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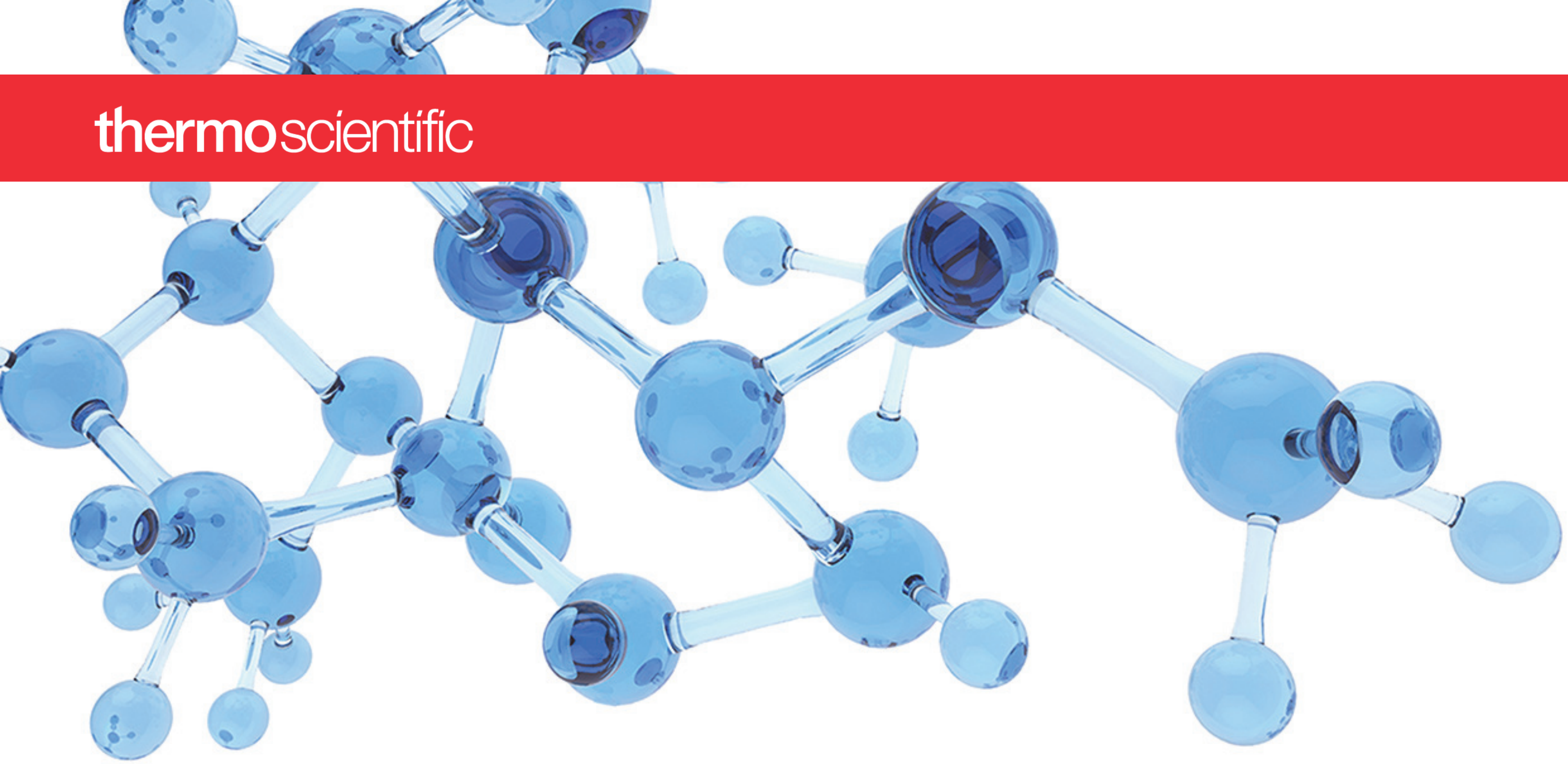

Thermo

Compound Discoverer

User Guide

Software Version 3.0

XCALI-97963 Revision A • July 2018

ThermoFisher
SCIENTIFIC

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Release history: Revision A June 2018

Software version: Compound Discoverer 3.0.x
For Research Use Only. Not for use in diagnostic procedures.

Contents

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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 or see "Getting Started with Data Processing and Data Review" on page 17.

Contents

Related Documentation

The Compound Discoverer application includes these manuals as PDF files:

- *Compound Discoverer User Guide*
- *Compound Discoverer E & L Tutorial*
- *Compound Discoverer Metabolism Tutorial*
- *Compound Discoverer Metabolomics Tutorial*
- *Compound Discoverer Stable Isotope Labeling Tutorial*
- *Compound Discoverer Reporting Quick Start*

The Compound Discoverer application also includes a Help system.

❖ To view the Compound Discoverer manuals

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

–or–

From the Microsoft™ Windows™ taskbar, choose **Start > All Programs** (or **Programs) > Thermo Compound Discoverer 3.0 >** ***Manual***.

❖ To download user documentation from the Thermo Scientific™ website

1. Go to thermofisher.com.
2. Point to **Services & Support** and click **Manuals** on the left.
3. In the Refine Your Search box, search by the product name.
4. From the results list, click the title to open the document in your web browser, save it, or print it.

   To return to the document list, click the browser **Back** button.

System Requirements

The Compound Discoverer 3.0 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 • DVD-ROM and USB drive • Display monitor resolution of 1920 × 1080 with 96 dpi setting
Software	• Microsoft Windows 7 Pro SP1 (64-bit) or Windows 10 64-bit operating system • Microsoft .NET Framework 4.7 • Microsoft Office 2010 • Adobe™ Reader™ 11 • Adobe Flash™ Player 15
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 data 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™ E5-2667 v4, 3.2 GHz) • 64 GB RAM • 1 TB SSD (solid-state disk) hard drive for OS • 2nd 3 TB (conventional disk) hard drive for data storage • DVD-ROM and USB drive • Two 27 in. UHD monitors: Display monitor resolution of 3840 × 2160

To check the access to the mass spectral databases, the time and date settings, and the Internet time, see Chapter 15, "Testing Communication to the Online Databases."

To verify that the system meets the minimum requirements, follow these procedures:

- To check the computer specifications
- To check the font DPI for a Windows 7 system
- To check the format setting for Region and Language

❖ 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. From the Windows Desktop, choose **Start > Control Panel > System and Security > System**.

   The System 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).

❖ To check the font DPI for a Windows 7 system

1. From the Windows taskbar, choose **Start > Control Panel**.
2. On the Adjust Your Computer's Settings page, do the following:
   a. For View By, select **Category**.

   b. Under Appearance and Personalization, click **Adjust Screen Resolution**.

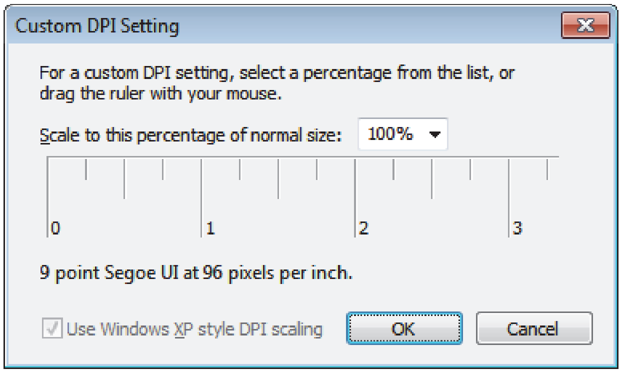
      The Screen Resolution page opens.

3. Click **Make Text and Other Items Larger or Smaller**.

4. On the left panel, click **Set Custom Text Size (DPI)**.

   The Custom DPI Setting dialog box opens (Figure 1).

Figure 1. Custom DPI Setting dialog box



For a custom DPI setting, select a percentage from the list, or drag the ruler with your mouse.

Scale to this percentage of normal size: 100%

9 point Segoe UI at 96 pixels per inch.

☑ Use Windows XP style DPI scaling

5. Make sure that the DPI setting is 96 pixels per inch.

❖ To check the format setting for Region and Language

1. From the Windows taskbar, choose **Start > Control Panel**.
2. On the Adjust Your Computer's Settings page, do the following:
   a. For View By, select **Category**.
   b. Select **Clock, Language, and Region**.
3. Select **Region and Language**.
4. On the Formats page of the Region and Language dialog box, select **English (United States)** from the Format list.

Installation Instructions

Thermo Compound Discoverer is a licensed application. Thermo Fisher Scientific provides a full version and a demo version of the application. For either version, you must use the license key provided to successfully install the software.

- Full version—Install the Compound Discoverer 3.0 application from the software media kit that includes a key-shaped USB flash drive with the installation executable and a small card with the license key.
- Demo version—Install the Compound Discoverer 3.0 application from the DVD. The license key is on the back of the DVD case.

IMPORTANT Read the following:

The Compound Discoverer 3.0 installation process requires the following:

- An Internet connection to validate the software license. If your computer does not have Internet access, see To install the Compound Discoverer application on a computer without Internet access.
- The Windows 7 SP1 64-bit or Windows 10 64-bit operating system. See "System Requirements" on page xv for the recommended hardware requirements and system settings.

The Compound Discoverer application is supported for US-English Only locale settings.

Do not install the mzVault™ 2.0 application on a computer that has an installation of the TraceFinder™ 4.1 or earlier application. These two applications are not compatible. Future versions of the TraceFinder application will be compatible with the mzVault 2.0 application.

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

Follow one of these procedures:

- To install the Compound Discoverer application on a computer with Internet access
- To install the Compound Discoverer application on a computer without Internet access

❖ To install the Compound Discoverer application on a computer with Internet access

1. Do one of the following:
   - For the full version, insert the Compound Discoverer USB flash drive into a USB port on your computer.
   - For the demo version, insert the Compound Discoverer DVD into the DVD drive on your computer.

2. Open Windows Explorer and select the USB or DVD drive to view its contents.

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

   The installation wizard starts (Figure 2).

   Figure 2. Compound Discoverer installation wizard

Adobe Acrobat Reader or an alternative PDF reader must be installed before you can read any of the documents provided as PDF files on this media. Validation certificate is also included. Adobe® Reader® XI Copyright © 1984-2012. Adobe® Flash® Player. Copyright © 1996-2010. Adobe Systems Incorporated. All Rights Reserved. Adobe Reader and Flash Player are either trademarks or registered trademarks in the Unites States and/or other countries.

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4. Click **Compound Discoverer 3.0** and continue the installation process.

   The Minimum Product Requirements screen appears with a product requirements scan summary. If the computer meets the system requirements, the box displays the following summary:

   > All the system minimum requirements checks passed.

5. When the License Activation dialog box opens, type the activation code in the Activation Code boxes.

   - For the full version, enter the license key from the small card in the Compound Discoverer 3.0 software media kit.
   - For the demo version, enter the license key from the back of the Compound Discoverer 3.0 DVD case.

6. Complete the installation process.

❖ To install the Compound Discoverer application on a computer without Internet access

> **Note** Installing the application on a Host computer without Internet access is a three-step process:
>
> 1. Export the Host computer information to a license request file, and then transfer the license request file to a computer with Internet access.
> 2. Activate the license request file, and then transfer the file back to the Host computer.
> 3. Import the activation information to the Host computer and complete the installation.

1. On the computer without Internet access, do the following:

    a. Follow step 1 through step 4 of "To install the Compound Discoverer application on a computer with Internet access" on page xviii.

    > **IMPORTANT** If an Activation Error dialog box opens, temporarily connect the computer to a network switch or hub that is turned on but is not connected to a network. Wait a few minutes. Then continue the installation process.

    b. When the License Activation dialog box opens, do the following:

        i. Type the activation code in the Activation Code boxes.

        ii. In the If You Do Not Have an Internet Connection on this Computer area, click **Export the License Request**.

        The Export License Request dialog box opens.

        iii. Select the directory where you want to store the license request file, name the file, and click **Save**.

    c. Eject the flash drive or DVD from the computer and leave the License Activation dialog box open.

    d. Transfer the license request file to a computer with Internet access.

    For example, copy the license request file to a read-writable USB flash drive. Insert the USB flash drive into a USB port on the computer that has Internet access and copy the *File Name*.licrequest file to an appropriate directory.

2. On a computer with Internet access, activate the license as follows:

    a. Verify that you transferred the *File Name*.licrequest file to this computer.

    > **Note** Ensure that the license request file is not write-protected.

b. Follow step 1 through step 3 of "To install the Compound Discoverer application on a computer with Internet access" on page xviii.

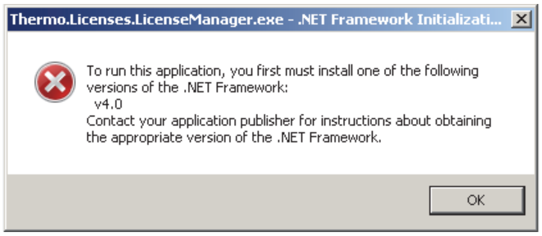
c. Click **Offline Activation**.

The Import License Activation Request dialog box opens with the Thermo License Activation dialog box in the background.

–or–

If the computer does not have the appropriate version of the .NET Framework, a message box appears in front of the installation screen (Figure 3).

Figure 3. .NET Framework initialization message box



Thermo.Licenses.LicenseManager.exe - .NET Framework Initializati...

To run this application, you first must install one of the following versions of the .NET Framework:
v4.0
Contact your application publisher for instructions about obtaining the appropriate version of the .NET Framework.

Note The License Activation dialog box requires Microsoft Visual C^{++} ™ redistributables and .NET Framework 4.0 or later. If the redistributables are not present on the computer, the program installs them automatically. If the appropriate version of the .NET Framework is not present, click **OK** to close the message box. Then, click **Microsoft .NET Framework 7.0** (see Figure 2 on page xix).

d. Browse to the license request file that you copied to this computer and click **Open**.

The Import License Activation Request dialog box closes, the Thermo License Activation dialog box becomes available, and the Activation Code boxes are populated with the license activation code from the license request file.

e. Enter the appropriate information in the Contact Information area.

f. Click **Activate**.

The program activates the license and stores it in the license request file.

g. Click **OK** when the following message appears:

Activation was successful.

h. Close the installation wizard.

i. Transfer the activated license request file back to the computer without Internet access.

For example, copy the activated license request file to a read-writable USB flash drive. Insert the USB flash drive into a USB port on the computer with no Internet access and overwrite the unactivated *File Name*.licrequest file with the activated *File Name*.licrequest file.

3. On the computer without Internet access, do the following:
    a. Verify that you transferred the activated *File Name*.licrequest file to this computer.
    b. In the License Activation dialog box that you left open in step 1c, click **Reimport the Activated License Request to Continue Activation**.

       The Import License Activation Request dialog box opens.
    c. Browse to the activated license request file and click **Open**.

       The Activation Success box opens and displays the following message:

       > Licenses successfully imported.
4. Complete the installation.

Special Notices

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

Special notices include the following:

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.

Contacting Us

Contact	Email	Telephone	QR Code[a]
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.		

Note To provide feedback for this document, go to surveymonkey.com/s/PQM6P62 or send an email message to Technical Publications (techpubs-lcms@thermofisher.com).

[a] You can use your smartphone to scan a QR Code, which opens your email application or browser.

❖ **For Compound Discoverer customer support questions**

Send an email message to CD.support@thermofisher.com.

1

Introduction

Compound Discoverer is a qualitative data-processing application that uses accurate mass data, isotope pattern 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 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 MS.

To familiarize yourself with the Compound Discoverer application, see these topics.

Contents

Tip Compound Discoverer is a licensed software application. For information about installing the application, see "Installation Instructions" on page xviii.

To get started with this application, follow these tutorials and guides:

- *Compound Discoverer 3.0 Metabolism Tutorial*
- *Compound Discoverer 3.0 Metabolomics Tutorial*
- *Compound Discoverer 3.0 Extractables and Leachables Tutorial*
- *Compound Discoverer 3.0 Stable Isotope Labeling Tutorial*
- *Compound Discoverer 3.0 Reporting Quick Start Guide*

To access these tutorials from the application window, choose **Help** > **Manuals**.

New Features and Enhancements

The application uses a study format to define the sample types, experimental study factors, sample groups, and group ratios. It uses a customizable node-based processing workflow to process Xcalibur™ RAW files and create a result file.

Some of the workflow nodes require input from the application's customizable lists and libraries, which include compound structures, mass lists, adduct ions, transformations, metabolic pathways, and fragment lists.

The result file includes a set of result tables and graphical views 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.

These topics describe the new features and enhancements:

- New Features
- Enhancements

New Features

Compound Discoverer 3.0 has the following new features:

- mzLogic scoring algorithm that combines mzCloud™ similarity searching (MS2 and MSn) with structure similarity matching to rank putative database results; for example, ChemSpider™ hits, mass list hits, and mapped compounds.

- Stable isotope labeling support for untargeted analyses including the new Labeled Compounds per File and the new Labeled Features result tables, the new Isotopologues Distribution Chart, and an enhanced Trend Chart where you can overlay the relative or average exchange rate for each detected compound by file, sample type, or study factor. For a brief introduction to this new feature, refer to the *Compound Discoverer 3.0 Stable Isotope Labeling Tutorial*.
- Built-in Metabolika pathway mapping that includes the ability to create and edit local Metabolika pathway files. The application includes a library of 378 metabolic pathway files.
- Manual creation of new mzVault libraries or new library entries from the Compounds result table or the Expected Compounds result table.
- Hierarchical cluster analysis with options to select the distance function, the linkage method, and the scaling type, and options to show or hide clusters and overlay the study factor information.
- Independent reprocessing for the compound identification, pathway mapping, and scoring sections of an analysis. Reprocessing specific nodes results in significant time savings by bypassing the spectrum processing and compound detection sections of the analysis.
- A new post-processing Xcalibur Inclusion/Exclusion List workflow node for the automated creation of Xcalibur Inclusion/Exclusion lists and a new shortcut menu command for the manual creation of Xcalibur Inclusion/Exclusion lists from the Compounds or Expected Compounds result tables.
- mzCloud, mzVault, and mass list searches for expected compounds as part of a targeted analysis. (The Group Expected Compounds workflow node now connects to the Search mzCloud, Search mzVault, and Search Mass Lists nodes.)
- A built-in mass list editor that is accessible from the Mass Lists library.
- FISh coverage score calculation that now uses full MSn tree (all MSn levels).
- Installation of mzVault 2.1 software for creating and editing mass spectral libraries. This version supports importing MSP files.

Enhancements

Compound Discoverer 3.0 has the following enhancements:

- Auto-save on closing a study or submitting an analysis
- Configuration option for specifying the scratch directory (the location for storing temporary files during data processing)
- Fail-safe mode for updating result files

- Custom layouts for processing workflows so that you can modify the layout of the workflow nodes for presentation purposes
- Custom color palettes for chart data
- A choice between large or small toolbar icons
- More mass spectral libraries
  - mzVault May 2018 library, which is a snapshot of the mzCloud spectral library with 7957 compounds and 233 718 spectra
  - Bamba lab lipid mediator spectral library (34 lipid mediators, contributed by Prof. Takeshi Bamba's lab of Kyushi University, Japan)
  - Bamba lab polar metabolite spectral library (598 polar metabolites, contributed by Prof. Bamba's lab of Kyushi University, Japan)
- More mass lists:
  - EFS HRAM Compound Database
  - Extractables and Leachables HRAM Compound Database with structures (1741 compounds)
  - Arita lab 6549 Flavonoid Structure Database (6549 compounds, contributed by the Arita Laboratory, National Institute of Genetics, Japan)
- A color-coded MS2 column in the Compounds and Expected Compounds result tables that shows the availability of MS2 scans for each compound
- Selectable search mode that specifies whether to search by formula, exact mass, or formula and exact mass for the Search ChemSpider, Map to KEGG pathways, Map to BioCyc pathways, and Map to Metabolika pathways workflow nodes
- Support for sorting and changing the hierarchical grouping of the study variables in the Trend Chart view (similar to the Grouping & Ratios page of a study)
- New ways to add selected files to the Analysis pane:
  - New shortcut menu command— Set As Input File—for the Input Files or Samples page of a study for automatically adding selected files to an analysis
  - Dragging and dropping files from the Samples page of a study (in addition to dragging and dropping the file from the Input Files page of a study)
- New shortcut menu command—Enable Row Grouping— for grouping table rows by a column heading
- Two new shortcut menu commands—Check All Up-Regulated Points and Check All Down-Regulated Points—for the Differential Analysis view

Supported File Formats

Table 3 describes the file types that the application can recognize or create.

Table 3. Supported file formats (Sheet 1 of 2)

File format	Description
Xcalibur RAW file	Contains unprocessed data acquired from a high-resolution, accurate mass LC/MS/MS instrument with a Thermo Scientific data system that is layered on the Thermo Foundation™ platform.
MOL format (.mol), compressed structure (.mcs), template (.tml)	You can open structure files by using the Structure Editor or the Custom Explanations Editor. For more information, see "Adding and Editing Compounds with the Compound Editor" on page 392 and "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162.
cdProcessingWF	Contains the data processing instructions for the application. To create a processing workflow, you must start or open an analysis in a study (see "Creating and Editing Processing Workflows" on page 115).
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. For more information about studies, see Chapter 3, "Editing Existing Studies."
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. For information about opening a result file and reviewing its contents, see Chapter 6, "Reviewing the Analysis Results."
cdResultView	Contains the layout settings that the application uses to display the result file's tables and graphical views. 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.
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).

Table 3. Supported file formats (Sheet 2 of 2)

File format	Description
Filter Set (.filterset)	Contains a set of result table filters. 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. For information about working with a defined filter set file, see “Using Result Filters for Data Reduction and Creating Filter Sets” on page 162.
mgf, mzML, mzDATA	You can export the MS scans in a raw data file to an open file format that can be read by third-party mass spectrometry applications. For information about exporting MS scans in a raw data file to an open file format, see “Export Spectra Node” on page 462.
XML	You can export each library to an XML file, and you can import library entries from an XML file. See Chapter 10, “Using the Lists and Libraries Manager.”
text (.txt)	You can save the data points in the graphical views to a text file. For more information, see “Copying or Saving Graphical Views for Publication” on page 185.
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. For more information, see “Copying or Saving Graphical Views for Publication” on page 185.
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.
DB	You can import mzVault libraries into the Spectral Libraries list.

Starting the Application

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

❖ To start the application

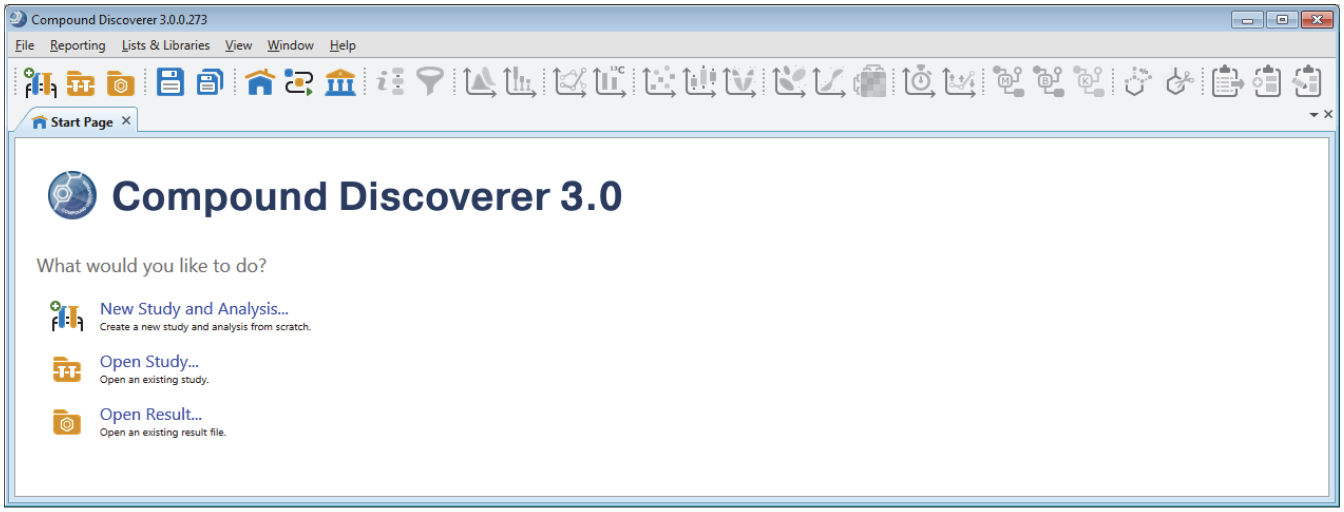
- From the taskbar, choose **Start > All Programs** (or **Programs**) **> Thermo Compound Discoverer**.

–or–

- From the computer desktop, double-click the **Compound Discoverer** icon, .

The Compound Discoverer window opens with the Start Page displayed as a tabbed document (Figure 4). As you create studies and process data, the application creates and populates recent file lists to the right of the What Would You Like to Do? hyperlinks.

Figure 4. Application window with the initial Start Page and large toolbar icons



Compound Discoverer 3.0

What would you like to do?

New Study and Analysis...
Create a new study and analysis from scratch.

Open Study...
Open an existing study.

Open Result...
Open an existing result file.

Choosing the Toolbar Icon Size

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

❖ 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**.

Application Window

The application 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 by clicking a toolbar icon.

> **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—A graphical element that accepts user input. Only one dialog box can be open at a time. When it is open, a dialog box blocks you from working in other parts of the application.
> - Pane—A defined area of an application view, page, or dialog box.

These topics describe the menu bar and toolbar:

- Application Menu Bar
- Application Toolbar

Application Menu Bar

Table 4 describes the menu commands in the menu bar at the top of the application window.

Table 4. Application menu bar (Sheet 1 of 7)

Menu command	Description
File menu These commands are always available.	
New Study and Analysis	Opens the New Study and Analysis Wizard that takes you through the process of selecting the studies folder for your study subfolders, creating a new study, and starting a new analysis (see "Starting a New Study and Setting Up an Analysis" on page 49).
Open Study	Opens the Open Study dialog box for selecting an existing study file to open. The CD study file type has the .cdStudy file name extension.

Table 4. Application menu bar (Sheet 2 of 7)

Menu command	Description
Open Result	Opens the Open Result File dialog box for selecting an existing result file or result view file (see "Opening, Closing, and Updating Result Files" on page 142). Opening result files does not require an active software license. The CD result file type, which contains the data processing results, has the .cdResult file name extension. The CD result view file type, which contains the display layout for the results tables and graphical views and the filter settings, has the .cdResultView file name extension. To restore the default layout for a result file, delete its associated CD result view file.
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 only available 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 (see "Generating a Report with an Existing Report Template" on page 332).
Create Report Template	Opens the Customize Report dialog box for setting up the main properties of a report template (see "Creating a Report Template with the Customize Report Dialog Box" on page 334).
Edit Report Template	Opens the Open Report Design Template dialog box for choosing an existing report template to edit (see "Editing an Existing Report Template" on page 344).

Table 4. Application menu bar (Sheet 3 of 7)

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 (see “Modifying the Expected Compounds List” on page 390). **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 (see “Modifying the Adducts List” on page 394).
Ion Definitions	Opens the Ion Definitions view for modifying the list of ion definitions (see “Modifying the Ion Definitions List” on page 397).
Adducts	Opens the Adducts view for modifying the list of adducts (see “Modifying the Adducts List” on page 394).
Mass Lists	Opens the Mass Lists view for modifying the list of mass list files or editing mass list files (see “Modifying the Mass Lists Library” on page 407).
Spectral Libraries	Opens the Spectral Libraries view for modifying the list of mzVault database files (see “Modifying the Spectral Libraries List” on page 418).
Metabolika Pathways	Opens the Metabolika Pathways view for modifying the list of Metabolika pathways or editing a Metabolika pathway (“Modifying the Metabolika Pathways List” on page 420).
Compound Classes	Opens the Compound Class view for viewing or modifying the list of compound class libraries (see “Modifying the Compound Classes List” on page 427).
View menu The Start Page and Job Queue commands from this menu are always available. The other View commands are only available 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 (see “Working with the Job Queue” on page 105).

Table 4. Application menu bar (Sheet 4 of 7)

Menu command	Description
View menu (continued)	
Result Summary	Opens the Summaries view (see "Viewing the Result Summary" on page 171).
Result Filters	Opens the Result Filters view for reducing the number of rows displayed in selected result tables (see "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162).
Chromatograms	Opens the Chromatograms view for viewing chromatogram plots (see "Working with the Chromatograms View" on page 188).
Mass Spectrum	Opens the Mass Spectrum view for viewing a spectral tree and the spectrum scans (see "Working with the Mass Spectrum View" on page 198).
Trend Chart	Opens the Trend Chart view for setting up a box-and-whisker (Box Whisker selection) chart or a trendline chart (see "Working with the Trend Chart View" on page 226).
Isotopologues Distribution Chart	Opens the Isotopologues Chart view (see "Working with the Isotopologues Distribution Chart" on page 271).
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 (see "Viewing Scatter Plots, Histograms, Bar Graphs, and Pie Charts" on page 204).
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 (see "Working with the Descriptive Statistics View" on page 239).
Differential Analysis	Opens the Differential Analysis view for viewing volcano plots and running differential analyses (see "Viewing a Volcano Plot and Running a New Differential Analysis" on page 244).
Principal Component Analysis	Opens the Principal Component Analysis view for evaluating multivariate data (see "Working with the Principal Component Analysis View" on page 233).
Partial Least Squares Discriminant Analysis	Opens the Partial Least Squares Discriminant Analysis view (see "Working with the Partial Least Squares Discriminant Analysis View" on page 250).
Hierarchical Cluster Analysis	Opens the Hierarchical Cluster Analysis view (see "Running a Hierarchical Clustering Analysis" on page 261).

Table 4. Application menu bar (Sheet 5 of 7)

Menu command	Description
View menu (continued)	
Retention Time Corrections	Opens the Corrected Retention Times view (see "Viewing the Corrected Retention Times of the Alignment Features" on page 257). 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 (see "Viewing the QC-Based Compound Area Correction Curves" on page 259). Available only when the active result file includes data from Quality Control samples.
Metabolika Pathways	Opens the Metabolika Pathways view for viewing the Metabolika pathways that are mapped to the compounds data (see "Viewing Metabolika Pathways" on page 256).
BioCyc Pathways	Opens the BioCyc Pathways view for viewing the BioCyc pathways that are mapped to the compounds data (see "Viewing BioCyc Pathways" on page 254). 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 (see "Viewing KEGG Pathways" on page 252). Available only when the active result file includes mapped KEGG pathways.
mzLogic Analysis	Opens the mzLogic Analysis view (see "Running an mzLogic Analysis" on page 269).
FISh Scoring Queue	Opens the FISh Scoring Queue view (see "Viewing the FISh Scoring Queue" on page 260).

Table 4. Application menu bar (Sheet 6 of 7)

Menu command	Description
Window menu Use these command 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.
License Manager	Opens the License Manager page where you can activate your Compound Discoverer license or scan for missing application features. See Chapter 11, “Using the License Manager.”
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. See Chapter 15, “Testing Communication to the Online Databases.”
Create Bug Report	Creates a report of your computer’s 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.

Table 4. Application menu bar (Sheet 7 of 7)

Menu command	Description
Help menu (continued)	These commands are always available.
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. See Chapter 12, "Setting Up the Configuration Options."
About	Opens the Compound Discoverer dialog box for viewing lists of the installed components and processing workflow nodes.

Application Toolbar

Figure 5 shows the application toolbar.

Figure 5. Application toolbar

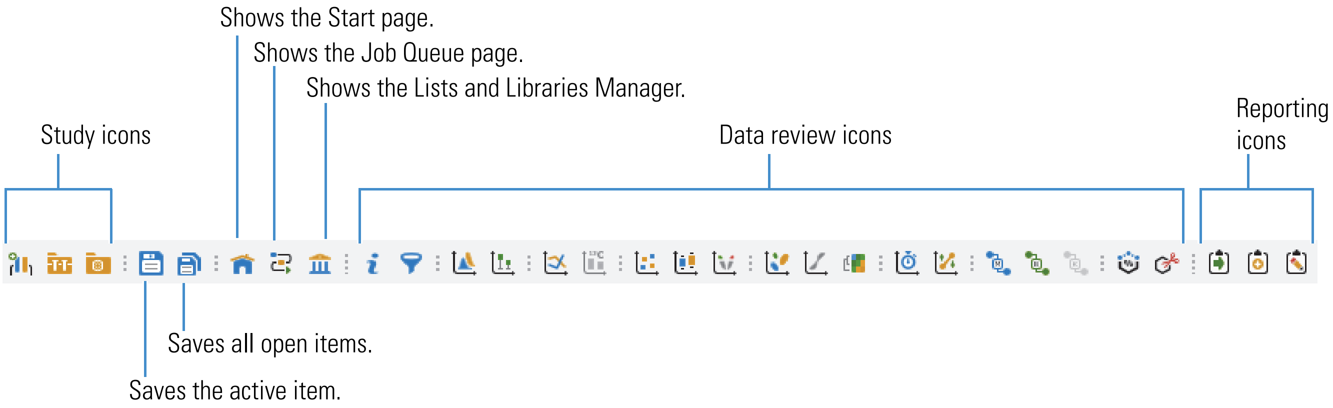


Table 5 describes the icons in the application toolbar from left to right.

Table 5. Toolbar icons (Sheet 1 of 4)

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.

Table 5. Toolbar icons (Sheet 2 of 4)

Icon	Description
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 if it is not already open and makes it the active page.
	Opens the Job Queue page if 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 lists or libraries: • Expected Compounds—For viewing or modifying a list of compounds • Transformations—For viewing or modifying a list of transformations • 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
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.	
i	Opens the Summaries view as a docked view. Available when the Summaries view is closed.
▽	Opens the Result Filters view as a floating window.
📈	Opens the Chromatograms view as a docked view.

Table 5. Toolbar icons (Sheet 3 of 4)

Icon	Description
Data review icons (continued)	
	Opens the Mass Spectrum view as a docked view.
	Opens the Trend Chart view as a docked view.
13C	Opens the Isotopologues Distribution Chart view as a docked view. Available when the opened result file includes an analysis of labeled compounds.
	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.
	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.
B	Opens the BioCyc Pathways view as a docked view. Available when the result file includes mapped BioCyc pathways.
K	Opens the KEGG Pathways view as a docked view. Available when the result file includes compounds mapped to KEGG pathways. Selecting an item in the KEGG Pathways result table opens the reference pathway for the item in the KEGG Pathway view.

Table 5. Toolbar icons (Sheet 4 of 4)

Icon	Description
Data review icons (continued)	
	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).

Getting Started with Data Processing and Data Review

The following steps summarize the application setup, data analysis, data review, and reporting processes for the Compound Discoverer application.

1. Setting Up the Libraries and Checking Access to the Online Databases
2. Setting Up a Study and an Analysis and Processing a Data Set
3. Opening the Result File, Reviewing the Data, and Creating a Report

Setting Up the Libraries and Checking Access to the Online Databases

To set up your libraries and lists and test your computer's access to the online databases, follow these procedures as needed.

❖ To find expected compounds

Add the compounds of interest to the Expected Compounds library. See "Modifying the Expected Compounds List" on page 390.

❖ To identify unknown compounds

Check the computer's access to the KEGG Pathways, BioCyc Pathways, mzCloud, and ChemSpider databases. If necessary, set up a BioCyc subscription. See Chapter 15, "Testing Communication to the Online Databases."

❖ To add your mzVault libraries to the Spectral Libraries list

1. From the application menu bar, choose **Lists & Libraries > Spectral Libraries**.
2. Click **Import**, locate your mzVault libraries (.db files), and click **Open**.

   The application comes with an mzVault library that includes all the compounds in the online mzCloud spectral database as of May 2018.

❖ To add a mass list to the list of available mass lists

1. From the application menu bar, choose **Lists & Libraries > Mass Lists**.
2. Click **Import**, locate the mass list (CSV file) of interest, and click **Open**.
3. The Define ‘CSV File Format for File Name.csv’ dialog box opens.

   > **Note** When the application recognizes an essential column in the CSV file, it selects the column heading in the respective list in the Essential Columns area and makes the check box for the column name unavailable in the Additional Columns table.

4. Define the Name and Molecular Weight columns or the Name and Formula columns.
5. (Optional) Define the Structure and Retention Time columns and any additional columns that you want to include in the mass list file.
6. Click **OK**.

Setting Up a Study and an Analysis and Processing a Data Set

A study is where you define your samples. An analysis is where you specify how you want to analyze the raw data (with a selected processing workflow), the samples (raw data files) that you want to process, (optional) the sample groups and ratios for a differential analysis, and the name of the result file for storing the processed data.

❖ To set up an new study and a new analysis

1. On the Start Page, click the **New Study and Analysis** link.

   The New Study and Analysis Wizard opens. To display instructions for each page of the wizard, click the **Show Description** icon, 💡.

2. On the Study Name and Processing Workflow page, name the study, select a processing workflow from the Common Templates folder, and read the processing workflow’s description.
3. On the Input File Selection page, click **Add Files** and add the files that you want to process to the study.

4. On the Input File Characterization page, define and assign the study factors for the sample set and assign the sample types.
5. (Optional) On the Sample Groups and Ratios page, set up the sample groups and ratios for a differential analysis.
6. Click **Finish** to exit the wizard.

   The Analysis pane lists the selected processing workflow, the name of the result file, and the selected raw data files. If the analysis is valid, the Run button is green.

❖ To troubleshoot the analysis when the Run button is unavailable

1. In the Analysis pane, point to the Caution symbol, ⚠.

   A pop-up message lists the missing analysis items.

   If you are working with one of the defined processing workflows, the most common errors are as follows:

   - Not selecting compounds for the Generate Expected Compounds and Create FISh Trace nodes
   - Not selecting a mass list for the Search Mass Lists node
   - Not selecting a spectral database for the Search mzVault node
   - Not selecting an isotope pattern for the Pattern Scoring node
   - Not selecting the isotope ratios for the Create Pattern Trace node
   - Not selecting a Compound Class fragment list for the Compound Class Scoring node
   - Not adding input files to the Files for Analysis area of the Analysis pane when running a new analysis

2. Fix the analysis errors until the Caution symbol disappears:

   - To fix a missing parameter error for a node (❗), select the node in the Workflow Tree pane on the Workflows page. Then, on the Parameters page for the node, select the missing item.
   - To fix a missing connection error for a node (⚠), make the appropriate connections.
   - If the Files for Analysis area is empty, add a set of input files from the Input Files page or Samples page of the study. You can select and drag the files or use the Set as Input File shortcut menu command.

❖ To start the analysis

1. In the Analysis pane, click **Run**.
2. If the Analysis Validation Issue prompt opens, decide whether to ignore the issue or cancel the run.

> **Tip** Not defining the ratios on the Grouping & Ratios page when the processing workflow includes the Differential Analysis node is one of the most common validation issues.

If there are no validation issues or you click Ignore to continue submitting the job, the Job Queue page opens.

Opening the Result File, Reviewing the Data, and Creating a Report

> **Note** When a graphical view or result table is the active item, pressing the F1 key opens the Help topic for the specific view or table.

❖ To open a result file

1. If the Job Queue page is closed, choose **View > Job Queue** from the application toolbar.
2. On the Job Queue page, double-click the completed job.

   The result file opens as a tabbed page.

❖ To review the data

1. Select the compounds of interest in the Compounds table or the Expected Compounds table.

   The respective XIC traces appear in the Chromatograms view and the best MS1 spectrum appears in the Mass Spectrum view.

2. Review the various result tables and other views as described in Chapter 6, “Reviewing the Analysis Results.”

❖ To filter the data to display only the compounds of interest

Use the Result filters view.

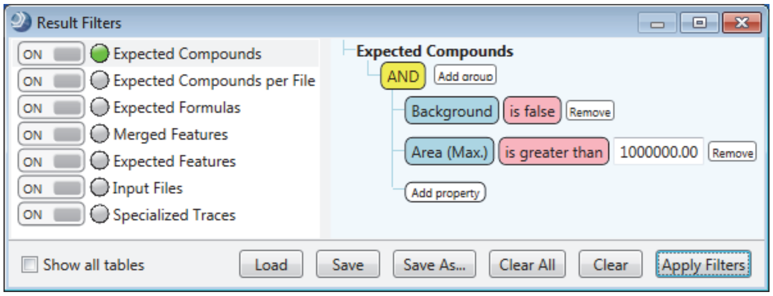
For example, to display only the compounds with a maximum peak area larger than 1e6, do the following:

a. From the application menu bar, choose **View > Result Filters**.

   The Result Filters view opens.

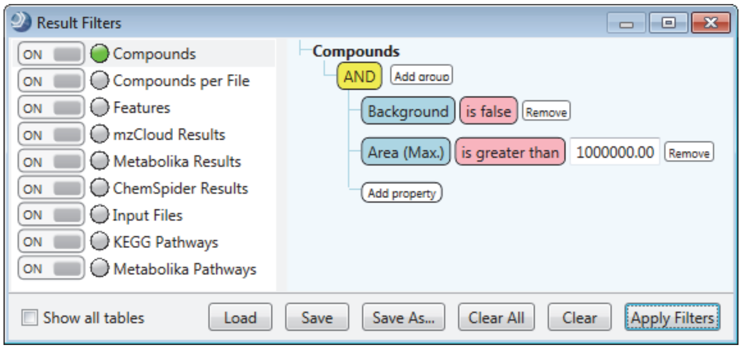
b. For the Expected Compounds table or the Compounds table, add the following filter: **Area (Max.) is greater than 1 000 000**.

Figure 6. Result filters for Expected Compounds table



Expected Compounds
AND
Background is false
Area (Max.) is greater than 1000000.00

Figure 7. Result filters for Compounds table



Compounds
AND
Background is false
Area (Max.) is greater than 1000000.00

c. Click **Apply Filters**.

For details, see "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162.

❖ To export the compounds data to a spreadsheet or an Xcalibur Inclusion/Exclusion list

1. Use the Result Filters view to filter the data or select the check boxes for the compounds of interest.

2. Right-click the Compounds table or the Expected Compounds table and choose the appropriate format:

   a. To export all the displayed columns, choose **Export > As Excel**.

      The Export to Excel dialog box opens.

   b. Select the result tables of interest.

   c. To export only the checked compounds, select the **Checked Items Only** check box.

   d. Click **Export**.

   –or–

   a. To create an Xcalibur Inclusion/Exclusion list, choose **Export > As Xcalibur Inclusion/Exclusion List**.

      The Export Xcalibur Inclusion/Exclusion List dialog box opens.

   b. Select the instrument type.
   c. To export only the checked compounds, select the **Checked Items Only** check box.
   d. Click **Export**.

❖ To print a report using a defined report template

1. Open the Expected Compounds table or the Compounds table.
2. Filter the table to display only the compounds of interest.
3. From the application menu bar, choose **Reporting > Create Report**.
4. In the Open Report Design Template dialog box, select one of the Compounds report templates or one of the Expected Compounds templates. Then, click **Open**.

   The report resolution page opens and the application resolves the data with the template.

5. On the report resolution page, click the **Print** icon, 🖶, in the toolbar to print the report.
6. In the Print dialog box, do the following:
   a. Select the appropriate printer and the page range that you want to print.

      > **Note** The report templates that come with the application default to printing on A4 paper.

   b. If you are not printing on A4 paper, change the printer setting.
   c. Click **OK** to print the report.

For details, see "Generating a Report with an Existing Report Template" on page 332.

Understanding Processing Workflows

The application uses a node-based method to create processing workflows. You can create your own custom processing workflows, use one of the many processing workflows provided with the application, or customize one of the existing processing workflows.

These topics describe the defined processing workflows and how the application processes data to find expected compounds (targeted analysis) or detect and identify unknown compounds (untargeted analysis):

- Targeted Workflows for Expected Compounds
- Untargeted Workflows for Identifying Unknown Compounds
- Marking Background Compounds in an Untargeted Analysis
- Nomenclature for the Defined Processing Workflows

To create custom workflows, see Chapter 5, "Creating and Editing Processing Workflows."

Targeted Workflows for Expected Compounds

Use the Expected Compounds workflow nodes to run an analysis that targets known analytes.

Figure 8 shows the workflow tree in the following processing workflow file:

Metabolism 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.

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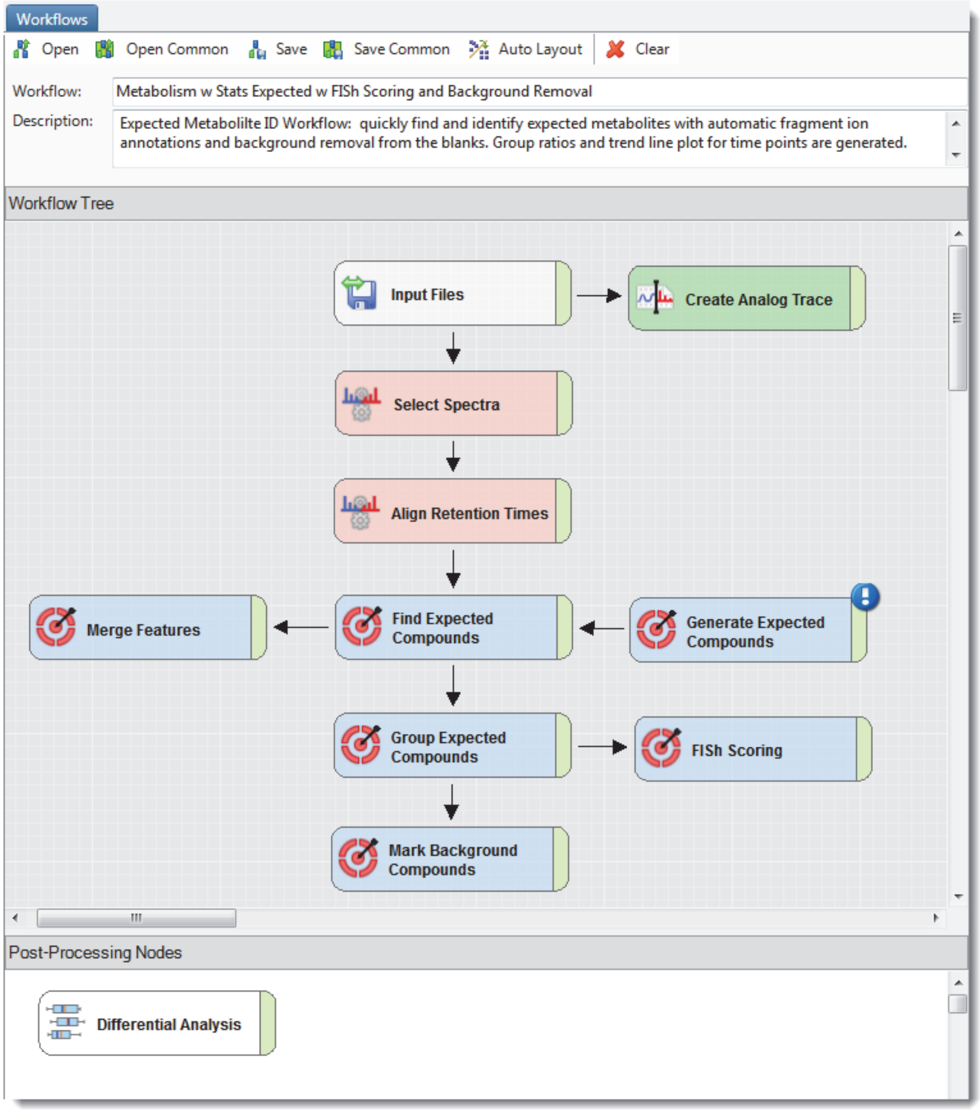
[1] A parent compound is the initial compound in a reaction or metabolic pathway.

Figure 8. Processing workflow for a metabolism study



Workflow: Metabolism w Stats Expected w FISh Scoring and Background Removal

Description: Expected Metabolilte ID Workflow: quickly find and identify expected metabolites with automatic fragment ion annotations and background removal from the blanks. Group ratios and trend line plot for time points are generated.

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.

IMPORTANT For a targeted analysis, which uses the Find Expected Compounds node, do not filter out all the full (MS1) scans, as this node requires the full scan data. When the processing workflow includes the FISh Scoring node, do not filter out the fragmentation scans, as this node uses them to provide a confirmation score for the expected precursor ions.

3. The Align Retention Times Node chromatographically aligns features across the input files in a sample set by using the specified alignment algorithm.

> **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:

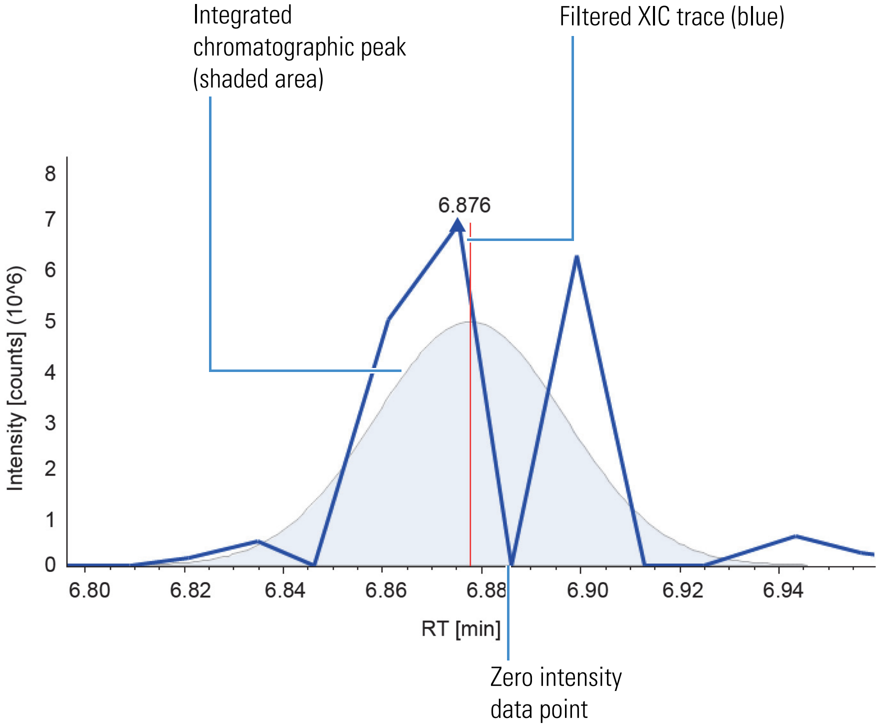
   - Charge
   - Theoretical *m/z* value

> **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 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 0 intensity value to the data point (Figure 9).
    c. For each expected compound found, the Find Expected Compounds 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.

Figure 9. Filtered XIC trace with a 0 intensity data point



Note A chromatographic peak with a 0 intensity value indicates one of the following:

- The user-specified mass tolerance, intensity tolerance, or number of required isotopes for the Find Expected Compounds node is not suitable for this sample set. Modify these parameter settings and rerun the analysis.

–or–

- The chromatographic peak does not represent the presence of an expected compound. Ignore this chromatographic peak.

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.
- 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]

   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 adduct 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 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.

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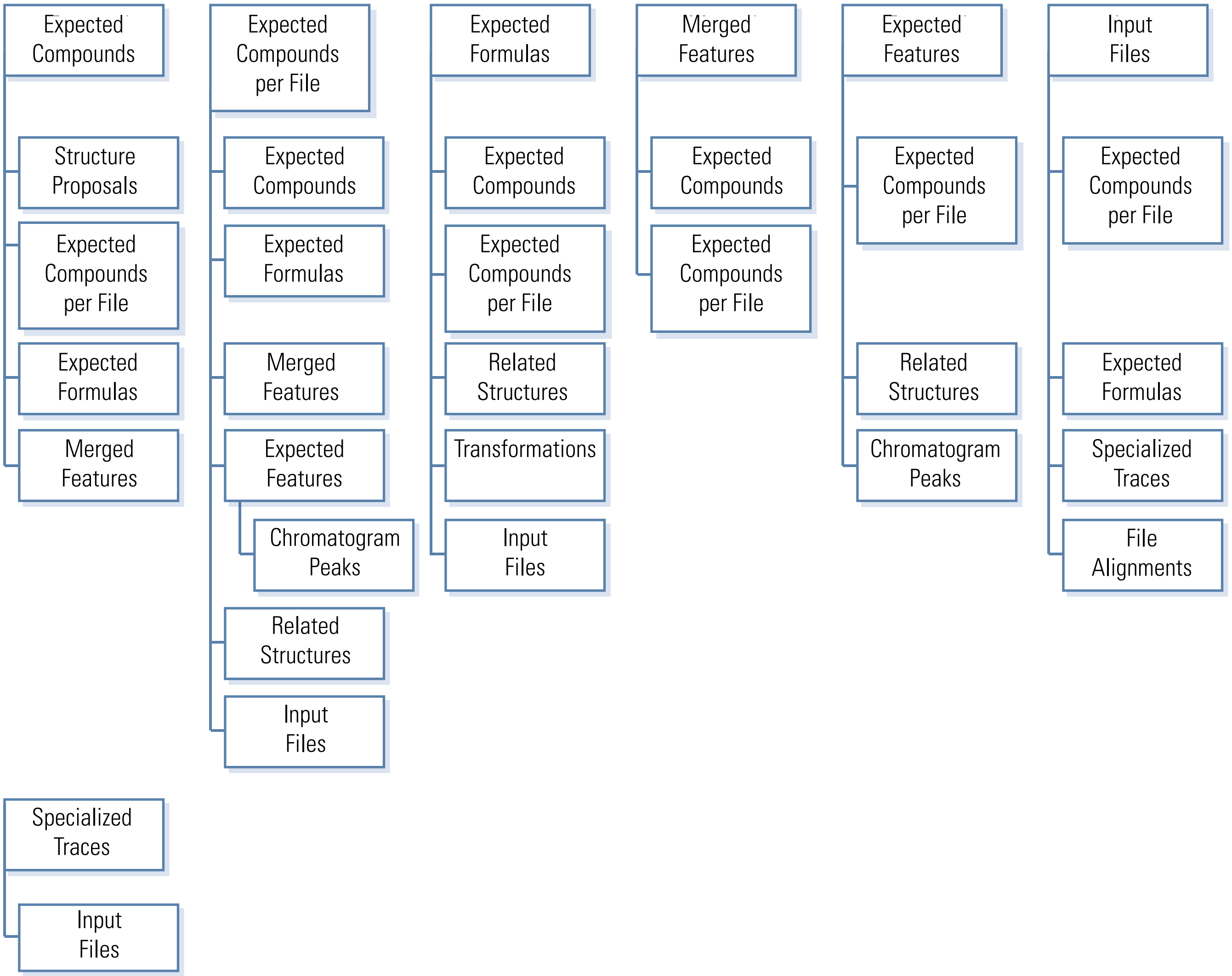
[2] For result files generated in Compound Discoverer 2.0, the Group Expected Compounds node also added the Best Compounds column to the Expected Compounds per File table. The Workflow page of the Result Summary view displays the Best Compound criteria for updated result files.

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 analysis includes group ratios, the Differential Analysis node runs the differential analysis.

Figure 10 shows a schematic of the main and related tables for the targeted workflow shown in Figure 8. The Structure Proposals table is empty until you populate it. For information about adding structure proposals or editing the compound annotations, see “Editing Compound Annotations” on page 156.

Figure 10. Result tables for a basic targeted workflow (with the Create Analog Traces and Merge Features nodes)



Untargeted Workflows for Identifying Unknown Compounds

Figure 11 shows the workflow tree for the metabolomics processing workflow that is provided with the application:

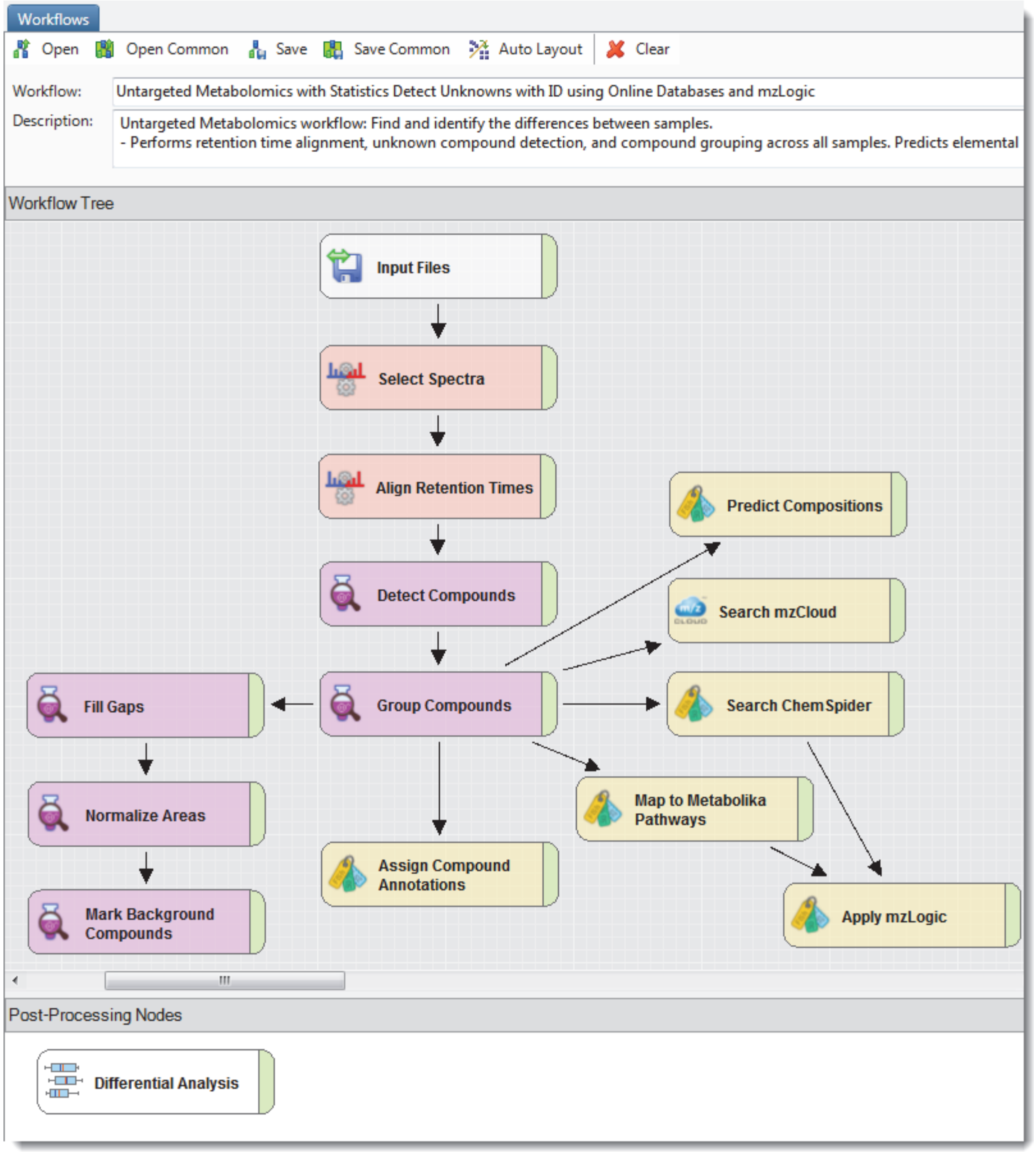
> Untargeted. Metabolomics with Statistics Detect Unknowns with ID using Online Databases and mzLogic.cdProcessingWF

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 MW or predicted formulas when available.
- The Search mzCloud node searches the mzCloud database of fragmentation scans by using the MW 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 11. Processing workflow that finds and identifies unknown compounds



Workflow: Untargeted Metabolomics with Statistics Detect Unknowns with ID using Online Databases and mzLogic

Description: Untargeted Metabolomics workflow: Find and identify the differences between samples.
- Performs retention time alignment, unknown compound detection, and compound grouping across all samples. Predicts elemental

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 by using the specified alignment algorithm.
4. The Detect Compounds node detects XIC traces in the full (MS1) scans by using the parameter settings for the mass tolerance and intensity threshold, groups isotopes and adducts by using the user-specified ions and base ions lists, and reports the unknown compounds (MW×RT) by occurrence in the Compounds per File table.

Note Make sure that the Preferred Ions list for the Group Compounds node includes the selections in the Base Ions list 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. 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.

11. The Mark Background Compounds node determines the background compounds in the Blank samples and labels these compounds as background compounds.

12. The Differential Analysis node runs a differential analysis on the defined sample ratios and calculates the p-values.

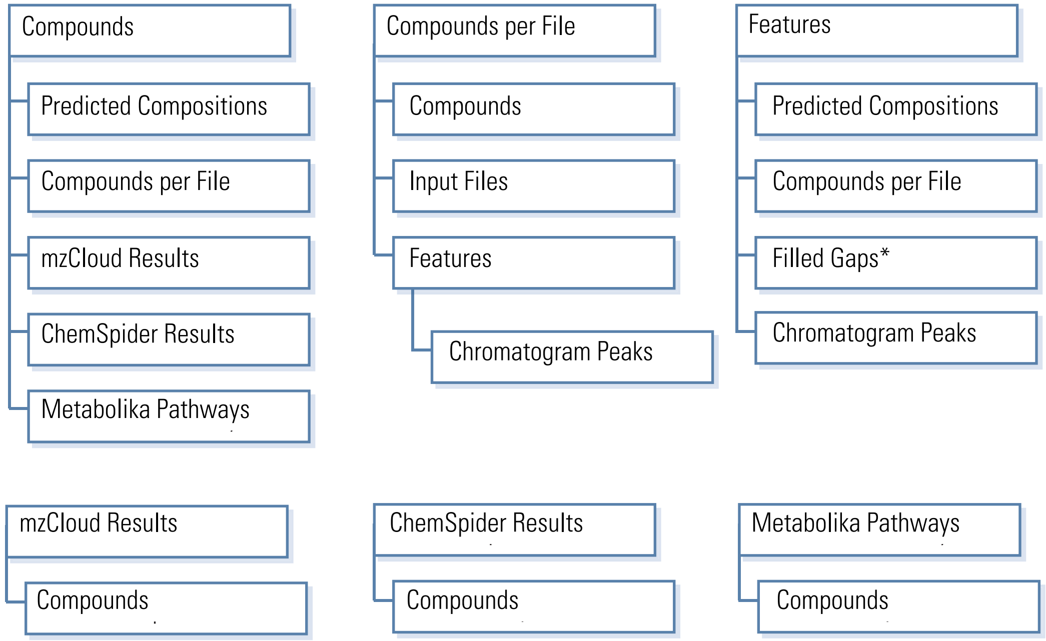
13. The Assign Compound Annotations node assigns and compares the annotations provided by the Predict Compositions, Search ChemSpider, Search mzCloud, and Search Mass Lists nodes.

14. 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 "Compound Detection Result Tables" on page 294.

Figure 12 shows a schematic of the main and related tables for a basic untargeted workflow.

Figure 12. Result tables for an untargeted workflow



*By default, the Filled Gaps table is hidden.

Marking Background Compounds in an Untargeted Analysis

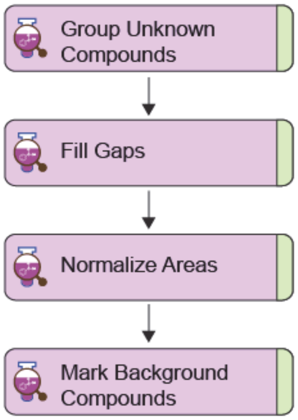
This topic describes how to make the appropriate node connections for an untargeted processing workflow that includes two or all three of these workflow nodes: Fill Gaps, Mark Background Compounds, and Normalize Areas. All three of these nodes process data across the input file set.

The Fill Gaps and Normalize Areas nodes automatically make the appropriate connections:

- The Fill Gaps node only takes input from the Group Compounds node. When you add the Fill Gaps node to a processing workflow that has a Group Compounds node, the Group Compounds node automatically connects to it.
- The Normalize Areas node only takes input from the Fill Gaps node. When you add the Normalize Areas node to a processing workflow that has a Fill Gaps node, the Fill Gaps node automatically connects to it.

The Mark Background Compounds node can take input from any of these three nodes—Group Compounds, Fill Gaps, or Normalize Areas. However, always add the Mark Background Compounds node to the end of the processing workflow.

When an untargeted processing workflow includes the Fill Gaps, Normalize Areas, and Mark Background Compounds nodes, the correct connection order is as follows: Group Compounds > Fill Gaps > Normalize Areas > Mark Background Compounds.



For more information about these optional nodes, see these topics:

- "Fill Gaps Node" on page 503
- "Normalize Areas Node" on page 506
- "Mark Background Compounds Node–Unknown Compounds" on page 505

Nomenclature for the Defined Processing Workflows

To access the defined processing workflows, open the Workflows page and choose **Open Common > Workflow Templates**. The Workflow Templates folder contains the following subfolders by field of study: Degradants, E and L (Extractables and Leachables), Environmental, Food Research, Forensics, Impurities, Metabolism, Metabolomics, and Stable Isotope Labeling.

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 + A to 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—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. The application includes three mzVault library files and the four mass lists.
>
> - mzVault libraries:
>   - mzVault May 2018 (snapshot of the mzCloud spectral database)
>   - Bamba Lab 34 Lipid Mediators Library Stepped NCE 10 30
>   - Bamba Lab 598 Polar Metabolites Stepped NCE 10 30 45
> - mass lists
>   - Anita Lab 6549 Flavonoid Structure Database
>   - EFS HRAM Compound Database
>   - Endogenous Metabolites Database 4400 Compounds
>   - Extractables and Leachables HRAM Compound Database

- 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—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.

- MDF—The workflow includes the Filter By Mass Defect Node.

The processing workflows installed with the application are as follows:

> **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.

- Degradants folder
  - Degradants Expected w FISh Scoring and Unknown w Database Searches
  - Degradants w Stats Expected w FISh Scoring and Unknown w Database Searches

- E and L 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
- Impurities folder
  - Impurities Expected w FISh and Unknown w Compound Class Scoring and Database Searches
  - Impurities Expected w FISh and Unknown w MDF Compound Class Scoring and Database Searches
  - Impurities w Stats Expected w FISh and Unknown w Compound Class Scoring and Database Searches
  - Impurities w Stats Expected w FISh and Unknown w MDF Compound Class Scoring and Database Searches
- Metabolism folder
  - Metabolism Pattern Scoring with Background Removal
  - Metabolism Generate Inclusion List For Acquisition Pos Mode
  - Metabolism Generate Inclusion List For Acquisition Neg Mode
  - Metabolism w Stats Expected No FISh Scoring w Background Removal
  - Metabolism w Stats Expected w FISh Scoring and Background Removal
  - Metabolism Advanced Expected and Unknown w Background Removal
  - Metabolism w Stats Advanced Expected and Unknown w Background Removal

- Metabolomics folder
  - Untargeted Metabolomics Quick Detection Unknowns No ID
  - Max ID - Detect Unknowns with ID Using Online Database Searches Single Sample
  - 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
- 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

Quality Control Samples for Batch Normalization

When acquiring raw data files for a large sample set, 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*.[3]

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

When the processing workflow includes the Normalize Areas Node and the input file set includes QC samples, the application uses the QC samples to create a regression curve of area versus acquisition time for each detected compound. The application 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 does not exceed the user-specified threshold.
- The number of samples acquired between the QC samples does not exceed the user-specified number.

---

[3] 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.

You can view the results of the batch normalization process in the Compounds result table and the Compound Area Corrections view (see Viewing the QC-Based Compound Area Correction Curves). 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. If the application excluded the selected compound during the QC signal correction step, the Compound Area Corrections view is empty.

Stable Isotope Labeling

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 high-resolution Orbitrap™ data and offers state-of-the-art analyses for unknown labeled compounds.

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. 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 > Stable Isotope Labeling

4. When using a label other than carbon-13, customize the parameter settings for the 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 compound's formula 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.

FISh Scoring for Targeted Compounds and Proposed Structures

Note In the current version 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, you can add FISh scoring to the automated analysis, and for unknown compounds, you can apply FISh scoring to your proposed structures.

The FISh scoring algorithm attempts to match 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 Expected Compounds table.

Using mzLogic to Score Candidates for Unknown Compounds

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

Running an Untargeted Analysis that Includes the mzLogic Node

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

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 a putative structure is to closely matching structures in the mzCloud spectral database.

During data processing, the 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 analysis 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 results.

For details, see "Running an mzLogic Analysis" on page 269.

Managing the Start Page's Recent Files Lists

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 a specific file at the top of each list, or open the folder where a specific study file or result file resides.

For details, see these topics:

- Keeping a File Name at the Top of a Recent File List
- Removing Files from the Recent File Lists
- Exploring File Folders from the Recent File Lists

Keeping a File Name at the Top of a Recent File List

❖ To keep a study name or result file name at the top of its list on the Start page

Click the pin icon to the left of the name.

The orientation of the pin changes from 📌 to 📌.

Removing Files from the Recent File Lists

You can remove individual files from the recent file lists or completely clear each list.

❖ To remove files from the recent files lists

- To remove a single file, right-click the file and choose **Remove From List**.

–or–

- To clear a list, right-click any file in the list and choose **Clear List**.

Note For information about using the File menu commands to manage the recent file lists, see “Application Menu Bar” on page 8.

Exploring File Folders from the Recent File Lists

You can access the file folder for a specific study or result file from the recent files list.

❖ To explore the contents of a folder for a study file or result file

Under the recent files list, right-click a study file or a result file and choose **Explore Path**.

Windows Explorer opens the folder for the selected study file or result file.

Working with Tabbed Pages and Dockable Views

A tabbed document is a top-level tabbed page below the toolbar in the Compound Discoverer window.

The following pages are tabbed documents in the application window:

- Start Page (Start Page ×)
- Study files (*Study Name* ×)
- Result files (*Result File Name* ×)
- Lists and Libraries manager (Lists & Libraries ×)
- Configuration (Configuration ×)

- Job Queue (Job Queue ×)
- Report Templates (*Report Template Name*)
- License Manager (License Manager ×)

> **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.

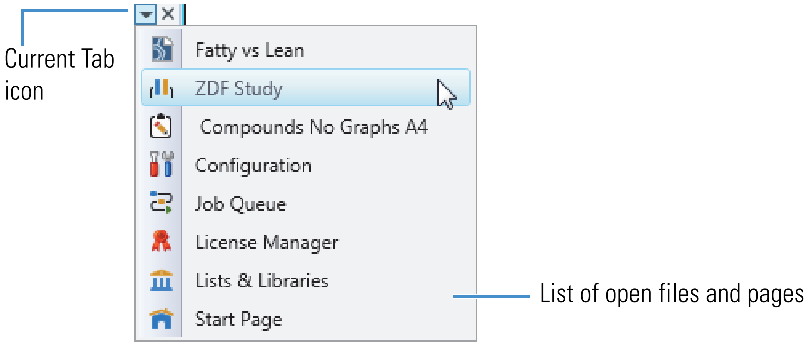
To display, dock, auto-hide, or group the tabbed pages and dockable views, see these topics:

- Tabbed Documents List
- Opening a Hidden Tabbed Document
- Auto-Hiding Views
- Tab Groups
- Shortcut Menu Commands for Tabbed Documents

Tabbed Documents List

Although you can have all tabbed 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 ⏷ (Figure 13).

Figure 13. List of open files and pages



Opening a Hidden Tabbed Document

❖ To display an open tabbed 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.

Auto-Hiding Views

To make more space for other views, you can auto-hide the Start Page and the Chromatograms and Mass Spectrum views. 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**.

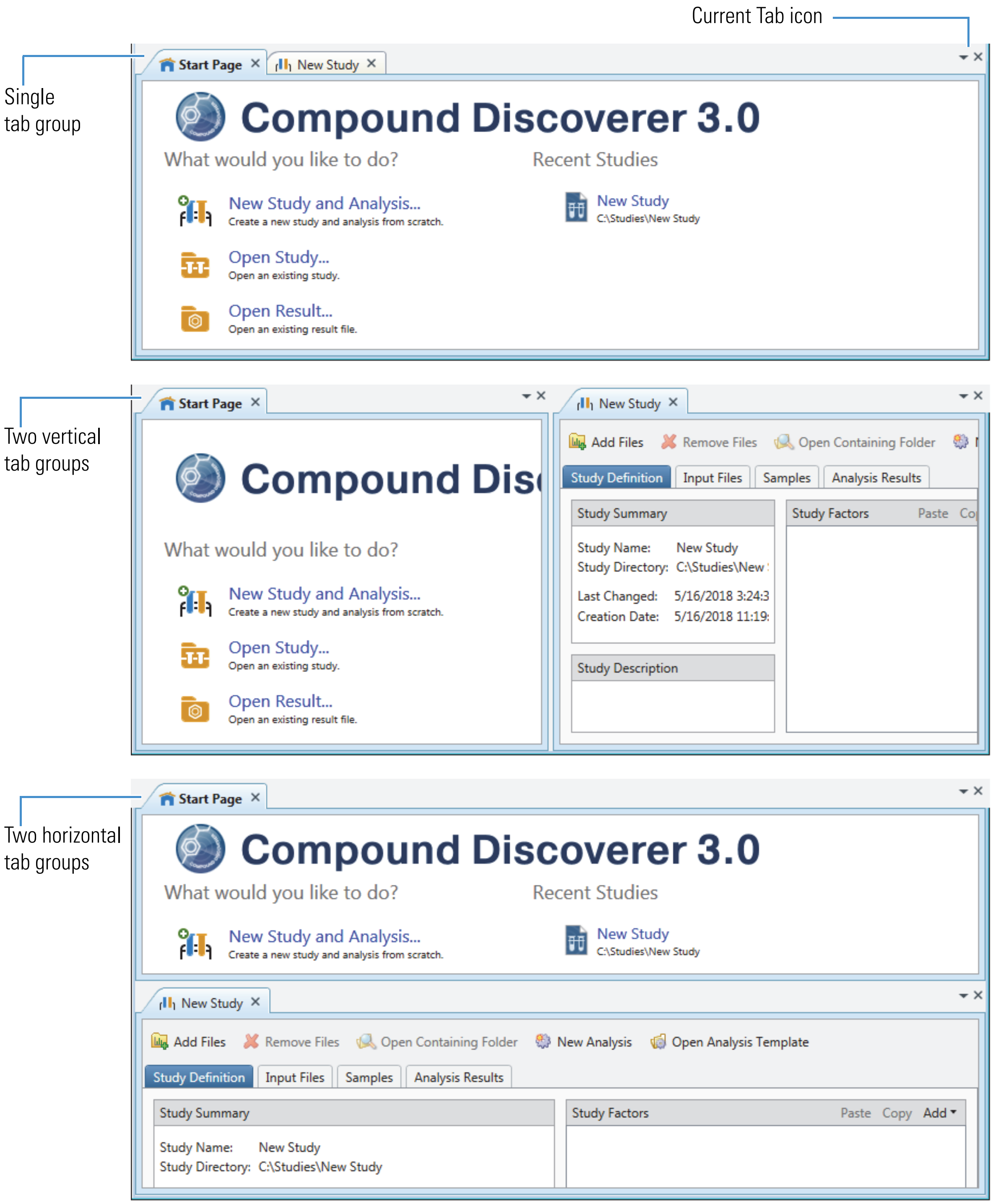
   The tab changes to a vertical tab on the left of the application window.

3. To view the hidden page, click its tab.
4. To hide the page, click anywhere in the application window outside the page borders.

Tab Groups

When you have two or more tabbed documents open in the same tab group, you can create more tab groups. Each tab group has its own Current Tabs icon, ▼. Figure 14 shows tab group examples.

Figure 14. Orientation of tab groups



What would you like to do?

New Study and Analysis... Create a new study and analysis from scratch.

Open Study... Open an existing study.

Open Result... Open an existing result file.

New Study C:\Studies\New Study

Study Name: New Study
Study Directory: C:\Studies\New Study
Last Changed: 5/16/2018 3:24:3
Creation Date: 5/16/2018 11:19:

Shortcut Menu Commands for Tabbed Documents

Table 6 describes the shortcut menu commands that control the tabbed document properties.

Table 6. Shortcut menu for tabbed documents

Command	Description
Dockable	Available for the Start Page and the result file views. This command is not available for the Job Queue page. Activates the Auto Hide command.
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	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. 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 tabbed document's position in the application window.
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 Start Page is a tabbed document that belongs to a vertical or horizontal tab group.
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.
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.

2

Starting a New Study and Setting Up an Analysis

To create a new study and optionally to set up an analysis, follow these topics.

Contents

About Studies and Analyses

In the Compound Discoverer application, you start analyses (data processing) from within the study environment.

For information about the studies and their components and analyses, see these topics:

- Studies
- Input Files
- Study Factors
- Sample Types
- Analyses

Studies

A study includes 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, the study factor values, and the sample type for each sample.

Creating a new study automatically creates a study file (.cdStudy) for storing the study information and a study folder for storing the study file and any result files (.cdResult) generated by running analyses within the study. The study file and its folder share the same name (see "Data Storage Architecture" on page 51).

For details about the sample information, see these topics:

- Input Files
- Study Factors
- Sample Types

Input Files

Input files are the raw data files acquired from an LC/MS/MS experiment. The file format for raw data files acquired with a Thermo Scientific MS is RAW.

To predict the elemental compositions of the sample components, the raw data must include high-resolution accurate-mass MS1 scans. To search the mass spectral libraries for matching fragmentation spectra, the raw data must include data-dependent MS2 or higher scans.

Study Factors

A study factor is an experimental variable that might have a statistically significant effect 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. See Appendix A, "Experiment Design for Comparison Statistics." You can add only one biological replicate factor to a study.

Sample Types

Table 7 describes the sample types that the application supports and how the it uses these sample types.

For more information, see "Selecting the Sample Types" on page 65.

Table 7. 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	Does not report the chromatographic peak areas for the sample's compounds. Uses the sample's fragmentation scans 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	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.

Analyses

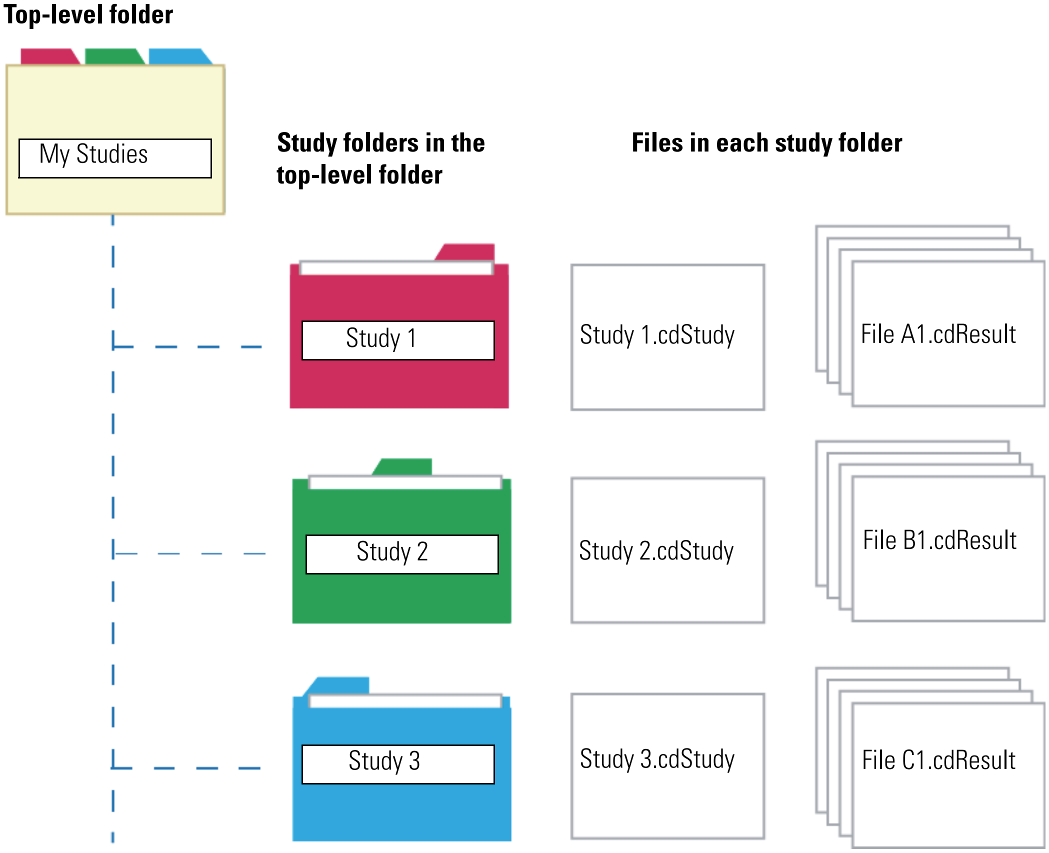
An analysis includes the processing workflow that extracts information from the raw data for each sample, such as the chromatographic peak areas and mass spectra for known and unknown compounds. It also includes the group ratios required to run a differential analysis, a list of input files, and the name of the result file where the processing results reside.

Data Storage Architecture

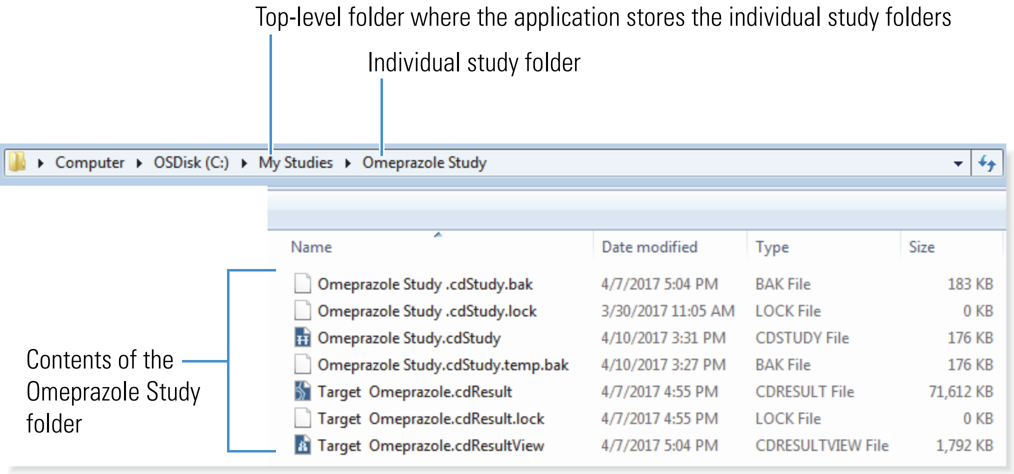
Figure 15 shows the hierarchy of the application folders. The studies folder is the top-level folder for all your studies or a particular set of studies. Each study folder within the studies folder holds one study file (.cdStudy) and one or more result files (.cdResult).

> **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.

Figure 15. 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.


Top-level folder where the application stores the individual study folders

Individual study folder

Contents of the Omeprazole Study folder

Name	Date modified	Type	Size
Omeprazole Study .cdStudy.bak	4/7/2017 5:04 PM	BAK File	183 KB
Omeprazole Study .cdStudy.lock	3/30/2017 11:05 AM	LOCK File	0 KB
Omeprazole Study.cdStudy	4/10/2017 3:31 PM	CDSTUDY File	176 KB
Omeprazole Study.cdStudy.temp.bak	4/10/2017 3:27 PM	BAK File	176 KB
Target Omeprazole.cdResult	4/7/2017 4:55 PM	CDRESULT File	71,612 KB
Target Omeprazole.cdResult.lock	4/7/2017 4:55 PM	LOCK File	0 KB
Target Omeprazole.cdResultView	4/7/2017 5:04 PM	CDRESULTVIEW File	1,792 KB

Starting the New Study and Analysis Wizard

You can access the wizard from the Start Page, the File menu, or the application toolbar.

❖ To start the New Study and Analysis Wizard

Do one of the following:

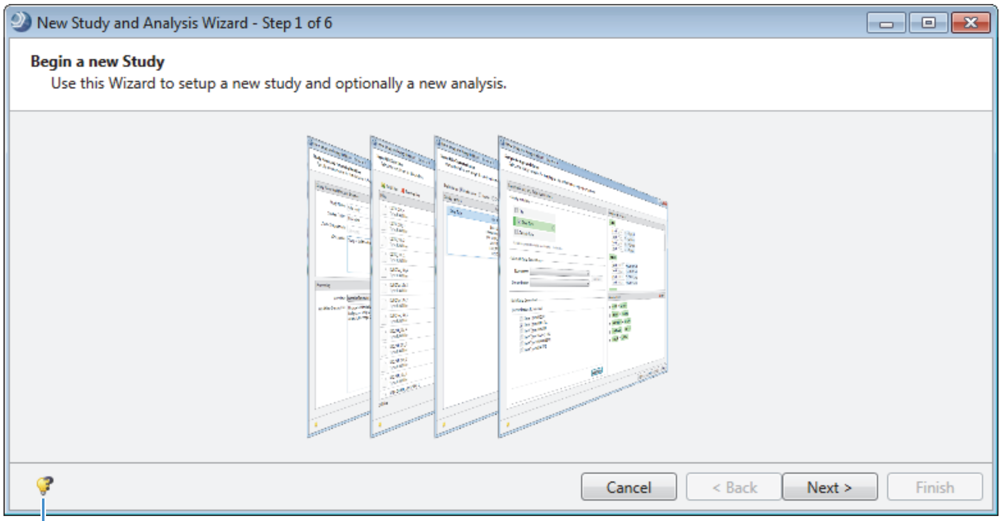
- From the menu bar, choose **File > New Study and Analysis**.
- In the toolbar, click the **Create a New Study and Analysis** icon, .

–or–

- On the Start page under What Would You Like to Do?, click **New Study and Analysis**.

The New Study and Analysis wizard opens. Unlike other areas of the application, the wizard has embedded "How To" instructions (see "About Accessing the Wizard Help" on page 80).

Figure 16. First page of the New Study and Analysis Wizard



New Study and Analysis Wizard - Step 1 of 6

Begin a new Study

Use this Wizard to setup a new study and optionally a new analysis.

Displays the embedded Help to the left of the page

Setting Up the Study Folders and Selecting a Processing Workflow

Use the Study Name and Processing Workflow page (step 2 of 6) of the New Study and Analysis Wizard to do the following:

- Name the current study and its storage folder.
- Select the top-level folder for storing all the study folders or a subset of the study folders.
- (Optional) Select a template file for the study.

Note A template file includes defined study factors.

- (Optional) Select a processing workflow for the analysis.

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

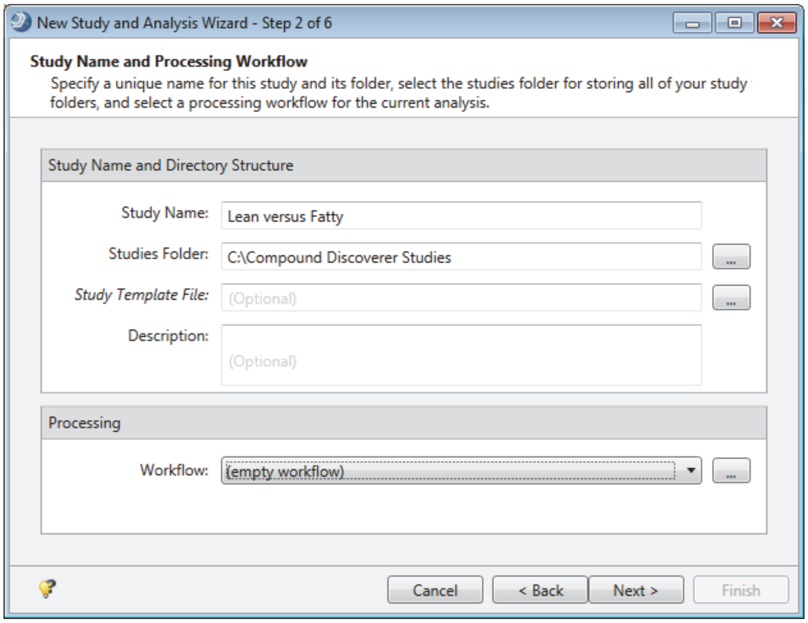
Follow these topics as needed:

- Naming a Study and Its Folder
- Creating or Selecting the Top-Level Folder for the Study
- Selecting a Study Template
- Selecting a Processing Workflow for the Analysis

After you complete this page of the wizard, go to the next page where you select the input files for the analysis.

Figure 17 shows page 2 of the wizard.

Figure 17. Study Name and Processing Workflow page of the wizard



New Study and Analysis Wizard - Step 2 of 6

Study Name and Processing Workflow

Specify a unique name for this study and its folder, select the studies folder for storing all of your study folders, and select a processing workflow for the current analysis.

Study Name and Directory Structure

Study Name: Lean versus Fatty

Studies Folder: C:\Compound Discoverer Studies

Study Template File: (Optional)

Description: (Optional)

Processing

Workflow: (empty workflow)

Naming a Study and Its Folder

The application uses the specified name for the study file (.cdStudy) and the study folder where it stores the study file. In addition, the application stores the result files from analyses run within the study in the same study folder (see "Data Storage Architecture" on page 51).

❖ To name the study and its folder

On page 2 of the wizard, in the Study Name box, type a name for the new study.

Creating or Selecting the Top-Level Folder for the Study

The studies folder is where the application stores the individual study folders.

❖ To specify the top-level folder where you want to store the new study folder

On page 2 of the wizard, do the following:

- Use the current folder name and location that is displayed in the Studies Folder box.

–or–

- Browse to or create a new folder.

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

Selecting a Study Template

A study template is a study that includes defined study factors.

❖ To extract the study factors for the current study from an existing study

1. On page 2 of the wizard, click the browse icon, ..., next to the Study Template File box.
2. In the Select Template Study File dialog box, locate a study file (.cdStudy) with the appropriate study factors, and click **Open**.

   The name and location of the study file appear in the Study Template File box.

Selecting a Processing Workflow for the Analysis

You can select a processing workflow on page 2 of the wizard or on the Workflows page of an analysis.

❖ To select a processing workflow for the current analysis

- Select a processing workflow from the Workflow list.

  The Workflow list displays the processing workflow files in the Common Templates folder (see "Nomenclature for the Defined Processing Workflows" on page 36).

–or–

- Select a processing workflow or result file from another folder as follows:

  a. Click the browse icon, ..., next to the Workflow list.

b. In the Select Workflow Template dialog box, locate a processing workflow file (.cdProcessingWF) or a result file (.cdResult), and click **Open**.

   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.

Adding Input Files to a New Study

Use the Input File Selection page (step 3 of 6) 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 adding input files to an existing study, see "Adding Input Files to an Existing Study" on page 87.

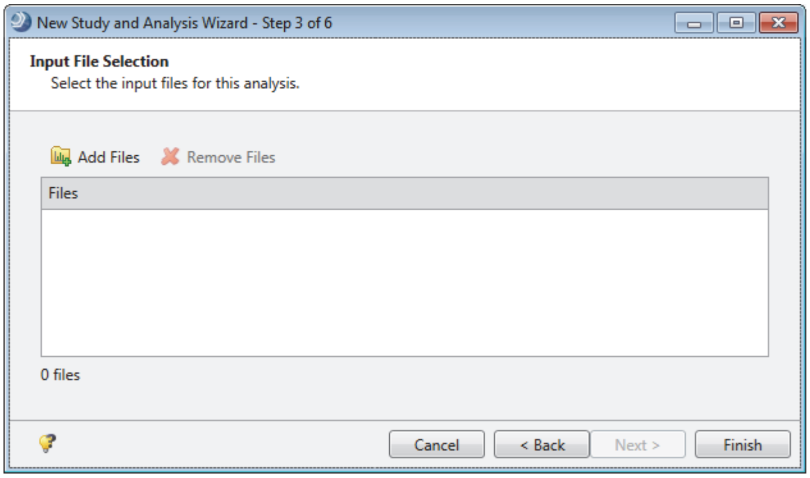
> **Note** The example Xcalibur RAW files for metabolism and metabolomics studies are on the Compound Discoverer USB key in the software media kit.

❖ To add or remove raw data files

1. On page 3 of the wizard, do the following:

   - To add files, click **Add Files**. Then, browse to the appropriate folder, select the Xcalibur RAW files of interest, and click **Open**.

   Figure 18. Input File Selection page of the wizard



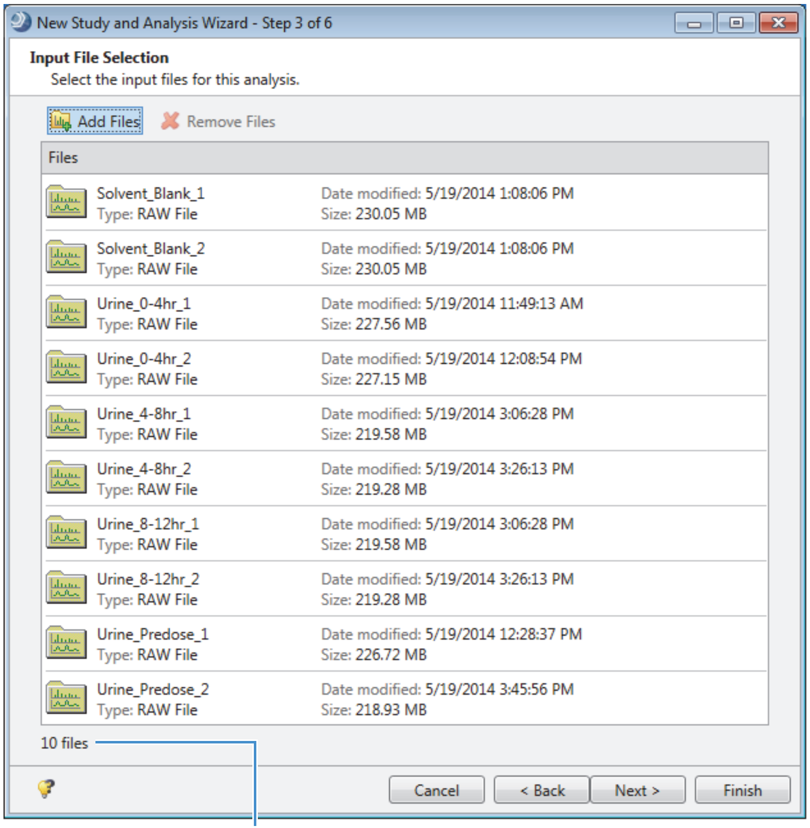
New Study and Analysis Wizard - Step 3 of 6

Input File Selection

Select the input files for this analysis.

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 19).

Figure 19. Input File Selection page with selected files



Input File Selection

Select the input files for this analysis.

Files	
Solvent_Blank_1 Type: RAW File	Date modified: 5/19/2014 1:08:06 PM Size: 230.05 MB
Solvent_Blank_2 Type: RAW File	Date modified: 5/19/2014 1:08:06 PM Size: 230.05 MB
Urine_0-4hr_1 Type: RAW File	Date modified: 5/19/2014 11:49:13 AM Size: 227.56 MB
Urine_0-4hr_2 Type: RAW File	Date modified: 5/19/2014 12:08:54 PM Size: 227.15 MB
Urine_4-8hr_1 Type: RAW File	Date modified: 5/19/2014 3:06:28 PM Size: 219.58 MB
Urine_4-8hr_2 Type: RAW File	Date modified: 5/19/2014 3:26:13 PM Size: 219.28 MB
Urine_8-12hr_1 Type: RAW File	Date modified: 5/19/2014 3:06:28 PM Size: 219.58 MB
Urine_8-12hr_2 Type: RAW File	Date modified: 5/19/2014 3:26:13 PM Size: 219.28 MB
Urine_Predose_1 Type: RAW File	Date modified: 5/19/2014 12:28:37 PM Size: 226.72 MB
Urine_Predose_2 Type: RAW File	Date modified: 5/19/2014 3:45:56 PM Size: 218.93 MB

10 files

Number of files field

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

2. Do one of the following:

    - Click **Next** to continue to the next page.
    - Click **Finish** to create the new study and close the wizard.

Characterizing New Input Files

To set up the study factors and the sample information for the study's input files, use one or both of the following:

- The Input File Characterization page (step 4 of 6) of the New Study and Analysis Wizard

–or–

- The Input File Characterization dialog box that opens when you add input files to an existing study

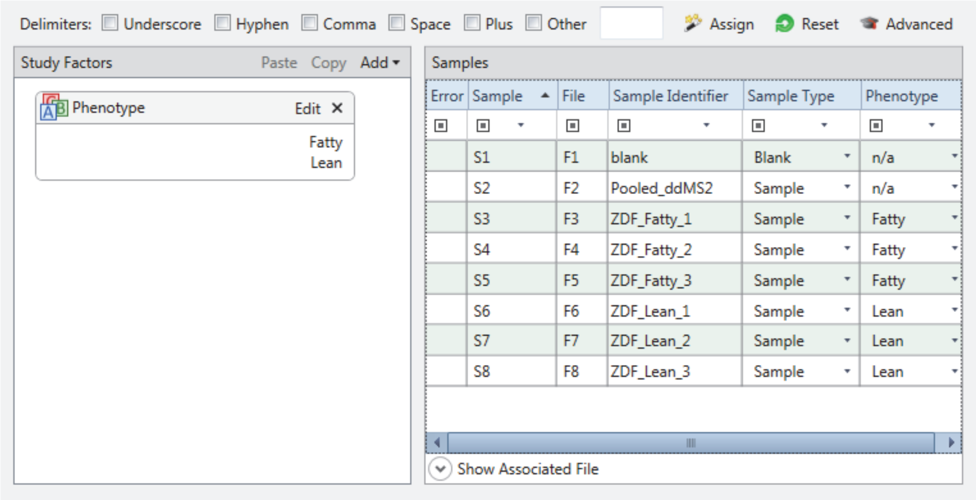
The sample information includes the sample type and study factor values for each sample.

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 (see "Editing the Study Factors and Study Description" on page 85).
- Select the sample types and study factor values on the Samples page (see "Editing the Sample Type and Study Factor Values" on page 91).

Figure 20 shows the functional area of the Input File Characterization page or dialog box.

Figure 20. Input File Characterization page of the wizard



Error	Sample	File	Sample Identifier	Sample Type	Phenotype
	S1	F1	blank	Blank	n/a
	S2	F2	Pooled_ddMS2	Sample	n/a
	S3	F3	ZDF_Fatty_1	Sample	Fatty
	S4	F4	ZDF_Fatty_2	Sample	Fatty
	S5	F5	ZDF_Fatty_3	Sample	Fatty
	S6	F6	ZDF_Lean_1	Sample	Lean
	S7	F7	ZDF_Lean_2	Sample	Lean
	S8	F8	ZDF_Lean_3	Sample	Lean

To set up the study factors and select or assign the sample types and factor values, follow these topics:

- Adding and Editing the Study Factors
- Assigning or Selecting the Study Factor Values
- Selecting the Sample Types

Adding and Editing the Study Factors

You can add and edit study factors from three locations:

- The Input File Characterization page of the New Study and Analysis Wizard
- The Input File Characterization dialog box that opens when you add files to an existing study
- The Study Definition page of an existing study

With the wizard, you can set up the study factors for the study in three ways:

- Import the study factors from another study (see "To extract the study factors for the current study from an existing study" on page 55).
- Add the study factors manually on the Input File Characterization page.
- Add and assign the study factors semiautomatically with the Extract Sample Information From Sample Names dialog box ("Using the Regular Expression Builder to Extract the Study Factors" on page 66).

The first two methods do not automatically assign study factor values to the samples. If you import the study factors from another study, you can edit them in the Study Factors pane of the Input File Characterization page or on the Study Definition page of a study.

> **Note** To open the Input File Characterization page of the wizard, you must select one or more input files on the previous page of the wizard.

To set up or edit the study factors, follow these topics as needed:

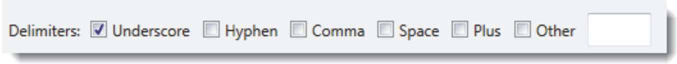
- Selecting the Delimiters for Parsing the File Names
- Adding Categorical Study Factors
- Adding Numeric Study Factors
- Adding Biological Replicate Study Factors
- Deleting a Study Factor
- Duplicating Study Factors
- Editing a Study Factor

Selecting 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 wizard or in the Input File Characterization dialog box.

❖ 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.



Delimiters: ☑ Underscore ☐ Hyphen ☐ Comma ☐ Space ☐ Plus ☐ Other

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:

Urine_0-4hr_1
Urine_0-4hr_2
Urine_4-8hr_1
Urine_4-8hr_2
Urine_8-12hr_1
Urine_8-12hr_2
Urine_Predose_1
Urine_Predose_2

In this case, the study factors are time period (0-4hr, 4-8hr, 8-12hr, or Predose) and replicate (1 or 2).

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

Adding Categorical Study Factors

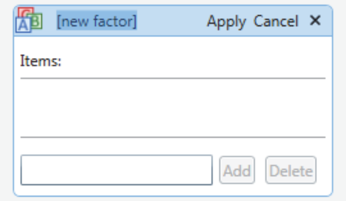
You can add study factors when you create a study, when you add files to an existing study, and on the Study Definition page of an existing study.

❖ To add a categorical study factor

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 21).

   Figure 21. Categorical factor editor

2. Type the name of the factor, for example, **Time Period**.

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

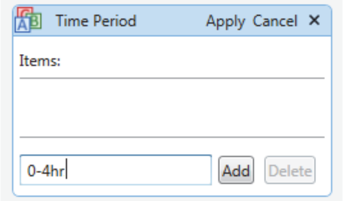
   a. In the Items box (to the left of the Add button), begin typing a factor, for example, **0-4hr**.

      If the file name contains a character delimiter and you selected the delimiter's check box, 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 (Figure 22).

      Figure 22. Entering items in the item box

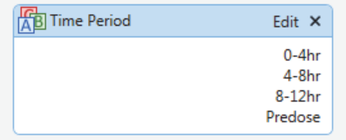
   b. Click **Add**.

      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 (Figure 23). The items appear in ascending order.

   Figure 23. Named factor with a list of items



Adding Numeric Study Factors

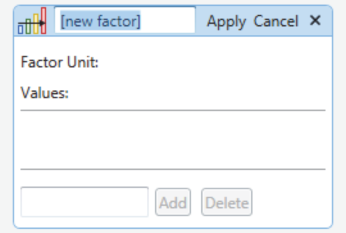
You can add study factors when you create a study, when you add files to an existing study, and on the Study Definition page of an existing study.

❖ To add a numeric factor

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 24).

   Figure 24. 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.

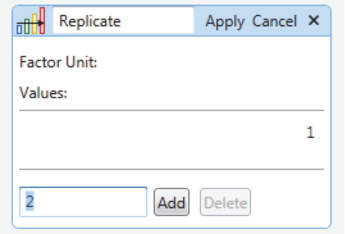
   The Factor Unit is only a text label; however, it must start with a letter.

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 25).

Figure 25. Entering numeric values in the values box



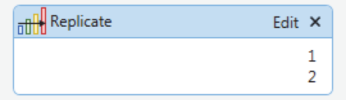
b. Click **Add**.

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 26).

Figure 26. Numeric factor with a list of values



Adding 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.

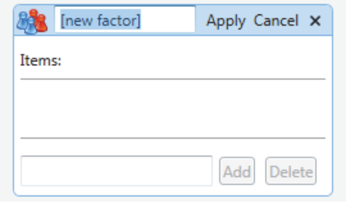
You can add only one biological replicate factor to a study. Use the biological replicate factor for nested statistical models—that is, for studies that include one study factor nested within another study factor.

❖ To add a biological replicate factor

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 27. Biological replicate factor editor

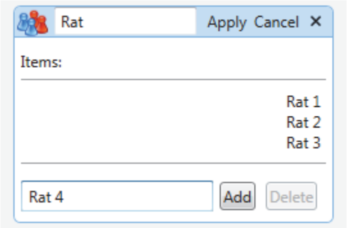


2. Type a factor name to replace [new factor], for example, **Rat**.

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, for example, **Rat 1**.

       The Add button becomes available.

       Figure 28. Biological replicate factor editor with added items

    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.

Deleting a Study Factor

❖ To delete a study factor

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.

Duplicating Study Factors

❖ 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**.

3. Click **Paste**.

   A copy of the selected factor appears.

4. Go to the next procedure "Editing a Study Factor."

Editing a Study Factor

You can edit 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 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.

Assigning or Selecting the Study Factor Values

You can assign the study factor values to the samples in the Samples pane of the Input File Characterization page or dialog box. When working with the Samples page of a study, you must manually select the study factor values, as this page does not include the Assign command.

Follow these topics as needed:

- Automatically Assigning Study Factor Values
- Manually Assigning Study Factor Values
- Resetting Sample Assignments

Automatically Assigning Study Factor Values

After you set up the study factors for the 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.

❖ 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 “Adding and Editing the Study Factors” on page 58).

2. In the command bar, click **Assign.**
3. Check the study factor columns, verify the sample assignments, and manually assign the study factor values if necessary.

Manually Assigning Study Factor Values

After you set up the study factors for the study, you can assign the study factor values to each sample. If the input file names do not follow a consistent pattern or do not include the study factor values, you must assign these values manually.

❖ **To manually select the study factor values**

On the Input File Characterization page (or dialog box), 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***.

Resetting 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.

Selecting the Sample Types

To select the sample type for each sample, use one of these locations:

- The Samples pane of the Input File Characterization page or dialog box
- The Samples page of a 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).

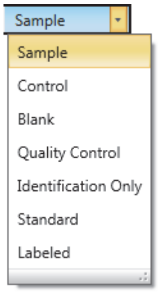
❖ To select the sample type for a sample

1. On the Input File Characterization page or dialog box, after setting up the study factors manually or by using the Extract Sample Information From Sample Names dialog box, click **Assign**.

   Clicking Assign assigns the Sample or Blank sample type to each sample. The Assign command is not available on the Samples page of a study.

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

   - To select the sample type for a single sample, in the Sample Type column, select **Sample**, **Control**, **Blank**, **Quality Control**, **Identification Only**, **Standard**, or **Labeled** from the list.

     For information about the sample types, see “Sample Types” on page 51.

   - 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.

Using the Regular Expression Builder to Extract the Study Factors

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.

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.

In the following example (Table 8), 0-4hr, 4-8hr, 8-12hr, and Predose are items for the time point categorical factor, and 1 and 2 are values for the replicate numeric factor.

Table 8. Example RAW files for metabolism studies (located on the installation media)

File Name	Time point	Replicate
Blank_1.raw	n/a	1
Blank_2.raw	n/a	2
Urine_0-4hr_1.raw	0-4hr	1
Urine_0-4hr_2.raw	0-4hr	2
Urine_4-8hr_1.raw	4-8hr	1
Urine_4-8hr_2.raw	4-8hr	2
Urine_8-12hr_1.raw	8-12hr	1
Urine_8-12hr_2.raw	8-12hr	2
Urine_Predose_1.raw	Predose	1
Urine_Predose_2.raw	Predose	2

These are the default expressions:

- Numeric factor [0-9]: (?<NumericalVariable_1>[0-9]+)
- Categorical factor [A-Z]: (?<CategoricalVariable_1>[0-9A-Z]+)
- Biological Replicate factor [A-Z]: Same as categorical factor.

If the default categorical factor expression cannot find the matching patterns in your input file names, review the examples in Table 9, and then modify the expression within the square brackets. For example, if a categorical factor contains a hyphen, the default regular expression cannot interpret it. Adding a hyphen to the default regular expression enables pattern matching for this factor value.

Table 9. Examples of regular expression operators (Sheet 1 of 2)

Operator	Quantifier	Matching pattern
[0-9]	none	A single integer
[0-9]	+	One or more integers
[A-Z]	none	One alphabetic character

Table 9. Examples of regular expression operators (Sheet 2 of 2)

Operator	Quantifier	Matching pattern
[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)

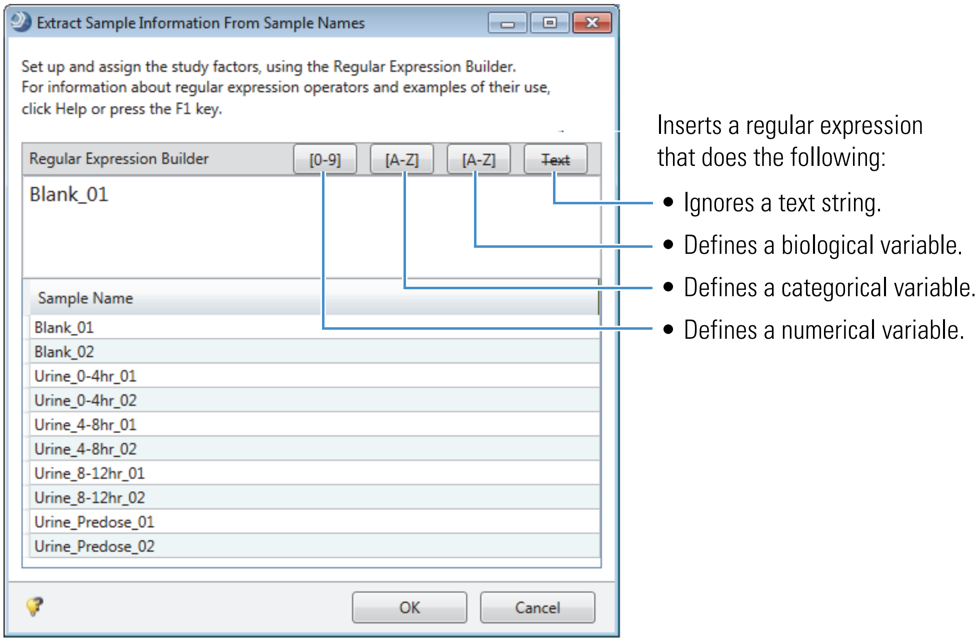
❖ To open the Extract Sample Information From Sample Names dialog box

1. Open the Input File Characterization page (step 4 of 6) of the wizard or the Input File Characterization dialog box from within an existing 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 (Figure 29).

Figure 29. Extract Sample Information From Sample Names dialog box



Extract Sample Information From Sample Names

Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their use, click Help or press the F1 key.

Regular Expression Builder: Blank_01

Sample Name
Blank_01
Blank_02
Urine_0-4hr_01
Urine_0-4hr_02
Urine_4-8hr_01
Urine_4-8hr_02
Urine_8-12hr_01
Urine_8-12hr_02
Urine_Predose_01
Urine_Predose_02

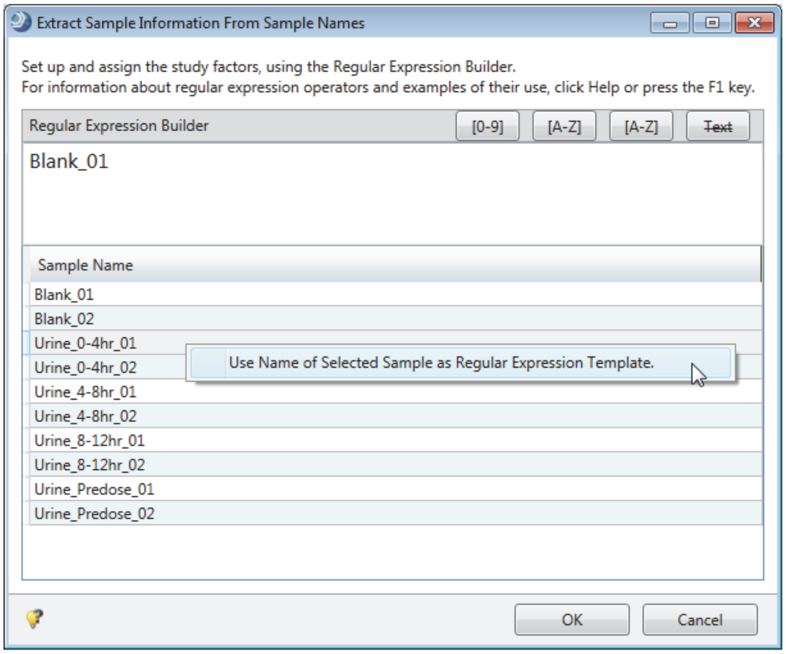
Inserts a regular expression that does the following:

- Ignores a text string.
- Defines a biological variable.
- Defines a categorical variable.
- Defines a numerical variable.

❖ To set up a regular expression that extracts the study factors from the input file names

1. 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 30).

Figure 30. Urine_0-4hr_01 sample name selected



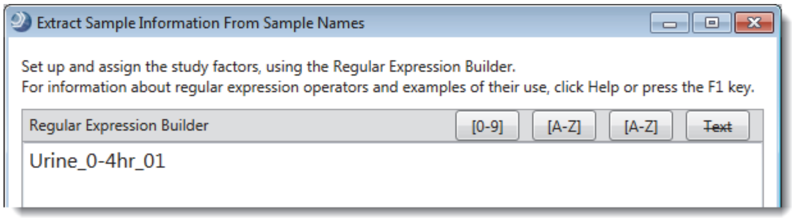
Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their use, click Help or press the F1 key.

Blank_01

Blank_01
Blank_02
Urine_0-4hr_01
Urine_0-4hr_02
Urine_4-8hr_01
Urine_4-8hr_02
Urine_8-12hr_01
Urine_8-12hr_02
Urine_Predose_01
Urine_Predose_02

The selected sample name replaces the nonrepresentative sample name (Figure 31).

Figure 31. Urine 0-4hr file name to be used as the regular expression template



Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their use, click Help or press the F1 key.

Urine_0-4hr_01

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

   - For each categorical study factor, select the corresponding 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. The column is not populated with study factor values for two reasons: the remaining portions of the sample names are not the same (for example, 1 and 2), and the default expression for a categorical factor does not recognize the hyphen special character.

     > **Note** For information about editing the column headings, see "To enter the study factor names" on page 73.

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

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

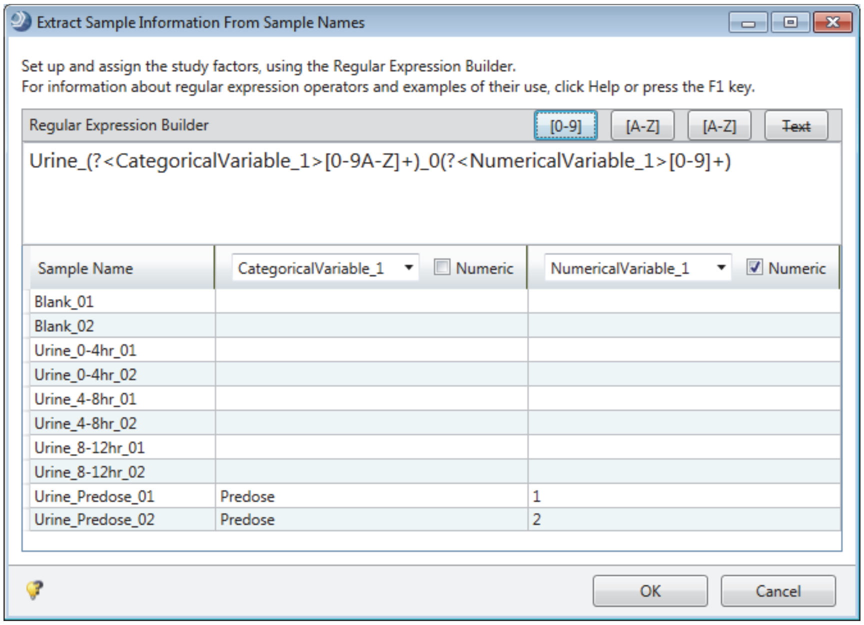
Urine_(?<CategoricalVariable_1>[0-9A-Z]+)_ (?<NumericalVariable_1>[0-9]+).

–and–

Only the study factor values for these file names appear in the table: Urine_Predose_1 and Urine_Predose_2 (Figure 32).

Figure 32 shows the new regular expression in the regular expression builder box. This expression cannot interpret the time periods that include hyphens (0-4hr, 4-8hr, 8-12hr). Only "Predose" matches the expression, which is looking for an alphanumeric string.

Figure 32. Building a regular expression with the default categorical and numeric operators



Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their use, click Help or press the F1 key.

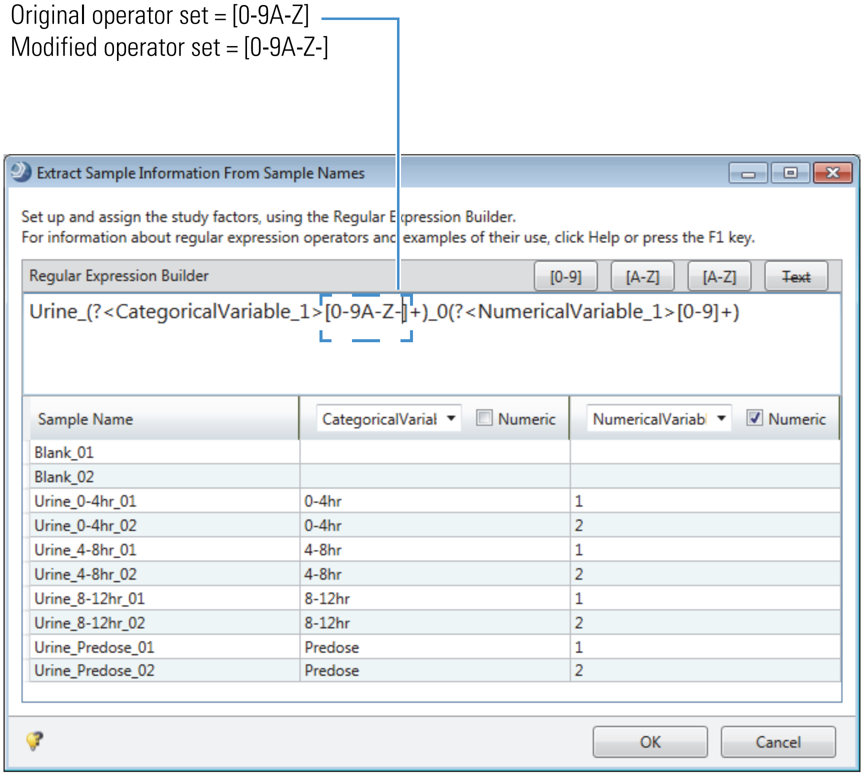
Urine_(?<CategoricalVariable_1>[0-9A-Z]+)_0(?<NumericalVariable_1>[0-9]+)

Sample Name	CategoricalVariable_1 ☐ Numeric	NumericalVariable_1 ☑ Numeric
Blank_01		
Blank_02		
Urine_0-4hr_01		
Urine_0-4hr_02		
Urine_4-8hr_01		
Urine_4-8hr_02		
Urine_8-12hr_01		
Urine_8-12hr_02		
Urine_Predose_01	Predose	1
Urine_Predose_02	Predose	2

3. If the study factor columns do not populate as expected, modify the regular expression operators within the square brackets (see Table 9).

   For example, to populate the rows for the other file names with defined time periods, add a hyphen to the operators in the categorical factor's square brackets. Figure 33 shows the hyphen character added to the operator set for a categorical factor.

Figure 33. Hyphen building block added to the regular expression for a categorical factor



Original operator set = [0-9A-Z]
Modified operator set = [0-9A-Z-]

Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their use, click Help or press the F1 key.

Urine_(?<CategoricalVariable_1>[0-9A-Z-]+)_0(?<NumericalVariable_1>[0-9]+)

Sample Name	CategoricalVarial ▾ ☐ Numeric	NumericalVariabl ▾ ☑ Numeric
Blank_01		
Blank_02		
Urine_0-4hr_01	0-4hr	1
Urine_0-4hr_02	0-4hr	2
Urine_4-8hr_01	4-8hr	1
Urine_4-8hr_02	4-8hr	2
Urine_8-12hr_01	8-12hr	1
Urine_8-12hr_02	8-12hr	2
Urine_Predose_01	Predose	1
Urine_Predose_02	Predose	2

4. 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 34 and Figure 35 show a different sample set than the previous figures.

For example, in the sample set shown in Figure 34, exclude all the characters to the right of the categorical variable by selecting **_01_MDF** and clicking ~~Text~~.

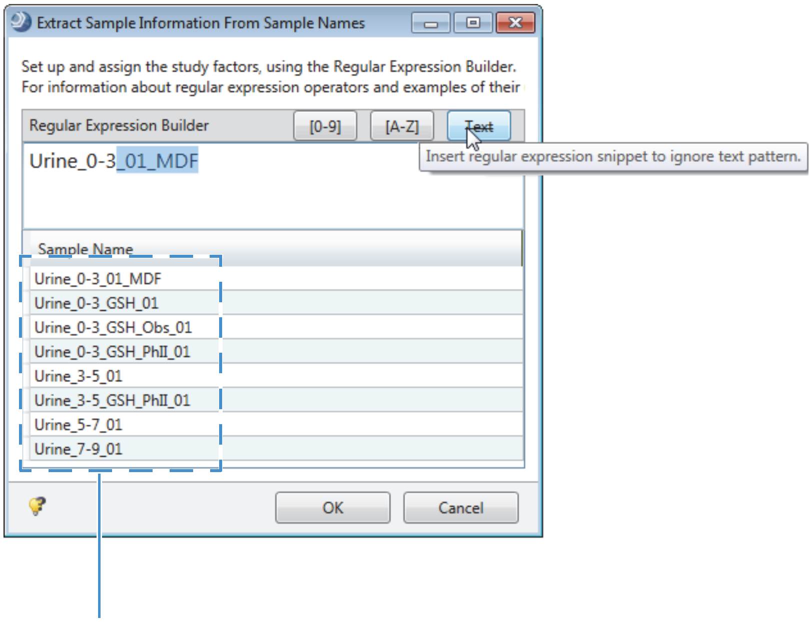
The regular expression builder replaces the selected text with the following expression:

(?:.+)?

Figure 35 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 34. Selecting the text that you want to exclude from the expression



Extract Sample Information From Sample Names

Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their

Regular Expression Builder

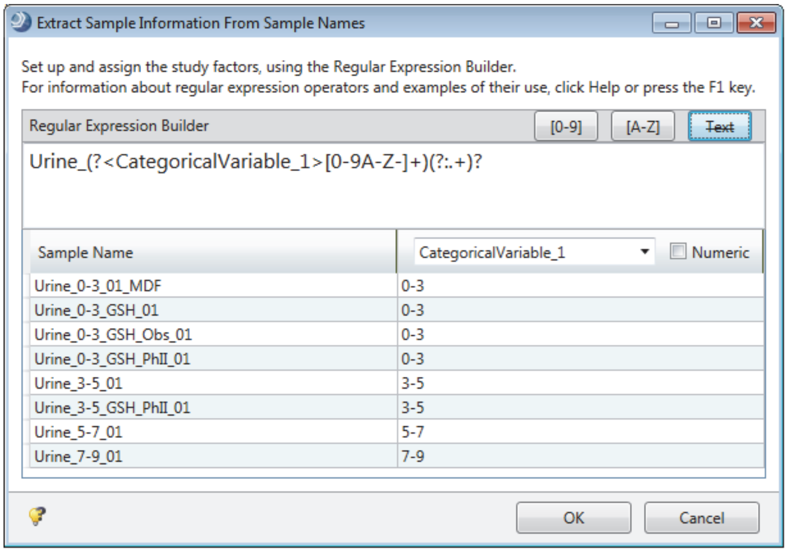
Insert regular expression snippet to ignore text pattern.

Urine_0-3_01_MDF

Sample Name
Urine_0-3_01_MDF
Urine_0-3_GSH_01
Urine_0-3_GSH_Obs_01
Urine_0-3_GSH_PhII_01
Urine_3-5_01
Urine_3-5_GSH_PhII_01
Urine_5-7_01
Urine_7-9_01

The application ignores the extra text when extracting the study factor values from these sample names.

Figure 35. Regular expression that defines the categorical variable and the text to ignore



Extract Sample Information From Sample Names

Set up and assign the study factors, using the Regular Expression Builder.
For information about regular expression operators and examples of their use, click Help or press the F1 key.

Regular Expression Builder

Urine_(?<CategoricalVariable_1>[0-9A-Z-]+)(?:.+)?

Sample Name	CategoricalVariable_1 ☐ Numeric
Urine_0-3_01_MDF	0-3
Urine_0-3_GSH_01	0-3
Urine_0-3_GSH_Obs_01	0-3
Urine_0-3_GSH_PhII_01	0-3
Urine_3-5_01	3-5
Urine_3-5_GSH_PhII_01	3-5
Urine_5-7_01	5-7
Urine_7-9_01	7-9

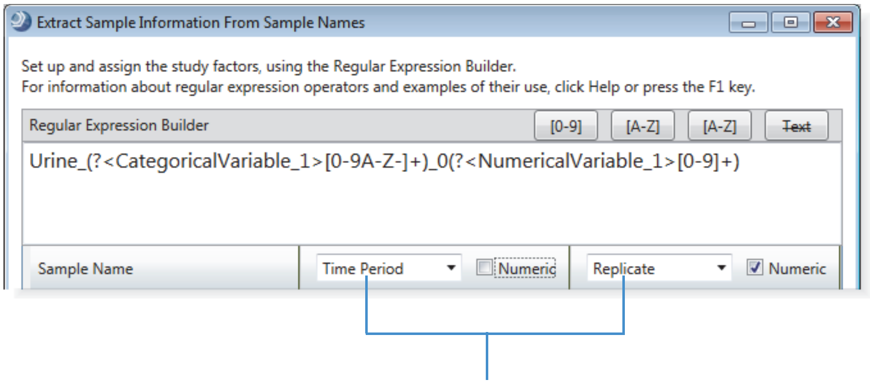
5. Go the next procedure "To enter the study factor names."

❖ To enter the study factor names

1. Type the study factor names in the column-heading boxes.

   For example, replace CategoricalVariable_1 with **Time Period** and NumericalVariable_1 with **Replicate** (Figure 33 and Figure 36).

   Figure 36. Study factors renamed

   Set up and assign the study factors, using the Regular Expression Builder.
   For information about regular expression operators and examples of their use, click Help or press the F1 key.

   ```
   Urine_(?<CategoricalVariable_1>[0-9A-Z-]+)_0(?<NumericalVariable_1>[0-9]+)
   ```

   Time Period ☐ Numeric
   Replicate ☑ Numeric

   Edited study factor names

   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.

2. 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 10 describes the parameters in the Extract Sample Information From Sample Names dialog box.

Table 10. 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.

Setting Up the Sample Groups and Ratios for a New Analysis

Use the Sample Groups and Ratios page (step 5 of 6) of the New Study and Analysis Wizard 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 You can also use the Sample Groups and Ratios page within an existing study to set up the sample groups and ratios. However, when you start a new analysis in an existing study, you cannot set up the sample groups without first adding the input files to the Files for Analysis area of the Analysis pane.

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.

❖ To open the Sample Groups and Ratios page of the wizard

1. From the menu bar, choose **File > New Study and Analysis** and click **Next**.
2. Make the appropriate selections on the Study Name and Processing Workflow page and click **Next**.

   The Input File Selection page opens.

3. Add all the input files for the study or add the input files for the current analysis and click **Next**.

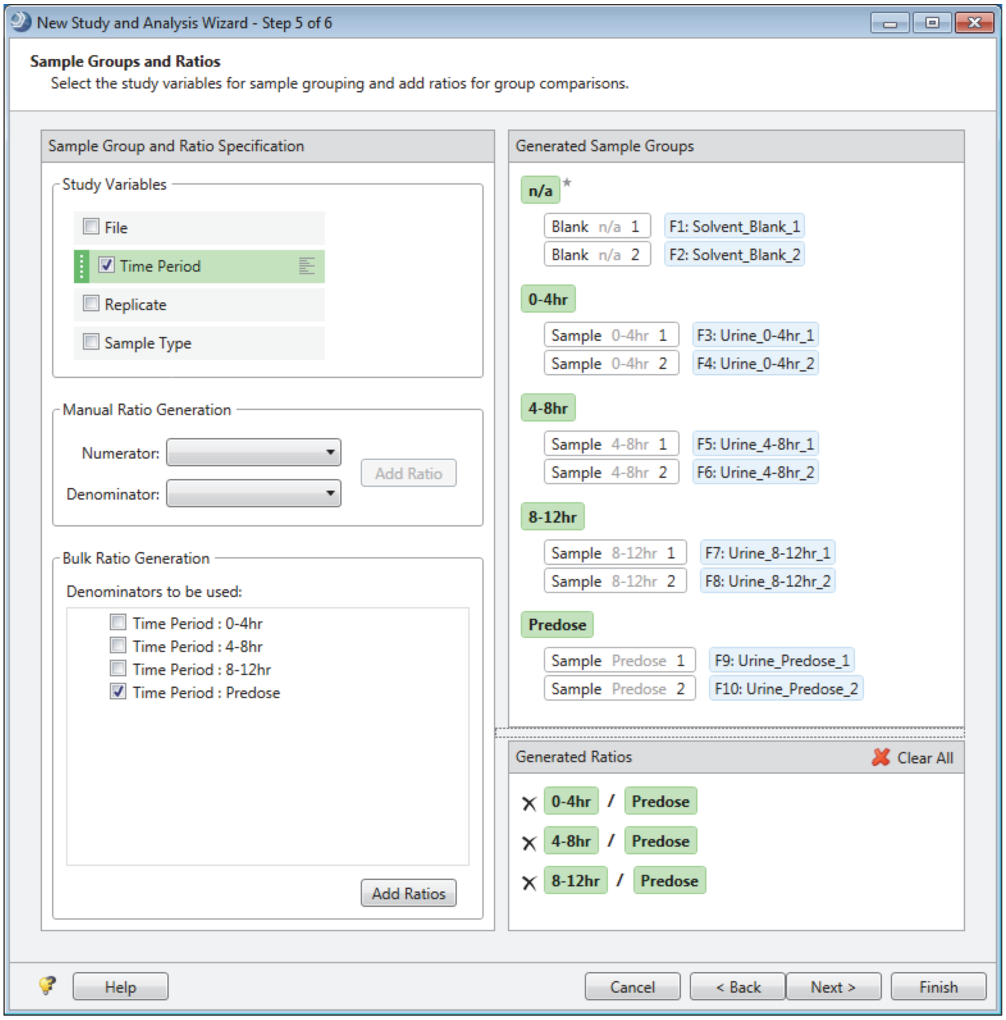
   If you selected a study template when you created the study, the Study Factors area of the Input File Characterization page contains one or more factors. Set up and assign the study factors and select the sample type for each sample.

4. Click **Next**.

   The Sample Groups and Ratios page opens. The Study Variables area contains a File check box and a Sample Type check box. If you added study factors on the Input File Characterization page, the Study Variables area also contains an additional check box for each study factor.

   Figure 37 shows a Sample Groups and Ratios page with generated sample groups and ratios.

Figure 37. Sample Groups and Ratios page of the wizard



New Study and Analysis Wizard - Step 5 of 6

Sample Groups and Ratios

Select the study variables for sample grouping and add ratios for group comparisons.

Sample Group and Ratio Specification

Study Variables

☐ File
☑ Time Period
☐ Replicate
☐ Sample Type

Manual Ratio Generation

Numerator:
Denominator:

Bulk Ratio Generation

Denominators to be used:

☐ Time Period : 0-4hr
☐ Time Period : 4-8hr
☐ Time Period : 8-12hr
☑ Time Period : Predose

Generated Sample Groups

n/a *

Blank n/a 1 — F1: Solvent_Blank_1
Blank n/a 2 — F2: Solvent_Blank_2

0-4hr

Sample 0-4hr 1 — F3: Urine_0-4hr_1
Sample 0-4hr 2 — F4: Urine_0-4hr_2

4-8hr

Sample 4-8hr 1 — F5: Urine_4-8hr_1
Sample 4-8hr 2 — F6: Urine_4-8hr_2

8-12hr

Sample 8-12hr 1 — F7: Urine_8-12hr_1
Sample 8-12hr 2 — F8: Urine_8-12hr_2

Predose

Sample Predose 1 — F9: Urine_Predose_1
Sample Predose 2 — F10: Urine_Predose_2

Generated Ratios

0-4hr / Predose
4-8hr / Predose
8-12hr / Predose

❖ To select the study variables for sample grouping

In the Study Variables area, select 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.

The Generated Sample Groups area displays the generated sample groups. The hierarchy of the study variables affects the sample group names and the denominator list for bulk ratio generation (see To change the hierarchy of the study variables).

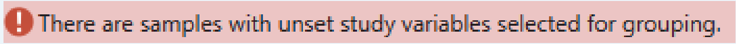
The naming scheme is as follows:

- 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.

❖ To fix an assignment error

IMPORTANT When selecting a study variable generates an N/A group with 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.

1. Return to the Input File Characterization page and do one 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.
   - Change the sample type assignment for samples without a study factor value to **Blank** or **Identification Only**.
2. Return to the Sample Groups and Ratios page and verify the assignments.

❖ 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.

Original hierarchy ------> **Dragging the variable ------> up in the list** **New hierarchy**

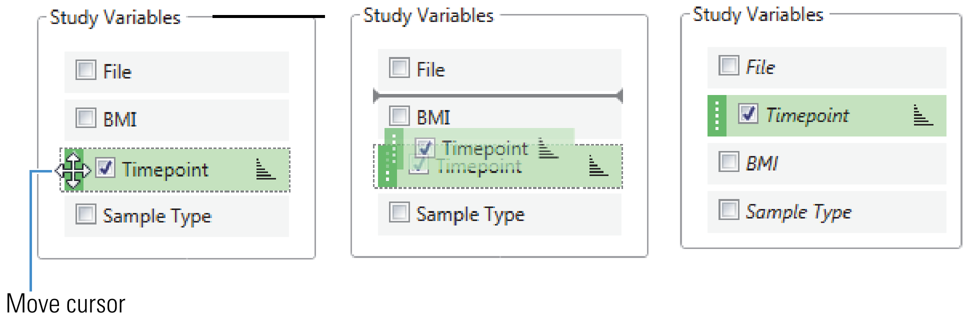
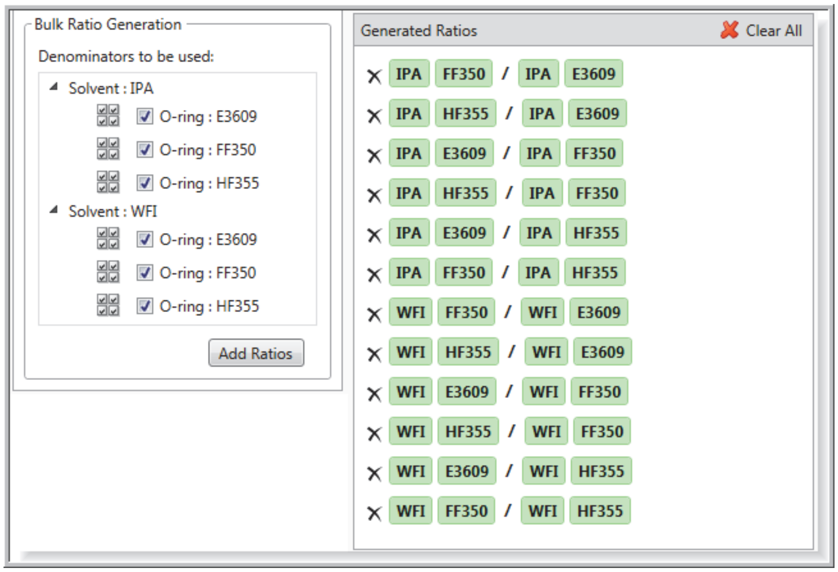


Figure 38 and Figure 39 show the effect of changing the study variable hierarchy for a study where either the extraction solvent (IPA or WFI) or the o-ring type (E3609, FF350, or HF355) is the primary study variable.

The ratios in Figure 38 compare the compounds extracted with the same solvent from different o-ring types.

The ratios in Figure 39 compare the compounds extracted from each o-ring type with the two solvents.

Figure 38. Extraction solvent is the primary variable

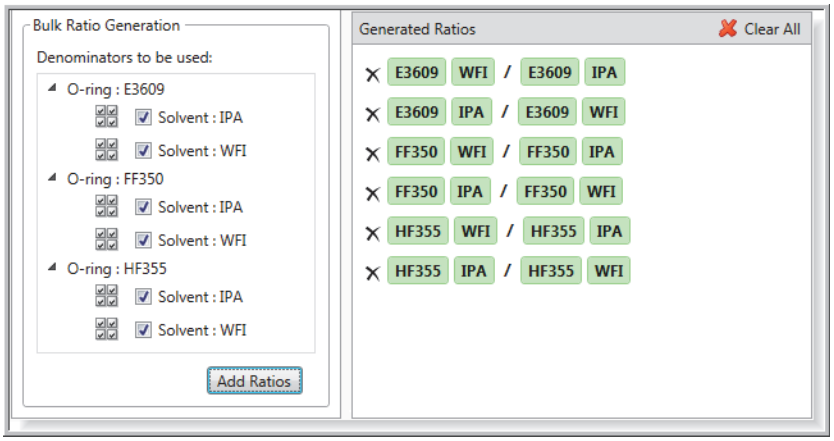


Solvent : IPA
- ☑ O-ring : E3609
- ☑ O-ring : FF350
- ☑ O-ring : HF355

Solvent : WFI
- ☑ O-ring : E3609
- ☑ O-ring : FF350
- ☑ O-ring : HF355

IPA FF350 / IPA E3609
IPA HF355 / IPA E3609
IPA E3609 / IPA FF350
IPA HF355 / IPA FF350
IPA E3609 / IPA HF355
IPA FF350 / IPA HF355
WFI FF350 / WFI E3609
WFI HF355 / WFI E3609
WFI E3609 / WFI FF350
WFI HF355 / WFI FF350
WFI E3609 / WFI HF355
WFI FF350 / WFI HF355

Figure 39. O-ring type is the primary study variable



O-ring : E3609
- ☑ Solvent : IPA
- ☑ Solvent : WFI

O-ring : FF350
- ☑ Solvent : IPA
- ☑ Solvent : WFI

O-ring : HF355
- ☑ Solvent : IPA
- ☑ Solvent : WFI

E3609 WFI / E3609 IPA
E3609 IPA / E3609 WFI
FF350 WFI / FF350 IPA
FF350 IPA / FF350 WFI
HF355 WFI / HF355 IPA
HF355 IPA / HF355 WFI

❖ To set up group ratios one-by-one

In the Manual Ratio Generation area, 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.

❖ To set up multiple ratios automatically

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 more than one value, 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, ⊞.

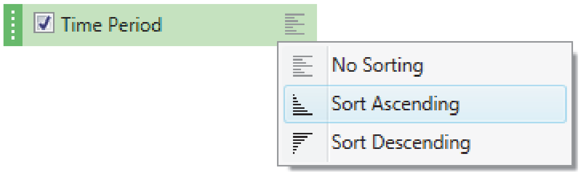
❖ To modify the group ratio list

To remove a ratio, click the delete icon (✕) to its left.

To clear the entire list, click **Clear All**.

❖ To sort the samples, groups, and ratio in ascending or descending order

Click the **Sorting** icon for the study variable that you want to sort by and choose **Sort Ascending** or **Sort Descending**. If you do not want to apply a sort order, choose **No Sorting**.



Preparing to Submit a Run 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.

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 pane. The Analysis pane 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 pane 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 (see "Customizing the Parameter Settings in a Defined Processing Workflow" on page 98). For example, for a targeted analysis, you must select the target compounds for the Generate Expected Compounds node.

If the processing workflow is valid and the Analysis pane contains one or more input files, the Run command at the top right of the Analysis pane is available. If the Run command is unavailable, point to the Caution symbol (⚠) to display a sequence of error messages. The application displays one error message at a time, so after you fix one error condition, another message might appear.

Fix all the error conditions until the Caution symbol disappears and the Run command (Run) becomes available. For more information about troubleshooting an analysis, see "Troubleshooting Common Analysis Errors" on page 101.

About Accessing the Wizard Help

The New Study and Analysis Wizard has two types of Help:

- Embedded instructions that appear to the left of each wizard page
- Context-sensitive Help topics that are part of the Help system

To …	Do the following …
Display the embedded instructions for the current page.	In the lower left corner of the wizard, click the light bulb icon (💡).
Hide the embedded instructions for the current page.	In the lower left corner of the wizard, click the light bulb icon (💡).
Open the context-sensitive Help topic for the current page.	Press the F1 key (F1) on your computer keyboard.

3

Editing Existing Studies

In the Compound Discoverer application, you process your raw data files (run analyses) within the study environment. These topics describe the study features and how to edit an existing Compound Discoverer study.

Contents

About Existing 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 Input Files page of a study tracks the status of the input files. These input files typically reside outside the study folder, for example, 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. Placing the cursor over the warning symbol displays the missing file's expected location and instructions for resolving the issue (see "To resolve the input files list when you move a study or the Xcalibur RAW files" on page 89).

The Analysis Results page of a study tracks the result files generated by analyses run within the study. Result files reside within the study's folder.

Opening an Existing Study

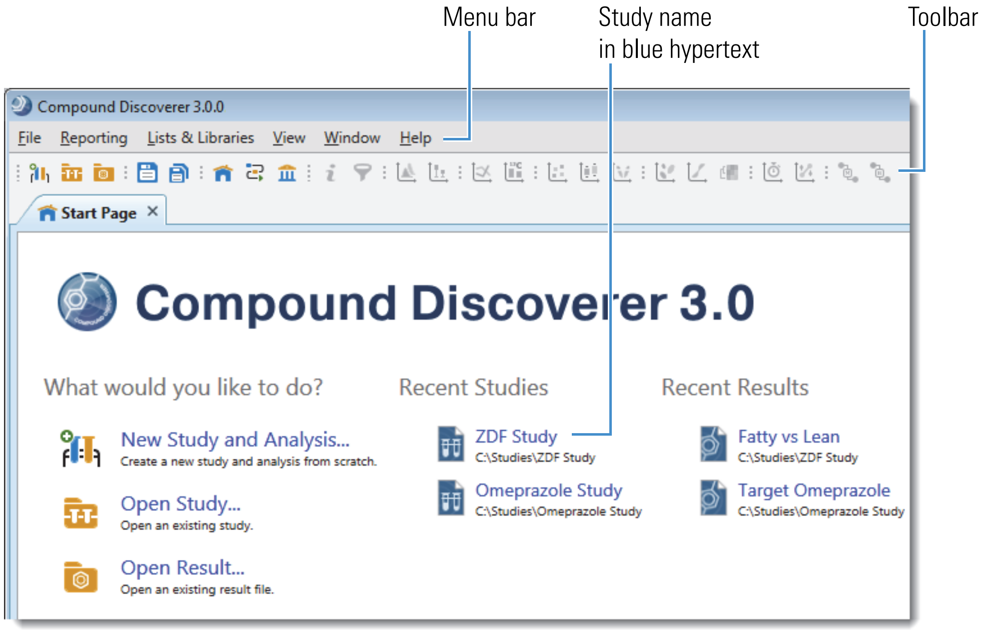
You can open an existing study from the Start Page or the Compound Discoverer window.

❖ To open an existing study

- 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.

  The Start Page lists the 20 most recent studies. The study name appears in blue hypertext. Placing the cursor over a study name underlines it (Figure 40).

  Figure 40. Application window and Start page

  Create a new study and analysis from scratch.

  Open an existing study.

  Open an existing result file.

- From the application menu bar, choose **File > Open Study** to open the Open Study dialog box. Then, select a study file and click **Open**.

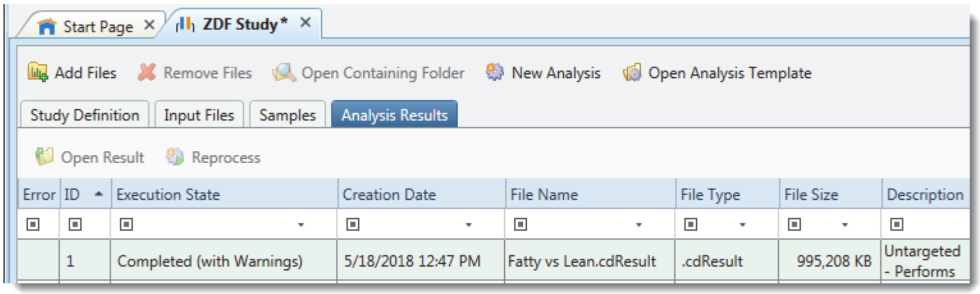
–or–

- 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. 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. When you make changes to a study, an asterisk (*) appears to the right of the study name to indicate unsaved changes (Figure 41).

Tip See the option for "Turning Off the Auto-Save Feature for Studies" on page 449.

Figure 41. Analysis Results page of a study



Error	ID	Execution State	Creation Date	File Name	File Type	File Size	Description
	1	Completed (with Warnings)	5/18/2018 12:47 PM	Fatty vs Lean.cdResult	.cdResult	995,208 KB	Untargeted - Performs

Study Page Commands and Tabs

The study page includes a command bar and four tabbed pages (Table 11).

Table 11. 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. For more information, see "Removing Input Files or Updating Their Location" on page 87.

Table 11. Study page parameters (Sheet 2 of 2)

Command or page	**Description**
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 pane and adds the Workflows tab to the tab set on the study page. The Workflows page itself is empty. This command is unavailable when the Analysis pane is open.
Open Analysis Template	Opens the Analysis Template dialog box where you select an analysis template. This command is unavailable when the Analysis pane is open.
Tabbed pages Use these pages as follows.	
Study Definition	Set up study factors and view the study name, file location, creation date, modification date, and description on this page (see Editing the Study Factors and Study Description).
Input Files	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 (see "Removing Input Files or Updating Their Location" on page 87). Clicking Add Files opens the Input File Characterization dialog box and the Input Files page, if it is not already open.
Samples	Select the sample type and study factors for each raw data file (see "Editing the Sample Type and Study Factor Values" on page 91).
Analysis Results	Access the result files created within the study, review the analysis details for the results files, and reprocess an analysis (see "Reviewing or Reprocessing an Analysis" on page 109).

Editing the Study Factors and Study Description

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.

Follow these topics as needed:

- Editing the Study Description
- Adding or Editing Study Factors in an Existing Study
- 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.

Editing the Study Description

You can edit the description of a study on its Study Definition page.

❖ **To add or edit a description of the study**

Type or edit the description in the Study description area.

Adding or Editing Study Factors in an Existing Study

> **Note** Unlike the Input File Characterization page or dialog box, the Study Factors area of the Study Definition page is not linked to the input file names on the Samples page. This means that the Study Definition page requires more user input to define the study factor values.

❖ **To add and edit study factors in an existing study**

See "Adding and Editing the Study Factors" on page 58.

Study Definition Page of a Study

Table 12 describes the parameters on the Study Definition page.

Table 12. 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.

Table 12. Study Definition page parameters (Sheet 2 of 2)

Parameter	Description
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	
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.
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.

Adding Input Files to an Existing Study

Use the Add Files button on the study command bar to add files to a study.

❖ To add input files to an existing study

1. Open the study of interest.
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 "Characterizing New Input Files" on page 57).
5. Click **OK**.

   The Input Files page of the study opens.

Removing Input Files or Updating 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 pane (see "Setting Up a New Analysis Within an Existing Study" on page 95).

Follow these procedures as needed:

- To sort the input files
- To display the file path for an input file
- To remove input files from the study
- To resolve the input files list when you move a study or the Xcalibur RAW files

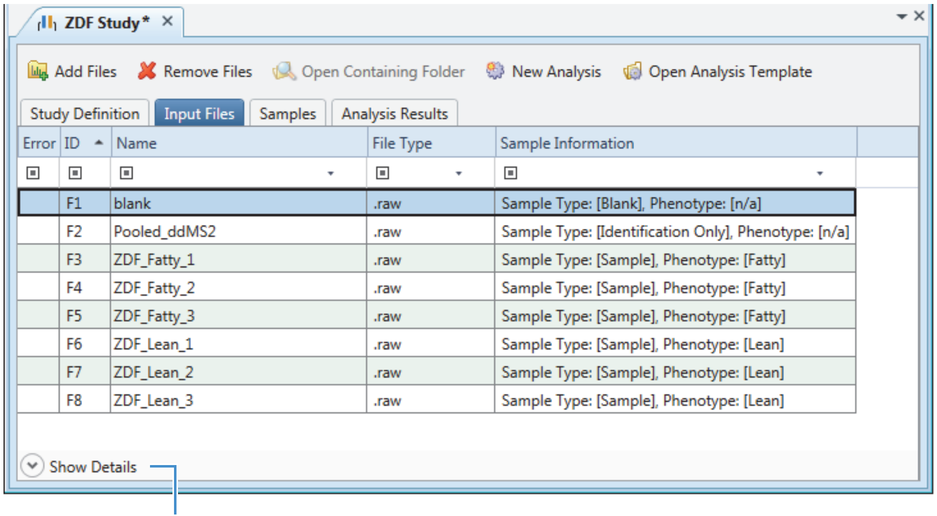
❖ To sort the input files

Click a column heading.

❖ To display the file path for an input file

1. In the input files table, select the input file of interest.
2. Below the table, click **Show Details** (Figure 42).

Figure 42. Input Files page



Error	ID	Name	File Type	Sample Information
	F1	blank	.raw	Sample Type: [Blank], Phenotype: [n/a]
	F2	Pooled_ddMS2	.raw	Sample Type: [Identification Only], Phenotype: [n/a]
	F3	ZDF_Fatty_1	.raw	Sample Type: [Sample], Phenotype: [Fatty]
	F4	ZDF_Fatty_2	.raw	Sample Type: [Sample], Phenotype: [Fatty]
	F5	ZDF_Fatty_3	.raw	Sample Type: [Sample], Phenotype: [Fatty]
	F6	ZDF_Lean_1	.raw	Sample Type: [Sample], Phenotype: [Lean]
	F7	ZDF_Lean_2	.raw	Sample Type: [Sample], Phenotype: [Lean]
	F8	ZDF_Lean_3	.raw	Sample Type: [Sample], Phenotype: [Lean]

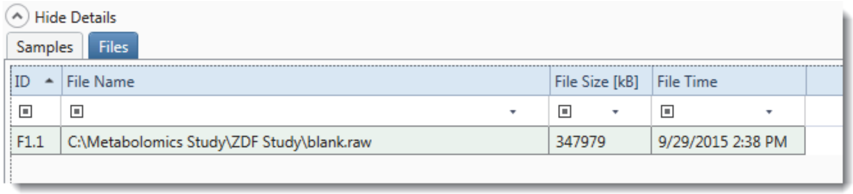
Show/Hide Details command

The Samples page opens below the input files table.

3. Click the **Files** tab.

   Figure 43 shows the hidden Files page that lists the selected input file's full file name, including its directory location.

Figure 43. File path of selected input file



ID	File Name	File Size [kB]	File Time
F1.1	C:\Metabolomics Study\ZDF Study\blank.raw	347979	9/29/2015 2:38 PM

❖ To remove input files from the study

1. 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.

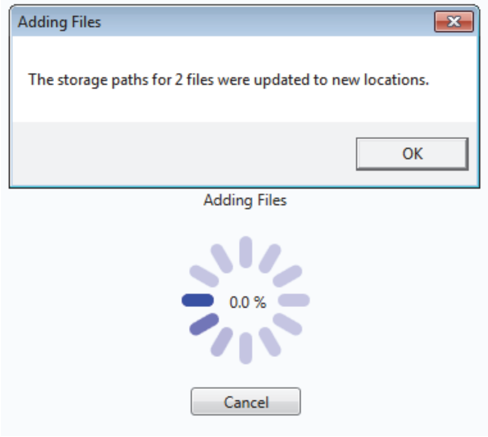
❖ To resolve the input files list when you move a study or the Xcalibur RAW files

> **Note** 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.

1. 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 (see "Adding Input Files to an Existing Study" on page 87).

   The Adding Files confirmation box opens. The progress remains at 0.0% until you click OK (Figure 44).

   Figure 44. Adding Files confirmation box with progress information

   Adding Files

   The storage paths for 2 files were updated to new locations.

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.

Table 13 describes the parameters on the Input Files page.

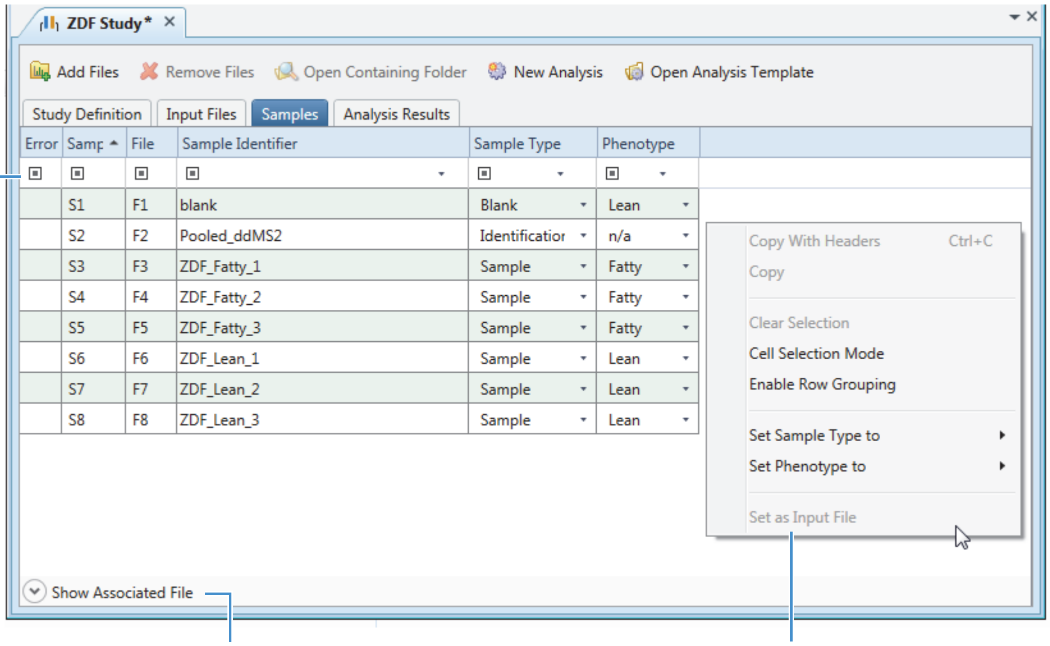
Table 13. Input Files page parameters

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.
Sample Identifier	Displays the file name of the raw data file.
Sample Type	Displays the sample type (see “Sample Types” on page 51).
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.

Editing the Sample Type and Study Factor Values

If you have not already characterized the study samples, use the Samples page (Figure 45) of an existing study to identify the sample type and study factors for each input file. Use the filter row to limit the sample list to specific samples.

Figure 45. Samples page and its shortcut menu



Error	Samp	File	Sample Identifier	Sample Type	Phenotype
	S1	F1	blank	Blank	Lean
	S2	F2	Pooled_ddMS2	Identificatior	n/a
	S3	F3	ZDF_Fatty_1	Sample	Fatty
	S4	F4	ZDF_Fatty_2	Sample	Fatty
	S5	F5	ZDF_Fatty_3	Sample	Fatty
	S6	F6	ZDF_Lean_1	Sample	Lean
	S7	F7	ZDF_Lean_2	Sample	Lean
	S8	F8	ZDF_Lean_3	Sample	Lean

Filter row

Shows the file information.

Shortcut menu

Select the sample type and study factors on the Samples page by following these procedures:

- To open the Samples page
- To select the sample type for each sample
- To select the study factor values for each sample
- To view additional information for a selected sample

❖ To open the Samples page

On the study page, click the **Samples** tab.

❖ To select the sample type for each sample

See "Selecting the Sample Types" on page 65.

❖ To select the study factor values for each sample

See "Assigning or Selecting the Study Factor Values" on page 64.

❖ To view additional information for a selected sample

Click **Show Associated File** below the table.

The following details appear—the full file name and location, the file size in kilobytes, and the acquisition time of the Xcalibur RAW file.

Table 14 describes the parameters on the Samples page.

Table 14. Samples page parameters (Sheet 1 of 2)

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. Selections: Sample, Control, Blank, Quality Control, Identification Only, Standard, or Labeled. For more information, see "Sample Types" on page 51.
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 "Working with the Application Tables" on page 531.	
Set Sample Type To	Assigns the selected sample type to a sample range.

Table 14. Samples page parameters (Sheet 2 of 2)

Parameter	Description
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 pane. Available when the Analysis pane is open.

Saving a Study File

By default, the application saves the study file when you close it. However, you can change this behavior by turning off the auto save feature ("Turning Off the Auto-Save Feature for Studies" on page 449).

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.

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 so on.

❖ To save a study file

Do one of the following:

- From the menu bar, choose **File > Save All**, or in the toolbar, click the **Save All Open Items** icon, .

–or–

a. Click the study tab to make it the active page.

b. From the menu bar, choose **File > Save**, or in the toolbar, click the **Save the Currently Active Item** icon, .

For information about reviewing an analysis during processing or after processing is finished, see "Reviewing or Reprocessing an Analysis" on page 109.

4

Creating, Running, and Reprocessing Analyses

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

Contents

Setting Up a New Analysis 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 pane. 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 pane.

Follow these topics in order:

1. Starting a New Analysis
2. Selecting a Processing Workflow for a New Analysis
3. Customizing the Parameter Settings in a Defined Processing Workflow
4. Selecting the Input Files for a New Analysis

5. (Optional) Naming the Result File for a New Analysis
6. (Optional) Setting Up the Sample Groups and Ratios for a New Analysis

Starting a New Analysis

❖ To start a new analysis

1. Open a study (see "Opening an Existing Study" on page 82).
2. Do one of the following:
   - To open an existing analysis for editing, select a run on the Analysis Results page and click **Reprocess**.

     The Workflows tab and the Grouping & Ratios tab appear to the right of the study page tabs. The Analysis pane opens to the right of the tabbed pages. The Workflows page, the Grouping & Ratios page, and the Analysis pane contain the analysis settings for the selected run. You can edit all of the analysis settings.
   - 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 pane opens to the right of the tabbed pages. Both the Workflows and Grouping & Ratios pages are empty.
   - In the study command bar, click **Open Analysis Template**.

     The Workflows and Grouping and Ratios tabs appear to the right of the study page tabs and an empty Analysis pane opens to the right of the tabbed pages. When you click the Workflows tab, the Workflows page opens with the processing workflow saved with the template. For information about editing the processing workflow, see "Editing a Processing Workflow" on page 119. The Grouping and Ratios page is unpopulated. To create sample groups and ratios, you must first add input files to the Analysis pane (see "To select the input files that you want to process" on page 99).

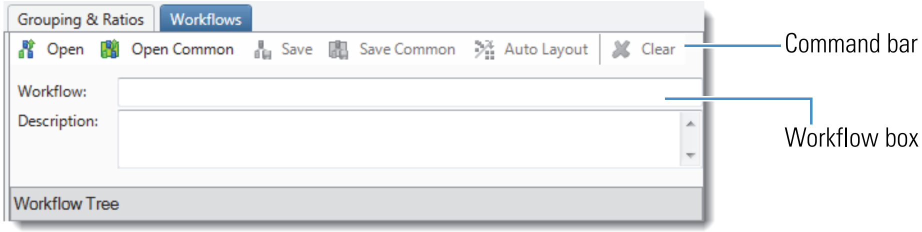
Selecting a Processing Workflow for a New Analysis

❖ To select a processing workflow for a new analysis

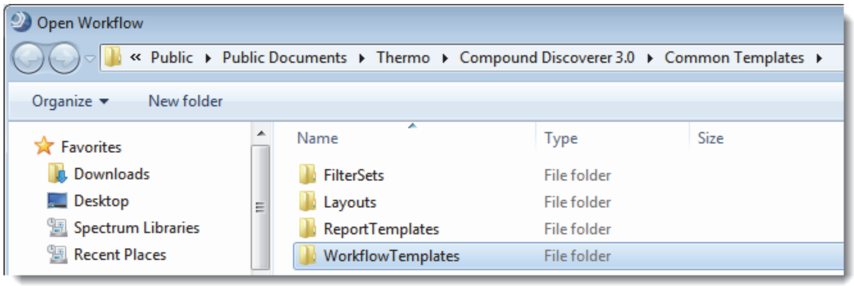
1. Follow the instructions in the previous topic "Starting a New Analysis."
2. Click the **Workflows** tab.

3. Do one of the following:

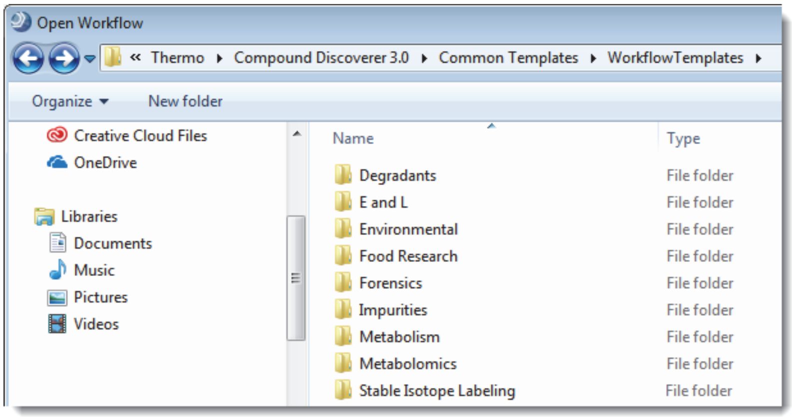
   a. To select a processing workflow from the Common Templates folder, click **Open Common** in the Workflows command bar.



   The Common Templates folder opens.



   b. Open the Workflow Templates folder, which contains a set of folders labeled by vertical market.



   c. Open the appropriate folder and select a processing workflow file.

   d. Click **Open**.

   –or–

   a. To select a processing workflow from another folder, click **Open** in the Workflows command bar.

   b. In the Open Workflow dialog box, locate a processing workflow file (.cdProcessingWF) or a result file (.cdResult), and click **Open**.

      - When you select a processing workflow file, the file name appears in the Workflow box.

- 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 Description box below the Workflow box.

Go to the next topic "Customizing the Parameter Settings in a Defined Processing Workflow."

Customizing the Parameter Settings in a Defined Processing Workflow

After you select a defined processing workflow or create your own processing workflow, you might need to modify the parameter settings for some of the workflow nodes.

Table 15 lists the workflow nodes that require custom settings.

To modify the workflow node settings, see "Editing a Processing Workflow" on page 119.

Table 15. Workflow nodes that require customization

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, define the ratio. In the defined workflow templates, the ratio has been set to C15S.
Search Mass Lists	From the Input Files list, select mass lists. In the defined workflow templates, one of the preinstalled mass lists has been selected, according to the vertical market.
Search mzVault	From the mzVault Library list, select mzVault libraries. In the defined workflow templates, the preinstalled mzVault May 2018 library has been 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.

Thermo Fisher Scientific has already optimized most of the parameter settings in the defined processing workflow templates. Table 16 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 (cdProcessingWorkflow).

Table 16. 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	See Table 17.

Table 17 lists the recommended range for the minimum peak intensity parameter. The optimal setting depends on the sensitivity of the mass spectrometer.

Table 17. 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

Go to the next topic "Selecting the Input Files for a New Analysis."

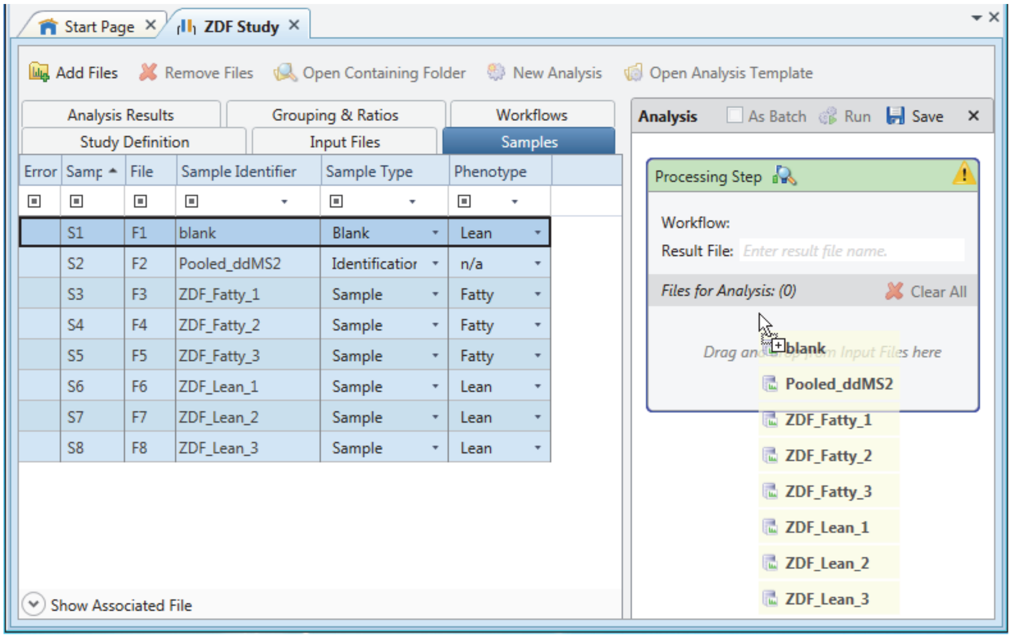
Selecting the Input Files for a New Analysis

Follow this procedure to select the input files for a new analysis. If you are reprocessing a previous analysis, the Files for Analysis area of the Analysis pane 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.
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 pane (Figure 46).

Figure 46. Dragging input files to the Analysis pane



Error	Samp	File	Sample Identifier	Sample Type	Phenotype
	S1	F1	blank	Blank	Lean
	S2	F2	Pooled_ddMS2	Identificatior	n/a
	S3	F3	ZDF_Fatty_1	Sample	Fatty
	S4	F4	ZDF_Fatty_2	Sample	Fatty
	S5	F5	ZDF_Fatty_3	Sample	Fatty
	S6	F6	ZDF_Lean_1	Sample	Lean
	S7	F7	ZDF_Lean_2	Sample	Lean
	S8	F8	ZDF_Lean_3	Sample	Lean

Workflow:
Result File: Enter result file name.
Files for Analysis: (0)

The file name of the last input file appears in the Result File box, and 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 As Batch check box becomes available.

If the Caution symbol in the Processing Step title bar remains, the processing workflow contains an error.

Naming the Result File for a New Analysis

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

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

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

Go to the next topic "Setting Up the Sample Groups and Ratios for a New Analysis."

Setting Up the Sample Groups and Ratios for a 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.

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

1. Add input files to the Analysis pane (see "Selecting the Input Files for a New Analysis" on page 99).
2. Follow the instructions for the Sample Groups and Ratios page of the New Study and Analysis Wizard ("Setting Up the Sample Groups and Ratios for a New Analysis" on page 75).

Go to the next topic, "Troubleshooting Common Analysis Errors."

Troubleshooting Common Analysis Errors

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

Tip The application does not know the polarity of the scan data or whether the data contains data-dependent fragmentation (DDF) or All Ions Fragmentation (AIF) scans. For best results, check the following:

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

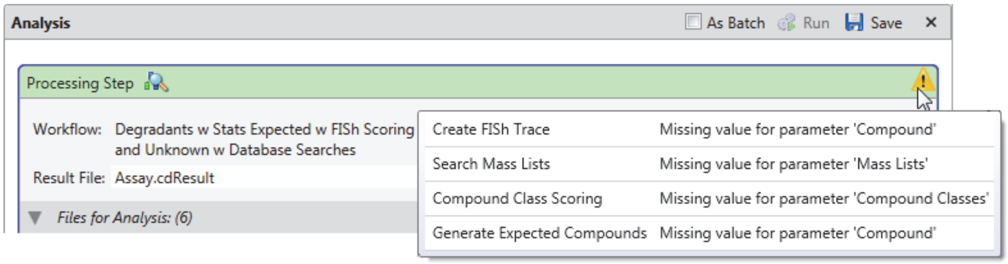
❖ To troubleshoot an analysis

1. In the Analysis pane, 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 48) 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 "Common Analysis Errors" on page 102).

   For example, Figure 47 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 47. Error messages for a defined processing workflow



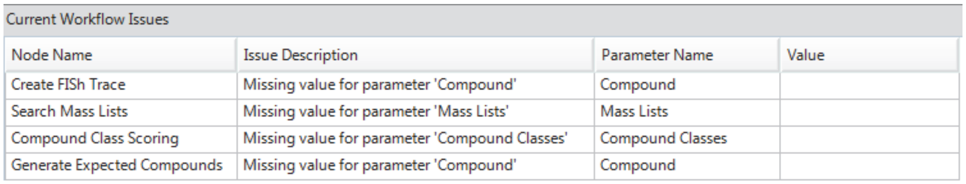
Workflow: Degradants w Stats Expected w FISh Scoring and Unknown w Database Searches

Result File: Assay.cdResult

Create FISh Trace	Missing value for parameter 'Compound'
Search Mass Lists	Missing value for parameter 'Mass Lists'
Compound Class Scoring	Missing value for parameter 'Compound Classes'
Generate Expected Compounds	Missing value for parameter 'Compound'

Figure 48 shows the corresponding error messages in the Current Workflow Issues pane.

Figure 48. Current Workflow Issues pane



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 To view new compounds in the Compound list or new mass lists in the Input Files list, close the current analysis and start a new analysis. This means that you must select the processing workflow on the Workflows page and add the input files that you want to process from the Input Files page to the Analysis pane.

Go to "Submitting an Analysis to the Job Queue" on page 103.

Common Analysis Errors

To troubleshoot common analysis errors, see Table 18.

Note To troubleshoot validation issues, which occur after you submit a run, see "Common Validation Issues" on page 104.

Table 18. Common analysis errors

Error message	Error	Solution
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 ("Selecting the Input Files for a New Analysis" on page 99).
The current pipeline does not contain any node.	You have not set up a processing workflow on the Workflows page.	Select or set up a processing workflow on the Workflows page.
Validation of processing node "*Node Name*" failed. Validation status was: Missing parameter value for: *Parameter*.	The processing workflow contains a node that requires a custom parameter setting.	Make the appropriate selections in the affected workflow nodes.
Validation of processing node "*Node Name*" failed. Validation status was: Missing connection: *Connection information*.	You have not connected all of the processing workflow nodes, or the Workflow Tree pane contains extra nodes that are not part of the processing workflow.	Connect workflow nodes that are part of the processing workflow and delete unnecessary nodes. Scroll up and down and left to right in the Workflow Tree pane to find unnecessary nodes.
Validation of processing node "Search ChemSpider failed! Validation status was: Missing parameter value for: Database(s). In addition to this error message, the node has an exclamation icon in its upper right corner.	Your processing computer does not have Internet access or its access to the external website is blocked.	Connect the computer to the Internet. If the computer has access to the Internet, verify that it has access to the external website.

Submitting 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 **As Batch** check box clear.
   - To create a separate result file for each input file, select the **As Batch** 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. For information about the job queue, see "Working with the Job Queue" on page 105.

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

4. At the prompt, do the following:

   a. Read the warning message.

   b. Do one of the following:

      - To modify the analysis, click **Abort** and remedy the error. See the next topic "Common Validation Issues."

      - To start data processing, click **Ignore**.

Common Validation Issues

To troubleshoot common validation issues, see Table 19.

Table 19. Validation issues (Sheet 1 of 2)

Validation issue	Remedy
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 samples 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.	
The processing workflow includes Compound Identification or Pathway Mapping nodes, but does not include the Assign Compound Annotations node.	On the Workflows page, add the **Assign Compound Annotations** node to the workflow.

Table 19. Validation issues (Sheet 2 of 2)

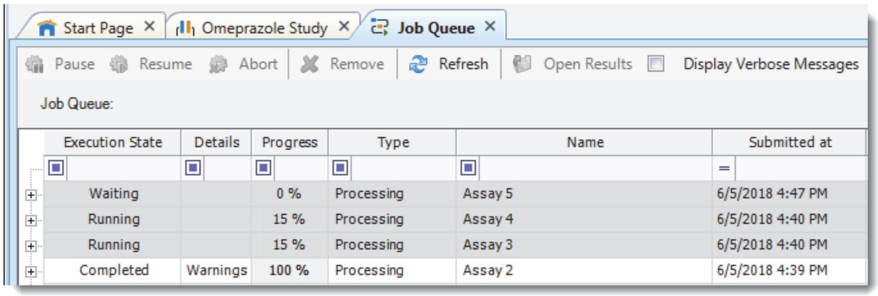
Validation issue	Remedy
IMPORTANT If the analysis does not include the Assign Compound Annotations node, the application does not assign names or formulas to compounds in the Compounds table of a result file.	
The processing workflow includes the Assign Compound Annotations node, but the processing workflow 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.

Working with the Job Queue

When you submit an analysis for processing, the Job Queue page opens (Figure 49). 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 (see "Selecting the Maximum Number of Parallel Processing Jobs" on page 447). If you submit a second run while the first run is being processed, the status of the second run goes to Not Queued, Running, or Execution Failed. If you submit a third run while the application is processing the first two runs, its status goes to Waiting. If you pause a run that is waiting, its status goes to Sleeping.

Figure 49. Job queue with runs in various processing states



Execution State	Details	Progress	Type	Name	Submitted at
Waiting		0 %	Processing	Assay 5	6/5/2018 4:47 PM
Running		15 %	Processing	Assay 4	6/5/2018 4:40 PM
Running		15 %	Processing	Assay 3	6/5/2018 4:40 PM
Completed	Warnings	100 %	Processing	Assay 2	6/5/2018 4:39 PM

Follow these procedures as needed:

- To open a hidden Job Queue page
- To pause a run that is waiting to be processed
- To resume a paused run
- To cancel a run that is being processed
- To remove a completed or failed run from the Job Queue list
- To refresh the Job Queue list

- To open a result file
- To display verbose messages
- To view the processing steps for a run
- To filter the Job Queue list

❖ To open a hidden Job Queue page

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

The Job Queue page opens as a tabbed document.

❖ To pause a run that is waiting to be processed

1. In the Job Queue list, select the run that you want to pause.

   You can only pause runs with a status of Waiting.

2. In the command bar, click **Pause**.

   The status of the run changes to Sleeping.

❖ To resume a paused run

1. In the Job Queue list, select the paused run.
2. In the command bar, click **Resume**.

❖ To cancel a run that is being processed

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

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

❖ To remove a completed or failed run from the Job Queue list

1. In the Job Queue list, select the run that you want to remove.
2. In the command bar, click **Remove**.

   The selected run disappears from the Job Queue list. The application does not remove the result file from the study.

❖ To refresh the Job Queue list

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

❖ To open a result file

In the Job Queue list, do one of the following:

- Select the completed run of interest and click **Open Results** in the command bar.

–or–

- Double-click a completed run of interest.

The Results page for the selected run opens as a tabbed document in the application window.

❖ To display verbose messages

Select the **Display Verbose Messages** check box.

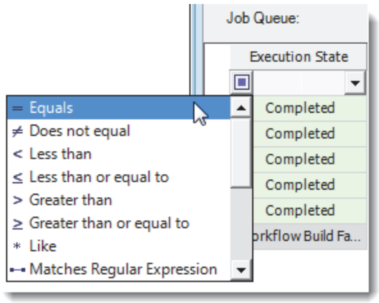
❖ To view the processing steps for a run

Click the expand icon, ⊞, to the left of the job row.

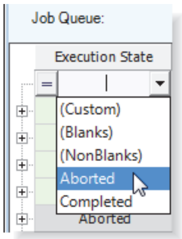
❖ To filter the Job Queue list

> **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.

Table 20 describes the command bar and progress table on the Job Queue page.

Table 20. Job Queue page features (Sheet 1 of 2)

Feature	Description
Command bar	
Pause	Pauses a job that is waiting to start. Selecting a job that is waiting to start activates this button.
Resume	Resumes a processing job that is sleeping. Selecting a job with a status of Sleeping activates this button.
Abort	Stops processing and removes the selected job from the queue. Selecting a job that is being processed activates this button.
Remove	Selecting a completed job activates this button.
Refresh	Refreshes the job queue list.
Open Results	Opens the result file for the selected job.
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 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. • Sleeping—You paused the job while it was waiting in the queue. • Completed—The application has completed the analysis and you can open the result file.
Details	Displays whether the job ran with or without warnings.

Table 20. Job Queue page features (Sheet 2 of 2)

Feature	Description
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.

Reviewing or Reprocessing 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.

To review or reprocess an analysis, follow these topics:

- Reviewing an Analysis
- Reprocessing an Analysis

Table 21 describes the command bar and progress table on the Analysis Results page of a study. For information about studies, see Chapter 3, “Editing Existing Studies.”

Table 21. Analysis Results page parameters (Sheet 1 of 2)

Feature	Description
Command bar	
Selecting an analysis in the list on this page activates these commands.	
Open Result	Opens the selected result file.

Table 21. Analysis Results page parameters (Sheet 2 of 2)

Feature	Description
Reprocess	Opens the Analysis pane 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.
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.
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 "Copying Table Entries to the Clipboard" on page 537 and "Grouping Table Rows" on page 533.
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 pane. You cannot start runs from this window.
Reprocess	Same functionality as the Reprocess command in the command bar.

Reviewing an Analysis

Use the Analysis Sequence Details window to review an analysis.

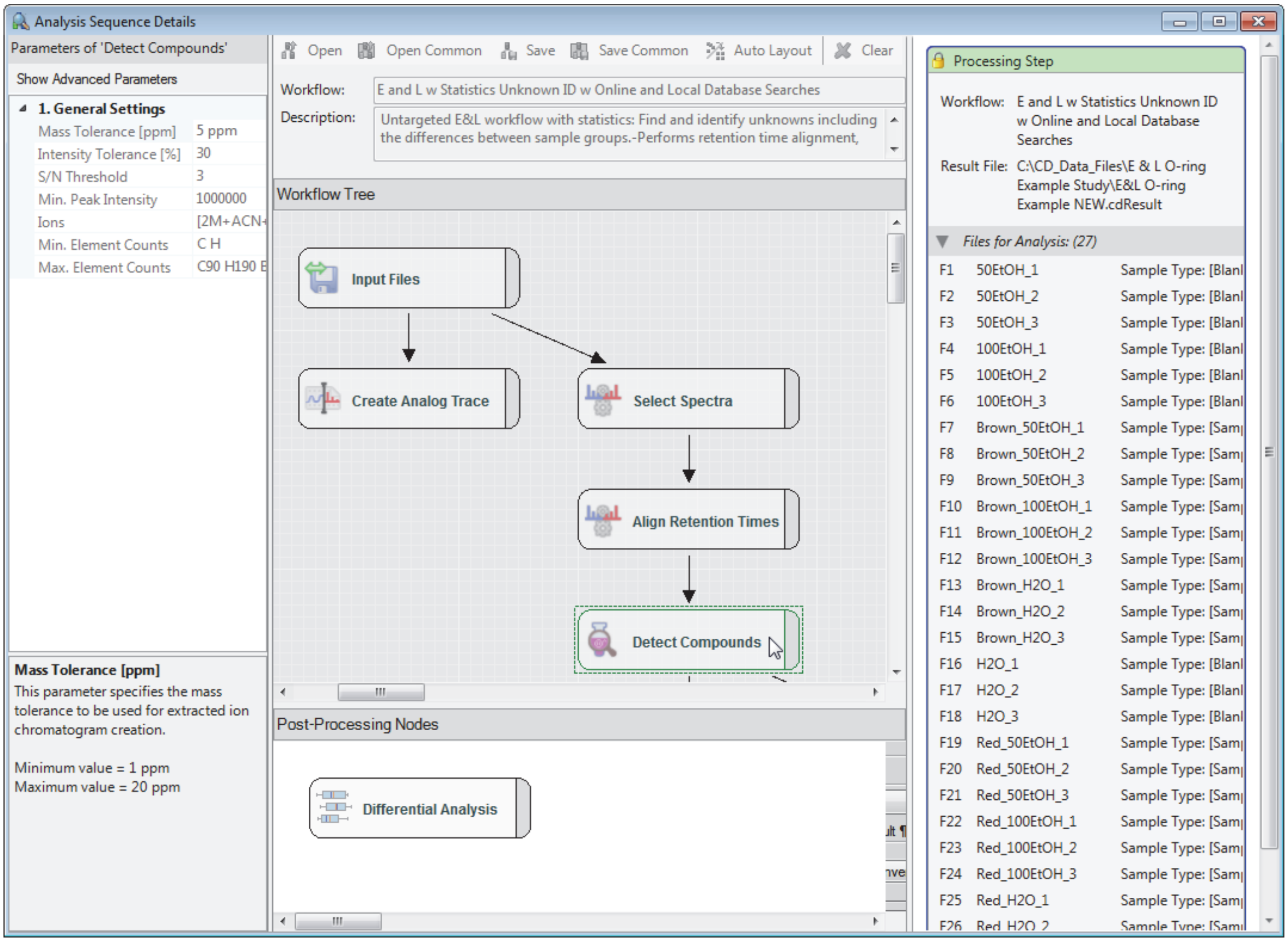
❖ To review an analysis

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 a workflow node's parameter settings, select it in the Workflow Tree pane to display its parameter settings in the Parameters pane on the left.

Figure 50. Analysis Sequence Details window showing the parameter settings for the Detect Compounds node



Parameters of 'Detect Compounds'

1. General Settings

Mass Tolerance [ppm]	5 ppm
Intensity Tolerance [%]	30
S/N Threshold	3
Min. Peak Intensity	1000000
Ions	[2M+ACN+
Min. Element Counts	C H
Max. Element Counts	C90 H190 E

Mass Tolerance [ppm]
This parameter specifies the mass tolerance to be used for extracted ion chromatogram creation.

Minimum value = 1 ppm
Maximum value = 20 ppm

Workflow: E and L w Statistics Unknown ID w Online and Local Database Searches

Description: Untargeted E&L workflow with statistics: Find and identify unknowns including the differences between sample groups.-Performs retention time alignment,

Workflow: E and L w Statistics Unknown ID w Online and Local Database Searches

Result File: C:\CD_Data_Files\E & L O-ring Example Study\E&L O-ring Example NEW.cdResult

Files for Analysis: (27)

F1	50EtOH_1	Sample Type: [Blan
F2	50EtOH_2	Sample Type: [Blan
F3	50EtOH_3	Sample Type: [Blan
F4	100EtOH_1	Sample Type: [Blan
F5	100EtOH_2	Sample Type: [Blan
F6	100EtOH_3	Sample Type: [Blan
F7	Brown_50EtOH_1	Sample Type: [Sam
F8	Brown_50EtOH_2	Sample Type: [Sam
F9	Brown_50EtOH_3	Sample Type: [Sam
F10	Brown_100EtOH_1	Sample Type: [Sam
F11	Brown_100EtOH_2	Sample Type: [Sam
F12	Brown_100EtOH_3	Sample Type: [Sam
F13	Brown_H2O_1	Sample Type: [Sam
F14	Brown_H2O_2	Sample Type: [Sam
F15	Brown_H2O_3	Sample Type: [Sam
F16	H2O_1	Sample Type: [Blan
F17	H2O_2	Sample Type: [Blan
F18	H2O_3	Sample Type: [Blan
F19	Red_50EtOH_1	Sample Type: [Sam
F20	Red_50EtOH_2	Sample Type: [Sam
F21	Red_50EtOH_3	Sample Type: [Sam
F22	Red_100EtOH_1	Sample Type: [Sam
F23	Red_100EtOH_2	Sample Type: [Sam
F24	Red_100EtOH_3	Sample Type: [Sam
F25	Red_H2O_1	Sample Type: [Sam
F26	Red_H2O_2	Sample Type: [Sam

Reprocessing an Analysis

You can reprocess an entire analysis or only the post-compound detection portions of an analysis.

❖ To reprocess an analysis

1. On the Analysis Results page of a study, right-click the analysis and choose **Reprocess**.
    - If the Analysis pane 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 pane 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 pane and decide whether you want to discard the current settings.
    b. Click **Yes** to replace the current settings in the Analysis pane 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 You can 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 (except the Mark Background Compounds node), or Expected Compounds (except the Mark Background Compounds and Merge Features nodes).

4. To reprocess only part of the 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.

    b. Right-click the nodes that you want to reprocess and choose **Reprocess**.

       The selected nodes and any related nodes revert to their original color, and the Run command becomes available in the Analysis pane.

    c. Go to step 7.

5. To reprocess the entire processing workflow, right-click the Input Files node and choose **Reprocess**.

6. If necessary, make changes to the sample groups and ratios on the Grouping & Ratios page and the settings in the Analysis pane.

   > **Note** When you change any of the settings on the Grouping & Ratios page or the files for analysis in the Analysis pane, the application automatically reprocesses the entire processing workflow.

7. To start the analysis, click **Run**.

Analysis Pane Parameters

The Analysis pane appears to the right of the analysis pages when you start a new analysis or open an existing analysis template. Table 22 describes the parameters in the Analysis pane.

Table 22. Analysis pane parameters (Sheet 1 of 2)

Parameters	Description
Title bar	
As Batch 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 pane, the Workflows page, and the Grouping & Ratios page.

Table 22. Analysis pane parameters (Sheet 2 of 2)

Parameters	Description
Processing Step area	
🔍 Show Workflow icon	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 Show Workflow icon (see “Common Analysis Errors” on page 102). To display the error list, point to the Caution symbol.
Workflow	By default, the text matches the text in the Workflow box on the Workflows page. You cannot change the text in the Analysis pane. To change the name of the processing workflow, edit the text on the Workflows page.
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.
Files for Analysis: (#)	Displays the number of input files in the Files for Analysis area.
Files for Analysis area	Displays the names of the input files after you add the input files from the Input Files page or the Samples page of the study to this area. To add files to the Files for Analysis area, see “Selecting the Input Files for a New Analysis” on page 99.

Creating and Editing Processing Workflows

The Compound Discoverer application uses a processing workflow to analyze the MS data acquired with a high-resolution, accurate-mass LC/MS/MS instrument. In addition to analyzing the MS data, the application can display chromatograms acquired with a photo-diode array (PDA) or ultraviolet-visible (UV-Vis) detector that is controlled by a Thermo Scientific data system or an analog detector that is connected to the mass spectrometer's analog input channels.

For information about each workflow node, see Chapter 13, "Workflow Nodes."

These topics describe how to create and edit processing workflows on the Workflows page of a study.

Contents

Workflows Page

Within an existing study, use the Workflows page to create or 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 information about opening the Workflows page and its command bar and shortcut menu, see these topics:

- Opening the Workflows Page
- Workflows Page Command Bar
- Workflows Page Shortcut Menu

Opening the Workflows Page

The Workflows page appears to the right of the four study pages and next to the Grouping and Ratios page after you set up a new study and a new analysis with the New Study and Analysis wizard. Closing a study erases the analysis settings, and reopening the study only opens the study pages.

❖ To open the Workflows page

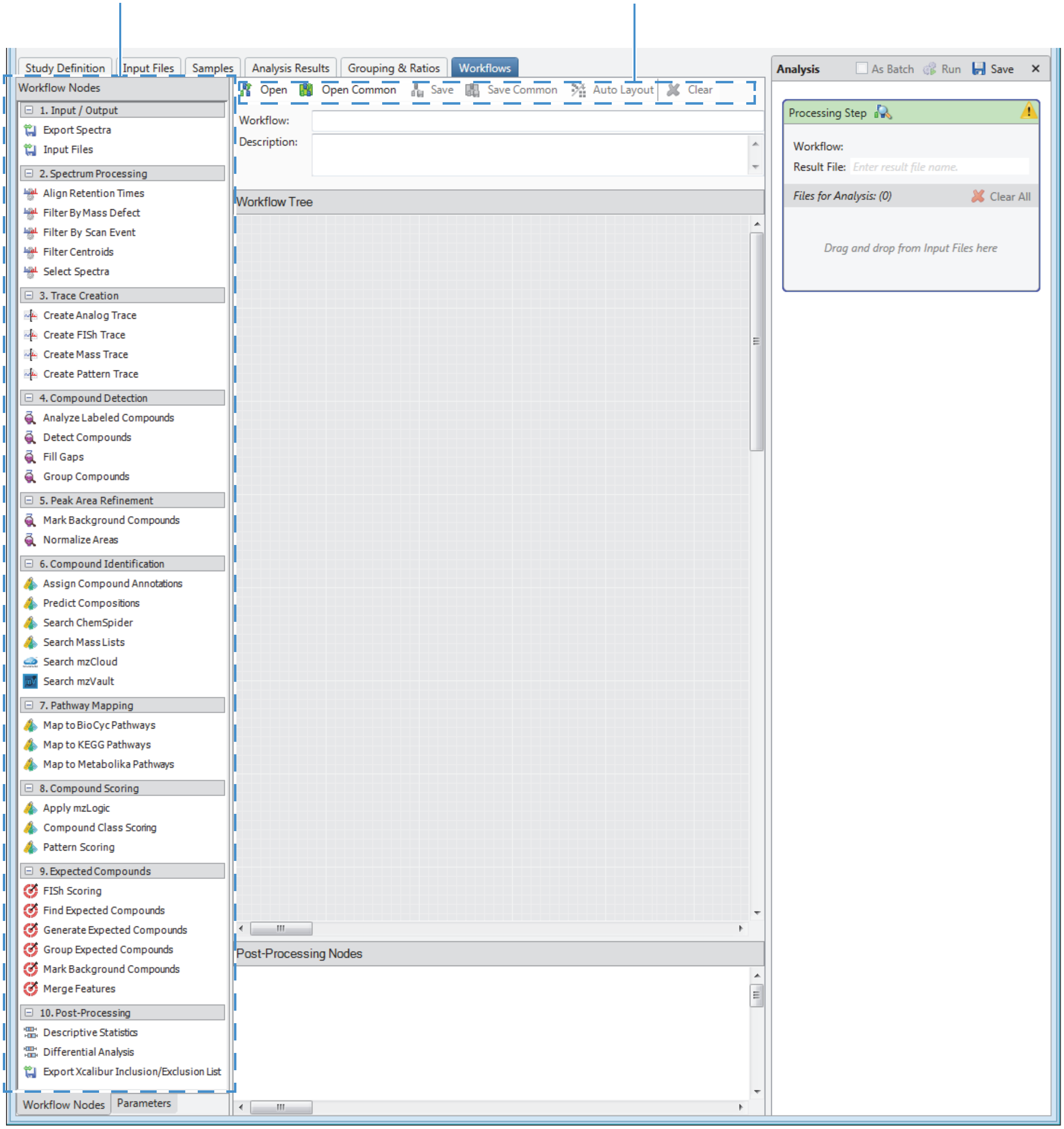
1. Start a new analysis or reprocess an existing analysis (see “Setting Up a New Analysis Within an Existing Study” on page 95 or “Reviewing or Reprocessing an Analysis” on page 109).
2. To open the Workflows page, click the **Workflows** tab, or click the **Show Workflow** icon ( ) in the title bar of the Processing Step area.

   The Workflow Tree and Workflow Nodes panes appear (Figure 51). For a new analysis, the Workflow Tree pane is empty. For an existing analysis template, the Workflow Tree pane usually contains a processing workflow.

Figure 51. Workflows page without a selected processing workflow

Workflow nodes list

Command bar



Workflows Page Command Bar

Table 23 describes the Workflows page commands.

Table 23. 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 3.0\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 24 describes the commands in the shortcut menu for the Workflow Tree pane or a workflow node.

Table 24. 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 enables this command.
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 enables this command.
Auto Layout	Automatically formats the layout of the workflow nodes.

Table 24. 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)].

Editing a Processing Workflow

You can modify a processing workflow by adding and deleting workflow nodes and by changing the parameter settings in the workflow nodes. For information about the defined processing workflows that come with the application, see “Nomenclature for the Defined Processing Workflows” on page 36.

These symbols on the upper right corner of a workflow node alert you to the following errors:

- An exclamation mark, ❗, appears when the node is missing a required parameter selection or the selected item is not found in its corresponding list or library.
- A Caution symbol, ⚠, appears when the node is missing a connection.

Follow these procedures as needed.

❖ 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 pane.

   A workflow node error typically begins with the following text: Validation of processing node.

2. Using the provided information, fix the workflow node error.

❖ 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 pane.

   A missing connection begins with the following text: Missing connection.

2. Make the appropriate node connections.

❖ To fix a missing parameter value

1. In the Workflow Tree pane, select the node with the missing parameter value.
2. In the Parameters of ‘*Workflow Node*’ page to the left, make a selection for the missing parameter value (see “Common Analysis Errors” on page 102).

❖ To delete a node in the Workflow Tree pane

Right-click the node in the Workflow Tree pane and choose **Cut**.

❖ 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.
2. If necessary, make the appropriate connections (see "Connecting the Workflow Nodes" on page 134).

> **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.

3. To display a node's parameters, click the node in the Workflow Tree pane.

   The Parameters page lists the parameters for the selected node.

4. Edit the parameter settings for the node as described in Chapter 13, "Workflow Nodes."

❖ To edit the parameter settings for each node

1. In the Workflow Tree pane, select the node of interest.

   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. See Chapter 13, "Workflow Nodes."

Setting Up Isotope Patterns for Pattern Scoring or Pattern Traces

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.

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, follow these procedures as needed:

- To open the Isotope Ratio Editor
- To set up the pattern for a compound by using its elemental composition

- To set up a custom pattern
- To export a mass spectrum from a raw data file to the Clipboard

❖ To open the Isotope Ratio Editor

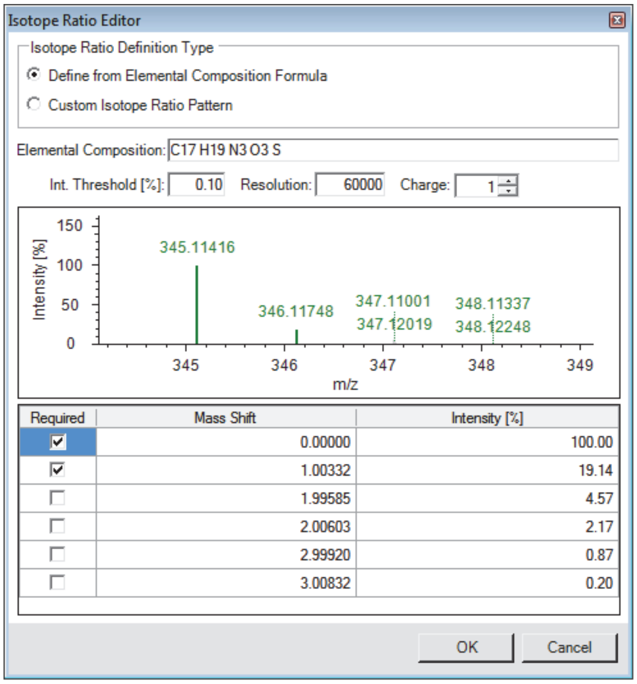
1. Open or create a processing workflow on the Workflows page.
2. Add one or both of these nodes to the processing workflow: **Create Pattern Trace** or **Pattern Scoring**.
3. In the workspace, click the **Create Pattern Trace** node or the **Pattern Scoring** node.

   The parameters for the node appear in the Parameters pane.
4. Depending on the node, do the following:
   - For the Create Pattern Trace node, click the **Isotope Ratios** box.
   - For the Pattern Scoring node, click the **Isotope Patterns** box.

   The browse icon appears.
5. Click the browse icon, ...
   - For the Create Pattern Trace node, the Isotope Ratio Editor dialog box opens (Figure 52).
   - For the Pattern List Editor node, the Pattern List Editor dialog box opens.
6. In the Pattern Editor dialog box, click **Add Patterns**.

   The Isotope Ratio Editor dialog box opens (Figure 52).

Figure 52. Isotope Ratio Editor dialog box with the elemental composition for omeprazole



● Define from Elemental Composition Formula
○ Custom Isotope Ratio Pattern

Elemental Composition: C17 H19 N3 O3 S

Int. Threshold [%]: 0.10 Resolution: 60000 Charge: 1

Required	Mass Shift	Intensity [%]
☑	0.00000	100.00
☑	1.00332	19.14
☐	1.99585	4.57
☐	2.00603	2.17
☐	2.99920	0.87
☐	3.00832	0.20

❖ To set up the pattern for a compound by using its elemental composition

1. In the Isotope Ratio Definition Type area, select the **Define from Elemental Composition Formula** option.

2. 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.

   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.

Tip To copy the elemental composition of a compound from the Expected Compounds library, do the following:

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.
7. Right-click in the Elemental Composition box and choose **Paste**.

3. Do the following:
   - 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.

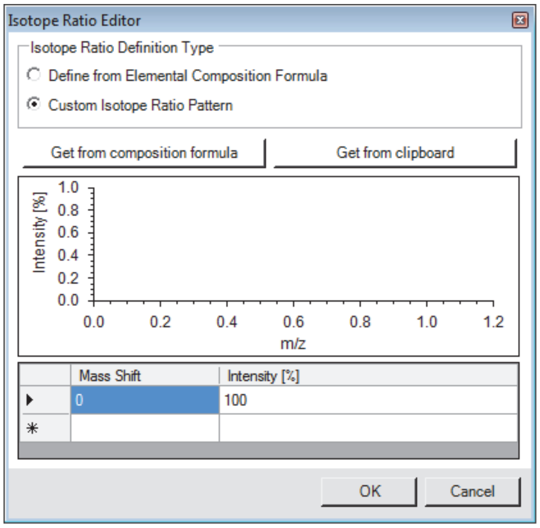
     The application uses the charge state to display the theoretical mass spectrum in the graphical display.

❖ To set up a custom pattern

1. Select the **Custom Isotope Ratio Pattern** option.

   Below the Isotope Ratio Definition Type area, the available parameters change (Figure 53).

Figure 53. Custom Isotope Ratio Pattern view



Isotope Ratio Editor

Isotope Ratio Definition Type

○ Define from Elemental Composition Formula

● Custom Isotope Ratio Pattern

	Mass Shift	Intensity [%]
▶	0	100
✳		

2. 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. For information about copying data points from a mass spectrum to the Clipboard, see the next procedure, "To export a mass spectrum from a raw data file to the Clipboard."

❖ 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 **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.

Table 25 describes the parameters in the Isotope Ratio Editor dialog box.

Table 25. Isotope Ratio Editor dialog box parameters (Sheet 1 of 2)

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
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

Table 25. Isotope Ratio Editor dialog box parameters (Sheet 2 of 2)

Parameter	Description
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.	
Mass shift and intensity table	
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 A0 isotope for the ion of interest.
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 Qual Browser 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.	

Creating an Isotope Patterns List

Follow these procedures to set up the isotope patterns for the Isotope Patterns node:

- To add isotope patterns to the Isotope Patterns node
- To add patterns to the Pattern List Editor

❖ To add isotope patterns to the Isotope Patterns node

- In the Isotope Patterns box of the Isotope Patterns node, type the elemental composition formulas for the defined isotope patterns that you want to compare. Separate each pattern with a semicolon.

–or–

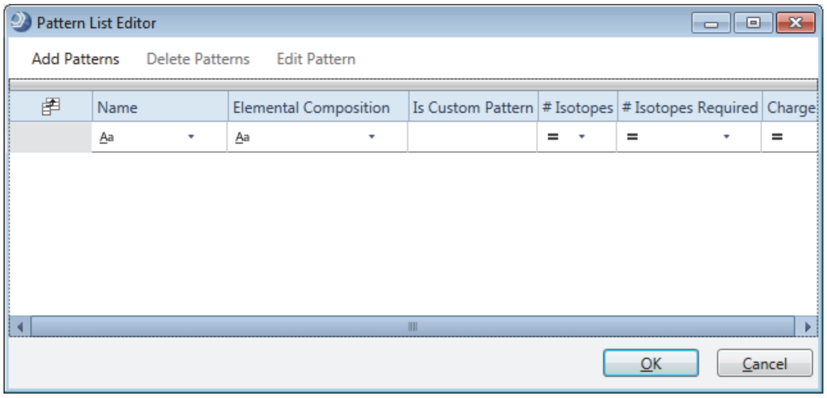
- Use the Pattern List Editor.

❖ To add patterns to the Pattern List Editor

1. Click the browse icon to the right of the Isotope Patterns box of the Isotope Patterns node.

   The Pattern List Editor opens (Figure 54).

   Figure 54. Pattern List Editor



2. For each pattern that you want to add, do the following:

   a. Click **Add Patterns**.

      The Isotope Ratio Editor dialog box opens ("Setting Up Isotope Patterns for Pattern Scoring or Pattern Traces" on page 120).

   b. Set up the isotope pattern and click **OK**.

      The pattern 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.

3. (Optional) To change a pattern name, type text in the Name column.

4. Click **OK**.

   The isotope patterns appear in the Isotope Patterns box of the Isotope Patterns node.

Table 26 describes the commands and table columns in the Pattern List Editor dialog box.

Table 26. Pattern List Editor parameters

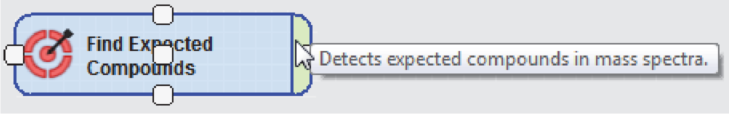
Parameter	Description
Commands	
Add Patterns	Opens the Isotope Ratio Editor dialog box for setting up an isotope pattern. For information about using the Isotope Ratio Editor dialog box, see "Setting Up Isotope Patterns for Pattern Scoring or Pattern Traces" on page 120.
Delete Patterns	Deletes the selected pattern.
Edit Pattern	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.

Creating a New Processing Workflow

A processing workflow is part of an analysis, and you can only perform analyses 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.

As the following figure shows, placing the cursor over a node name in the Workflow pane or a node in the Workflow Tree pane displays a ToolTip that describes the node's function.



Detects expected compounds in mass spectra.

For details about the node parameters, see Chapter 13, "Workflow Nodes."

To create a completely new processing workflow, follow these steps:

1. Clearing an Existing Workflow or Starting a New Analysis
2. Building a Processing Workflow
3. Connecting the Workflow Nodes

For information about editing the parameter settings for the workflow nodes, see "Editing a Processing Workflow" on page 119.

Clearing an Existing Workflow or Starting a New Analysis

To create a new processing workflow, begin with an empty Workflow Tree pane on the Workflows page of an analysis.

To begin with an empty Workflow Tree pane, follow the appropriate procedure:

- To clear an existing workflow
- To open an empty Workflow Tree pane

❖ To clear an existing workflow

1. If the Workflows tab is available, click it to open the Workflows page.
2. If the Workflows Tree area contains a processing workflow that you do not want to edit, click **Clear**.

❖ To open an empty Workflow Tree pane

1. In the study command bar, click **New Analysis**.

   The Grouping and Ratios and Workflows tabs appear to the right of the study page tabs and the Analysis pane appears to the right of the tabbed pages.

2. Click the **Workflows** tab.

   The Workflows page contains the following items:

   - The Workflow Nodes and Parameters panes to the left of the Workflow Tree pane
   - A toolbar and two input boxes above the Workflow Tree pane
   - The Workflow Tree pane, which is a workspace, at the bottom right of the page

Go to the next procedure, "Building a Processing Workflow."

Building a Processing Workflow

This topic describes how to build a completely new processing workflow in an empty Workflow Tree pane of the Workflows page for an analysis.

❖ To build a completely new processing workflow

1. If you have not already done so, open the Workflows page for an analysis (see Clearing an Existing Workflow or Starting a New Analysis).

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** node to the Workflow Tree pane. Then, connect the Select Spectra node to it.

   The Align Retention Times node chromatographically aligns the MS scan data in the input files.

5. To find expected compounds, do the following:

   a. Check whether your Expected Compounds library contains the compounds of interest (see "Modifying the Expected Compounds List" on page 390).

b. Drag the **Find Expected Compounds** node to the Workflow Tree pane. Then, connect the Align Retention Times node to it.

> **Note** The Find Expected Compounds node accepts input from any of the Spectrum Processing nodes.

> **IMPORTANT** For analyses with multiple input files, always add the Align Retention Times node to the processing workflow.

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” on page 491).

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 10.

6. To detect unknown compounds, do the following:
   a. Drag the **Detect Compounds** node to the Workflow Tree pane. Then, connect the Align Retention Times 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. To identify unknown compounds, do the following:

   Note The Group Compounds node automatically connects to all the Compound Identification nodes. In addition, the Group Expected Compounds node automatically connects to the Search Mass Lists, Search mzCloud, and Search mzVault nodes.

   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 (see "Search Mass Lists Node" on page 515).
   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.

8. To map detected compounds to a biochemical pathway, do any of the following:

   Note The Group Compounds node automatically connects to all the Pathway Mapping nodes.

   - 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. The Group Compounds node automatically connects to it.

- To search the BioCyc database, drag the **Map to BioCyc Pathways** node to the Workflow Tree pane.

  The Group Compounds node automatically connects to it.

Note For information about adding the Mark Background Compounds nodes to an untargeted workflow, see "Marking Background Compounds in an Untargeted Analysis" on page 35. For information about using the Normalize Areas node for batch normalization, see "Quality Control Samples for Batch Normalization" on page 39.

9. 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 it.

10. 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 it.

11. 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 it.

Note In this example, you connect the Align Retention Times node to the Create Pattern Trace, Create FISh Trace, and Create Mass Trace nodes. These nodes accept input from any of the Spectrum Processing nodes.

- 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 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 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 node to each Create Mass Trace node.

12. 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, and so on) for each detected compound.

      Note In a result file, the descriptive statistics columns are hidden by default. See "Expected Compounds Table" on page 285 and "Compounds Table" on page 295.

13. 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 instructions to connect the Workflow Nodes, see Connecting the Workflow Nodes. For detailed information about each node, see Chapter 13, "Workflow Nodes."

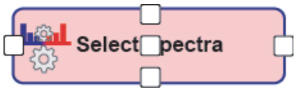
Connecting the Workflow Nodes

This topic describes how to use the mouse pointer to connect the workflow nodes and the specific connections for each workflow node.

❖ To connect the 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.

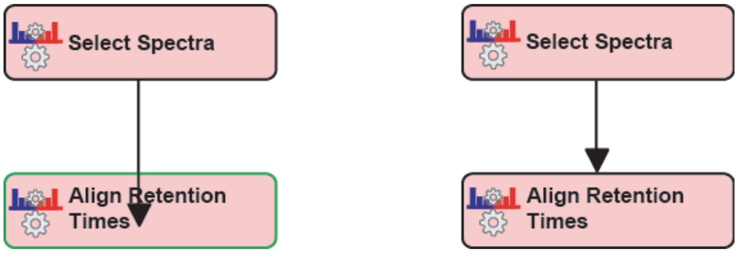


2. Click one of the white boxes and hold down the mouse button until a red border and an arrowhead appear.

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.



> **Note** The Input Files node automatically connects to the Create Analog Trace node and the Select Spectra node.

4. To automatically format the layout of the workflow nodes, click **Auto Layout** in the Workflows command bar (see "Workflows Page Command Bar" on page 118).

You can use the following nodes multiple times in a processing workflow: the Generate Expected Compounds node, all the Trace Creation nodes, and all the Spectrum Processing nodes, except for the Align Retention Times node.

While most of the nodes connect automatically, you must manually connect these nodes:

- Spectrum Processing nodes
- Find Expected Compounds node
- Trace Creation nodes (except for the Create Analog Trace node)

Table 27 describes the node connections.

Table 27. Input and output nodes for each workflow node (Sheet 1 of 4)

Workflow node	Input nodes	Output nodes
1.0 Input/Output		
Export Spectra Node	Select Spectra	Filter Centroids
Input Files (Begins every processing workflow.)	None	• Select Spectra • Create Analog Trace

Table 27. Input and output nodes for each workflow node (Sheet 2 of 4)

Workflow node	Input nodes	Output nodes
2.0 Spectrum Processing		
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
Align Retention Times Node	Spectrum Processing	• 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
3.0 Trace creation		
Create Analog Trace Node	Input Files	None
Create Mass Trace Node	Spectrum Processing	None
Create FISh Trace Node	Spectrum Processing	None
Create Pattern Trace Node	Spectrum Processing	None
4.0 Compound Detection		
Analyze Labeled Compounds Node	Assign Compound Annotations	None
Detect Compounds Node	Spectrum Processing	• Group Compounds • Merge Features
Fill Gaps Node	Group Compounds	• Normalize Areas • Mark Background Compounds
Group Compounds node	Detect Compounds	• Compound Identification • Pathway Mapping • Fill Gaps • Mark Background Compounds

Table 27. Input and output nodes for each workflow node (Sheet 3 of 4)

Workflow node	Input nodes	Output nodes
5. Peak Area Refinement		
Mark Background Compounds Node–Unknown Compounds	See “Marking Background Compounds in an Untargeted Analysis” on page 35.	None
Normalize Areas Node	Fill Gaps	Mark Background Compounds
6. Compound Identification		
Assign Compound Annotations Node	Group Compounds	None
Predict Compositions Node	Group Compounds	None
Search ChemSpider Node	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
7. Pathway Mapping		
All	Group Compounds	None
8. Compound Scoring		
Apply mzLogic Node	• Search Mass Lists • Search ChemSpider • Map to Metabolika Pathways • Map to BioCyc Pathways	None
Compound Class Scoring Node	Group Compounds	None
Pattern Scoring Node	Group Compounds	None
9. Expected Compounds		
FISh Scoring Node	Group Expected Compounds	None
Find Expected Compounds 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
Mark Background Compounds Node–Expected Compounds	Group Expected Compounds	None

Table 27. Input and output nodes for each workflow node (Sheet 4 of 4)

Workflow node	Input nodes	Output nodes
Merge Features Node	• Find Expected Compounds • Detect Compounds	None
7.0 Post-Processing (white nodes)		
Descriptive Statistics Node	None	None
Differential Analysis Node	None	None
Export Xcalibur Inclusion or Exclusion List Node	None	None

Saving a 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 later on. 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 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 to the last folder that you opened or to another folder, 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 pane is open.

Reviewing the Analysis Results

The Compound Discoverer application stores the results of an analysis in a result file (cdResult).

Note For details about the graphical views and result tables, see these chapters:

- Chapter 7, "Working with the Graphical Result Views."
- Chapter 8, "Reviewing the Tabular Result Data."

These topics describe how to open result files, filter the result tables to remove non-pertinent data, edit the compound annotations, propose custom structures, and modify and store the layout of the current result file. They also describe how to export mass lists and spectral data.

Contents

Opening, Closing, and Updating 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).

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:

- Opening Result Files Created in the Current Application Version
- Opening Result Files Created in Previous Versions of the Application
- Closing a Result File

For information about result page layouts, see "Modifying Result File Layouts" on page 145.

Opening Result Files Created in the Current Application Version

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).

For information about the result page, see "Factory Default Layout for a Result Page" on page 145.

❖ To open a result file 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***.

❖ To open a result file from the Start Page

Do one of the following:

- Under Recent Results, click the blue hyperlink for the result file of interest.
- Under What Would You Like to Do?, click **Open Result**.

❖ To open a 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**.

❖ To open a result file 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.

Opening Result Files Created in Previous Versions of the Application

When you attempt to open a legacy result file, the application prompts you to select an update process (Figure 55):

- 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.

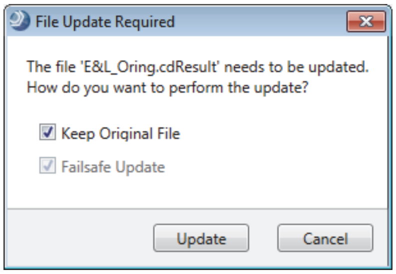
If the update process fails, the application does not rename the original file.

❖ 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 55).

   Figure 55. File Update Required dialog box

   File Update Required

   The file 'E&L_Oring.cdResult' needs to be updated.
   How do you want to perform the update?

   ☑ Keep Original File
   ☑ Failsafe Update

2. Select one of the following update processes:

   - To retain the original result file, select the **Keep Original File** check box.

     The application automatically selects the Failsafe Update check box as well.

   - 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**.

Closing a Result File

You can close a result file (CDRESULT) in 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 (see "Working with Tabbed Pages and Dockable Views" on page 44).

Modifying Result File Layouts

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, the applied result filters, and custom annotations and structure proposals.

For information about modifying result tables, filtering result tables, and adding custom annotations and structure proposals, see these topics: "Working with the Application Tables" on page 531, "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162, "Editing Compound Annotations" on page 156, and "Adding and Deleting Proposed Structures for a Compound" on page 158.

To modify the result file layout, create new layouts, and specify the default layout, follow these topics as needed:

- Factory Default Layout for a Result Page
- Rearranging the Views on a Result Page
- Grouping, Coloring, and Filtering the Data by Study Variable
- Showing or Hiding Result Tables
- Saving, Restoring, and Managing Layouts

Factory Default Layout for a Result Page

When you open a result file (see Opening, Closing, and Updating Result Files), it appears as a tabbed page in the application window.

The factory default layout for a result page includes the following items:

- A tab with the result file name
- A Chromatograms view on the top left that is populated with XIC traces for the component (based on the MW×RT dimensions of the chromatographic peak) 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.
- A Mass Spectrum view on the top right that 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)
- A set of tabbed main tables below the two graphical views
- A collapsed area for the related tables below the main tables

You cannot drag the tabbed result tables to a second monitor. However, you can change the following:

- The location of the tabbed result tables with respect to the tabbed documents that are open in the application window (see "Working with Tabbed Pages and Dockable Views" on page 44)
- The views that you want to display and their location (see "Rearranging the Views on a Result Page" on page 147)
- 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 "Showing or Hiding Result Tables" on page 153 and "Working with the Application Tables" on page 531)
- The data (table rows) displayed or hidden in the result tables (see "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162)
- The annotations in the Name, Structure, and FISh Coverage columns of the Compounds and Expected Compounds tables (see "Editing Compound Annotations" on page 156)

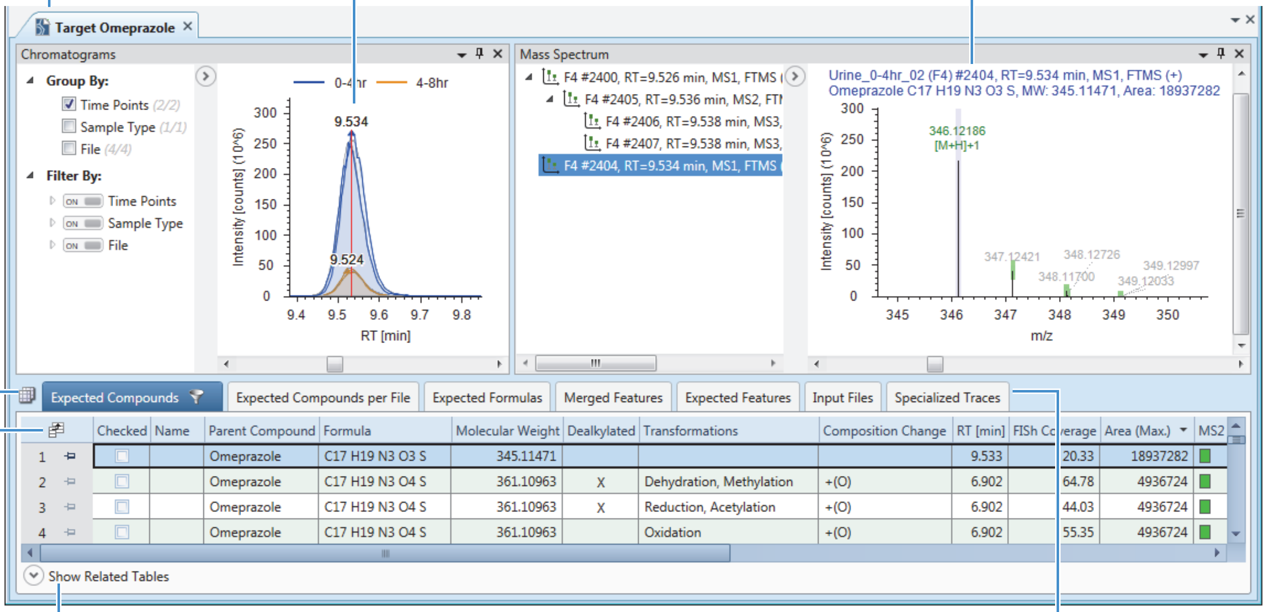
Figure 56 shows a tabbed result page. The result file is the product of processing a set of input files with a targeted processing workflow that includes the following nodes: Input Files, Select Spectra, Align Retention Times, Create Mass Trace, Generate Expected Compounds, Find Expected Compounds, Group Expected Compounds, and FISh Scoring.

Figure 56. Default layout for a result page

Result file tab

Chromatograms view with a collapsible pane on the left

Mass Spectrum view with a mass spectral tree on the left



		Checked	Name	Parent Compound	Formula	Molecular Weight	Dealkylated	Transformations	Composition Change	RT [min]	FISh Coverage	Area (Max.)	MS2
1		☐		Omeprazole	C17 H19 N3 O3 S	345.11471				9.533	20.33	18937282	🟩
2		☐		Omeprazole	C17 H19 N3 O4 S	361.10963	X	Dehydration, Methylation	+(O)	6.902	64.78	4936724	🟩
3		☐		Omeprazole	C17 H19 N3 O4 S	361.10963	X	Reduction, Acetylation	+(O)	6.902	44.03	4936724	🟩
4		☐		Omeprazole	C17 H19 N3 O4 S	361.10963		Oxidation	+(O)	6.902	55.35	4936724	🟩

Tabbed result tables

Click to open the tabbed related tables.

Field Chooser icon

Select Table Visibility icon

Working with Tabbed Pages and Dockable Views and Shortcut Menu Commands for the Result Tables describe the shortcut menu commands that are available by right-clicking the result page tab. Saving, Restoring, and Managing Layouts describes how to save a custom layout or restore the default layout.

Rearranging the Views on a Result Page

For an overview of a result page’s default layout, see Factory Default Layout for a Result Page.

The default layout for the views on a result page are as follows:

- The Chromatograms view appears as a docked view on the upper left.
- The Spectrum view appears as a docked view on the upper right.
- The main result tables appear as a tabbed pane below the two docked views.
- The Result Filters and Result Charts views open as floating windows.

- The Trend Chart, Isotopologues Distribution Chart, Principal Component Analysis, Descriptive Statistics, Differential Analysis, Partial Least Squares and Discriminant Analysis, Hierarchical Cluster Analysis, mapped pathways, Retention Time Corrections, and Compound Area Corrections views open as tabbed documents to the right of the tabbed result tables.
- The FISh Scoring Queue view opens to the right of the tabbed result tables and to the left of the statistical views.
- The Result Summary view opens as a separate panel below the statistical analysis views.

You can move the docked views from one dock position to another dock position or to a second monitor. You can also change the docked views to floating windows and move them anywhere on the screen or to a second monitor.

Figure 57 shows a result file page with the Statistics layout applied.

Figure 57. Result file page with the Statistics layout

	Checked	Name	Formula	Annotation Source	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)
1	☐	Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N2 O8	🟩🟩⬜🟩		292.09007	0.935	1217654417
2	☐	[Similar to: Dipropyl sulfoxide; ΔMass: -106.1141 Da]	C15 H28 S	🟩🟥⬜⬜		240.19066	7.081	663551286
3	☐	4V290005U9	C12 H10 O S	⬜🟥⬜🟩		202.04495	0.834	315866471

Data Source: Compounds
Comparison: Fatty vs. Lean
P-value: 0.001
Log₂ Fold Change: 3

Color By:
☐ Phenotype (2/3)
☐ Sample Type (1/2)
☐ File (6/7)
Filter By:
ON Phenotype
ON Sample Type
ON File
Other Settings:
Column Settings:
☑ Show Clusters
☑ Show Labels
Row Settings:
☑ Show Clusters
☐ Show Labels
Color Scheme:
Distance Function: Euclidean
Linkage Method

Data Source: Compounds
Scale Values: Scale Before Clustering
☑ Use normalized areas
Refresh

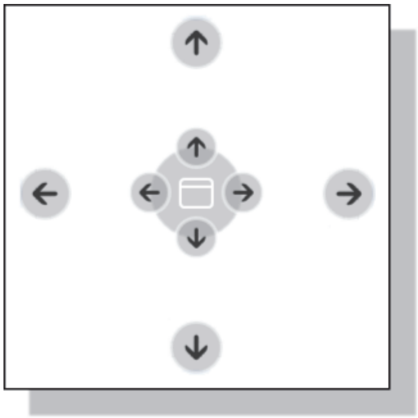
To rearrange the graphical views, follow these procedures as needed:

- To move a view to another dock position
- To move the view to the top of the page
- To move the view below the result tables
- To change a docked window to a floating window
- To enlarge a view to fill the screen
- To restore the previous size of a floating window

❖ To move a view to another dock position

1. Drag the view by its title bar.

   As you drag the window, a guide tool appears along the vertical median of the window. The guide tool consists of four directional arrows that are arranged in a diamond pattern around a central circle. In addition to the guide tool, a directional arrow appears in the middle of each of the window's four edges.



2. Drag the pointer until it aligns with the appropriate directional arrow. In some cases, you might need to move the view twice to dock it in the position you want.

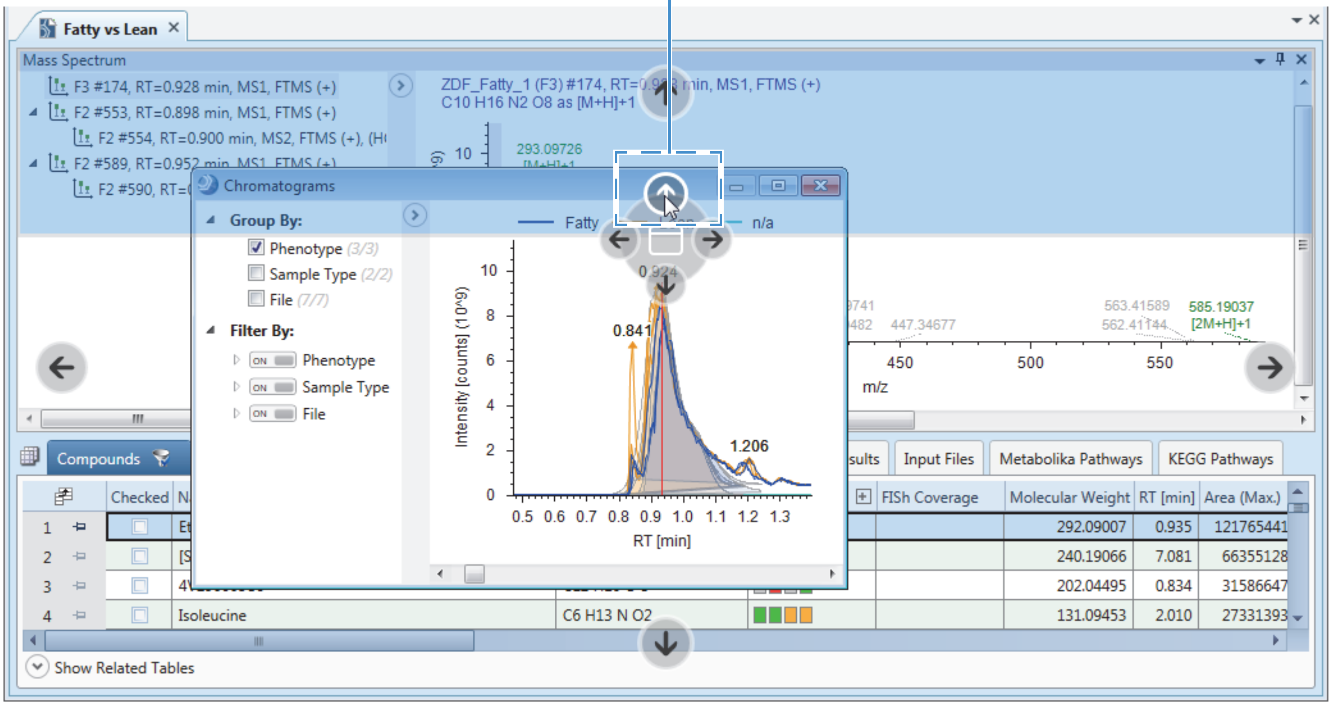
❖ To move the view to the top of the page

1. Drag the pointer over the arrow at the top of the page.

   A blue full-page-width rectangle appears in the top half of the page (Figure 58).

Figure 58. Dragging the Chromatograms view to the top of the page

Pointer aligned with the directional arrow



2. Release the mouse button to replace the blue rectangle with the view.

❖ To move the view below the result tables

1. Drag the pointer over the arrow at the bottom of the page.

   A blue, full-page-width rectangle appears in the bottom half of the page.

2. Release the mouse button.

   The view appears, expanded to the full width of the page, below the result tables.

❖ To change a docked window to a floating window

Do one of the following:

- Right-click the window’s title bar and choose **Floating**.

–or–

- Double-click the window’s title bar.

❖ To enlarge a view to fill the screen

Double-click the window’s title bar.

❖ To restore the previous size of a floating window

Double-click the window’s title bar.

Grouping, Coloring, and Filtering the Data by Study Variable

These four views include a collapsible pane of filtering options and grouping, coloring, or discriminating by options:

- Chromatograms view (see “Working with the Chromatograms View” on page 188)
- Trend Chart view (see “Working with the Trend Chart View” on page 226)
- Principal Component Analysis view (see “Working with the Principal Component Analysis View” on page 233)
- Partial Least Squares Discriminant Analysis (see “Working with the Partial Least Squares Discriminant Analysis View” on page 250)
- Descriptive Statistics view (see “Working with the Descriptive Statistics View” on page 239)

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.

Use the check boxes under Filter By to remove or display data points by sample type, study factor value, or individual file. The application selects all the check boxes with the exception of Blank sample types.

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.

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.

For the Principal Least Squares–Discriminant Analysis view, use the Discriminate By check boxes to select the study variables for the supervised analysis.

Follow these procedures to filter and group the samples in the result file:

- To open the collapsible pane if it is closed
- To group the data by the study variables or by the individual files

- To filter the data by selected study variable values
- To filter the data by selected files

❖ To open the collapsible pane if it is closed

Click the icon, ‹, in the upper left corner of the view.

❖ To group the data by the study variables or by the individual files

1. Select a row in the active result table.
2. To view a color legend of the sample groups, right-click the Chromatograms view and choose **Display Options > Show Legend**.
3. Depending on how you want to group the data points to display the traces in different colors, select one or more check boxes under Group By.

❖ To filter the data by selected study variable values

1. Under Filter By, click the expand icon to the left of the study variable name to open the values list.
2. Clear the check boxes for the items that you want to hide or values that you want to remove from the statistical calculations.

❖ 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.

Table 28 describes the Group By and Filter By options in the collapsible pane.

Table 28. 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 28. 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. By default, for the Chromatograms view, the application selects all sample types. 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.

Showing or Hiding 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. For example, the Adducts table is hidden for both targeted and untargeted analyses and the Filled Gaps related table is hidden for an untargeted analysis.

❖ To show or hide result tables

1. Open a result file (see "Opening, Closing, and Updating Result Files" on page 142).
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.

   By default, the Adducts and Filled Gaps tables are hidden.

4. Click **OK** to accept the changes.

Saving, Restoring, and Managing 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:

- Identification—Adds the Structure column to the Compounds and Expected Compounds tables. Opens the primary set of related tables to the Structure Proposals table. Closes the search result tables if they are visible.
- Quantification—Opens the Trend Chart view. Opens the primary set of related tables to the Structure Proposals table. Closes the search result tables if they are visible.
- Stable Isotope Labeling—Opens the Isotopologues Distribution Chart, the Trend Chart, and the Metabolika Pathways view. In the Compounds table, hides the following columns: #Metabolika Pathways, Avg. Exchange, FISh Coverage, and Metabolika Pathways,
- Statistics—Opens the Differential Analysis, Trend Chart, Principal Component Analysis, and Partial Least Squares Discriminant Analysis views. Closes the Chromatograms and Mass Spectrum views. Closes the search result tables if they are visible.

Follow these procedures as needed:

- To save the current layout of the result file
- To reset the layout to the factory default settings
- To create a custom layout
- To apply a custom layout
- To manage the layouts

❖ To save the current layout of the 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, 💾.

–or–

- From the menu bar, choose **File > Save** (save the currently active item).

❖ To reset the layout to the factory default settings

With the result file selected as the active page, from the menu bar, choose **Window > Reset Layout**.

The application closes the result file, and then reopens the result file to the factory default layout.

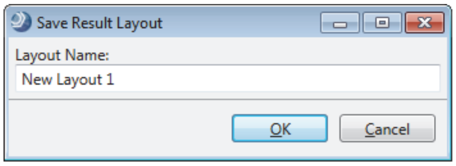
❖ To create a custom layout

1. Open a result file and modify its layout.

   For details, see "Opening, Closing, and Updating Result Files" on page 142 and "Modifying Result File Layouts" on page 145.

2. From the menu bar, choose **Window > Save Layout**.

   The Save Result Layout dialog box opens.



Layout Name: New Layout 1

3. Name the layout and click **OK**.

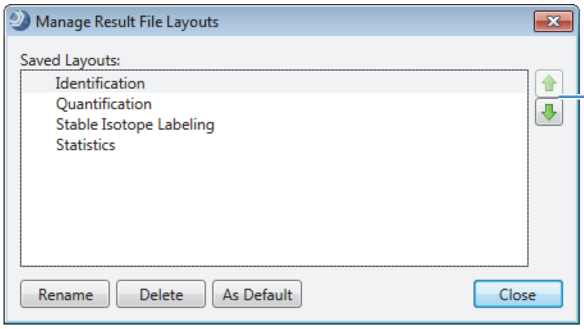
❖ To apply a custom layout

1. With the result file selected as the active page, from the menu bar, choose **Window > Apply Layout**.
2. Select a layout from the list or use the hot keys.

❖ 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.



Saved Layouts:
Identification
Quantification
Stable Isotope Labeling
Statistics

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 needed:

   - 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.

Editing Compound Annotations

Use the Compound Annotation Editor dialog box to edit the annotations for compounds of interest in the Compounds Table, Expected Compounds Table, and the Structure Proposals Table. Saving a custom annotation overwrites the original processing results.

Annotations include the compound name, formula, annotation source, FISh coverage score, and structure.

For information about applying the FISh scoring algorithm, see "Applying FISh Scoring" on page 159.

For information about the Compound Annotation Editor's shortcut menu, see Table 114 in "Adding and Editing Compounds with the Compound Editor" on page 392.

❖ To edit a compound annotation

1. Double-click the row of interest in the Compounds table, Expected Compounds table, or related Structure Proposals table.

   The Compound Annotation Editor dialog box opens (Figure 59).

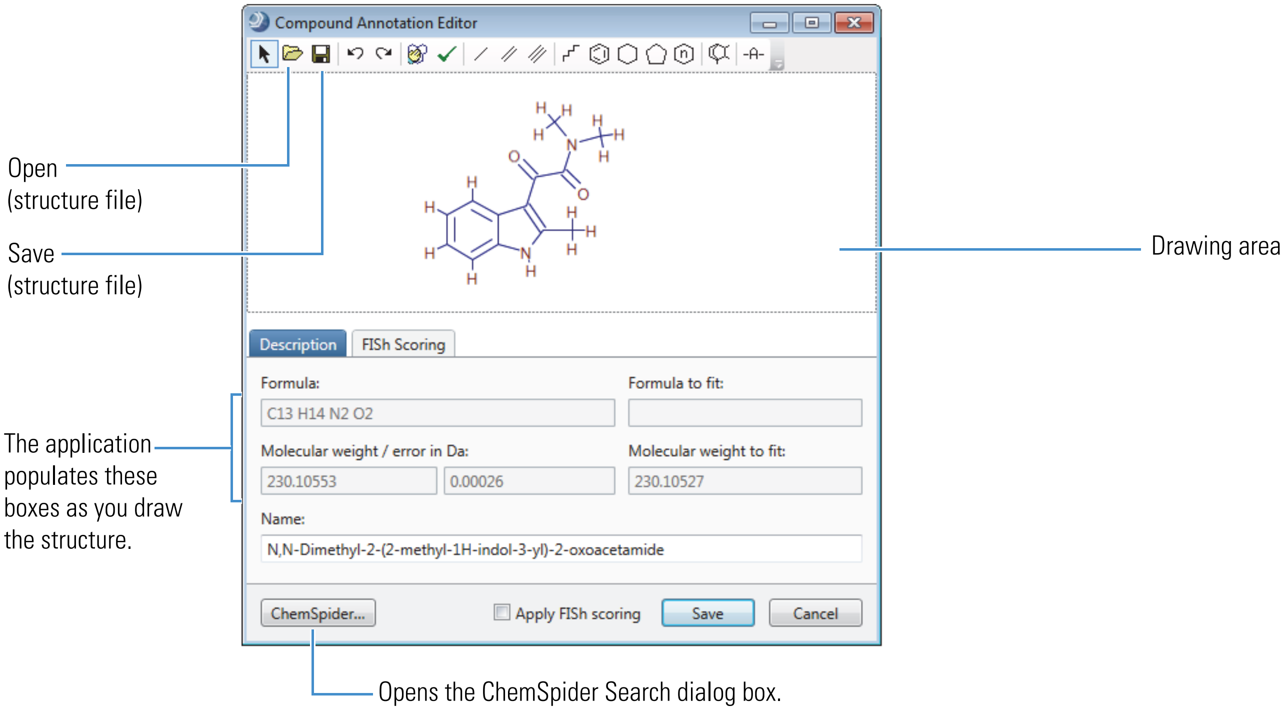
   The application automatically populates the Molecular Weight/Error in Da, and Molecular Weight to Fit boxes. If the formula, structure, and name are available, the application also populates these fields.

2. To add a structure to the drawing area, do any of the following:

   - Use the structure drawing tools. See "Using the Structure Drawing Tools or Commands" on page 434.
   - Open a structure file. See "To open a structure file" on page 393.
   - Run a ChemSpider search and select one of the hits. See "Finding a Structure in the ChemSpider Database" on page 433.

3. Click **Save** to save your custom annotations in the result file.

Figure 59. Compound Annotation Editor dialog box



Formula: C13 H14 N2 O2

Formula to fit:

Molecular weight / error in Da: 230.10553 0.00026

Molecular weight to fit: 230.10527

Name: N,N-Dimethyl-2-(2-methyl-1H-indol-3-yl)-2-oxoacetamide

Open (structure file)

Save (structure file)

Drawing area

The application populates these boxes as you draw the structure.

Opens the ChemSpider Search dialog box.

Table 29 describes the parameters in the Compound Annotation Editor dialog box.

Table 29. Compound Annotation Editor parameters (Sheet 1 of 2)

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.
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.

Table 29. Compound Annotation Editor parameters (Sheet 2 of 2)

Parameter	Description
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 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 Table 30 on page 161.	

Adding and Deleting Proposed Structures for a Compound

The result file contains a Structure Proposals Table for each compound (row) in the Expected Compounds and Compounds tables.

❖ To add structure proposals to a Structure Proposals table

1. Select a compound in the main Compounds or Expected Compounds table.
2. Click **Show Related Tables** below the Compounds or Expected Compounds table.
3. Click the **Structure Proposals** tab.
4. For each structure proposal, do the following:
   a. Right-click anywhere below the Structure Proposals tab and choose **Structure Proposals > Add Structure Proposal**.
   b. To edit the structure proposal, follow the instructions in “Editing Compound Annotations” on page 156.

❖ To delete a structure proposal

Right-click the row and choose **Structure Proposals > Delete Structure Proposal**.

❖ To replace the annotations for a compound in the main result table

Right-click a row in the Structured Proposals table and choose **Structure Proposals > Use As Compound Annotation**.

Applying FISh Scoring

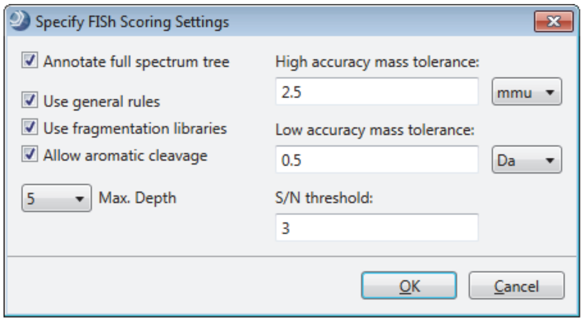
You can apply FISh scoring to a selected entry in the Compounds table, the Expected Compounds table, or the entries in the following compound-related search result tables: Structure Proposals, mzCloud Results, mzVault Results, Mass List Search Results, BioCyc Results, and ChemSpider Results. You can 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.

❖ 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 60), do one of the following:
    - To submit a compound in the Compounds or Expected Compounds table, 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 60. Specify FISh Scoring Settings dialog box


Specify FISh Scoring Settings

☑ Annotate full spectrum tree
☑ Use general rules
☑ Use fragmentation libraries
☑ Allow aromatic cleavage
Max. Depth: 5

High accuracy mass tolerance: 2.5 mmu
Low accuracy mass tolerance: 0.5 Da
S/N threshold: 3

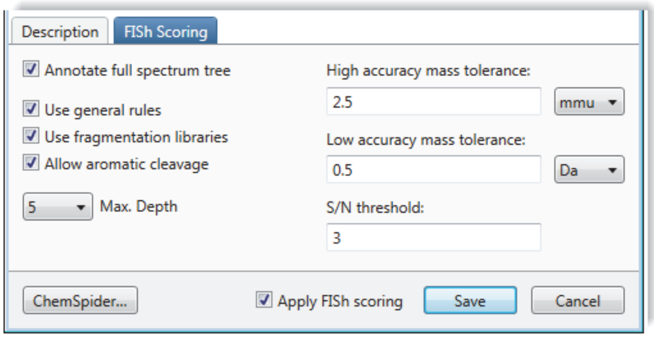
3. Set up the parameters (see "To set up the FISh scoring parameters" on page 160).
4. Click **OK**.

    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.

❖ 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 or the Expected 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 61).

Figure 61. FISh Scoring page of the Compound Annotation Editor dialog box



☑ Annotate full spectrum tree
☑ Use general rules
☑ Use fragmentation libraries
☑ Allow aromatic cleavage
5 Max. Depth
High accuracy mass tolerance: 2.5 mmu
Low accuracy mass tolerance: 0.5 Da
S/N threshold: 3
☑ Apply FISh scoring

5. Specify the parameter settings (see To set up the FISh scoring parameters and Table 30).
6. Click **Save**.

❖ 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 30 describes the parameter settings for the FISh scoring algorithm.

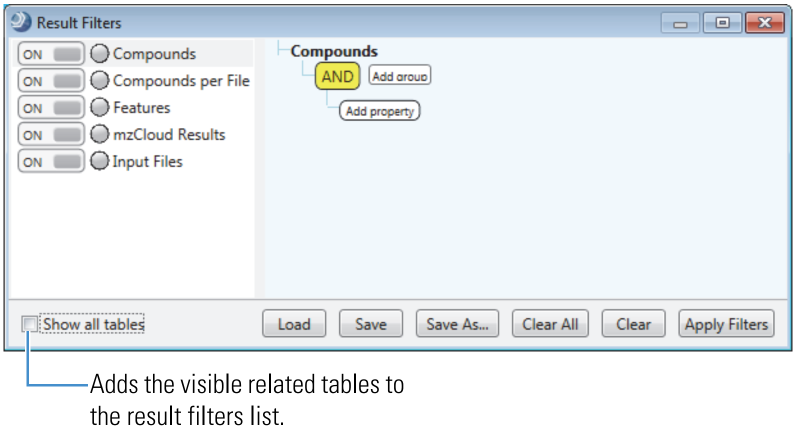
Table 30. FISh scoring parameters

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.

Using Result Filters for Data Reduction and Creating Filter Sets

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 lists the filters for the first table in the left pane (Figure 62). For information about the panes and buttons in the Result Filters window, see Table 31 on page 170.

Figure 62. Result Filters view with an empty filter for the Compounds table



Adds the visible related tables to the result filters list.

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 use the data reduction filters, follow these procedures as needed:

- To open the Result Filters view
- To set up filter conditions
- To display a filter tree that includes all the visible result tables in the result file
- To create a filter set using the AND logical conjunction
- To create a filter set using the OR logical conjunction
- To create a filter set using both the AND and the OR logical conjunctions
- To apply the filter conditions in the current filter set
- To save a filter to a file
- To load a saved filter set
- To turn off the filter conditions for a specific table
- To clear the filter conditions for a specific table

- To clear all of the filters conditions in a filter set
- To set up filters for the status columns

❖ To open the Result Filters view

1. Open a result file.
2. 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.

❖ To display a filter tree that includes all the visible result tables in the result file

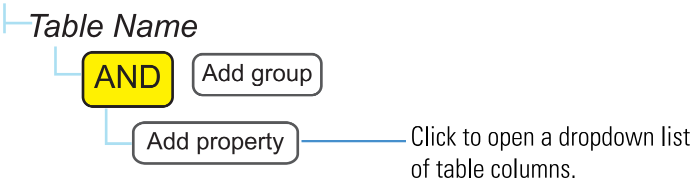
Select the **Show All Tables** check box.

Note To change which tables are visible, use the Select Visible Tables dialog box (see "To show or hide result tables" on page 153).

❖ To set up filter conditions

1. Select the table of interest.

   The table name appears in the right pane. The following selection tree appears below the table name.



2. Click **Add Property**.

   A list that includes the columns in the selected table and the AND and OR logic selections appears. The Add Property list appears below the current filter.

3. Select the table column (property) that you want to filter by.

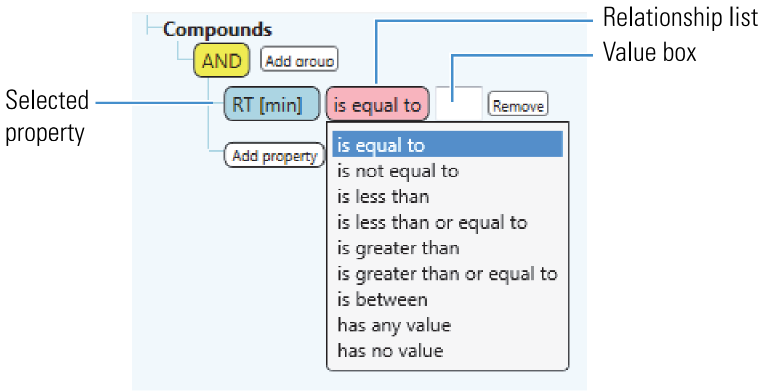
   A (pink) dropdown relationship list with a default selection appears. For numeric properties and most non-numeric properties, an empty value box appears next to the relation list.

4. Do one of the following:

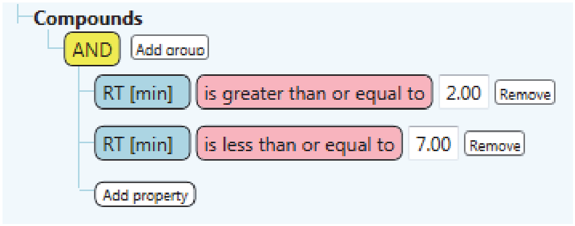
   - For a numeric property, such as retention time (RT), select a mathematical relationship and type a value in the adjacent box, if applicable.

     > **Tip** When you select the Is Equal To relationship, 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 relationship list for numeric properties.

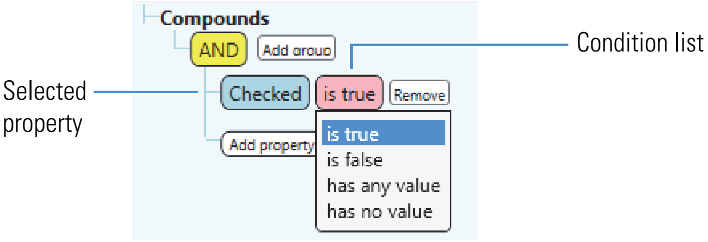


     This figure shows a set of filter conditions that limits the displayed results to chromatographic peaks from 2 to 7 minutes.


Compounds
AND
RT [min] is greater than or equal to 2.00
RT [min] is less than or equal to 7.00

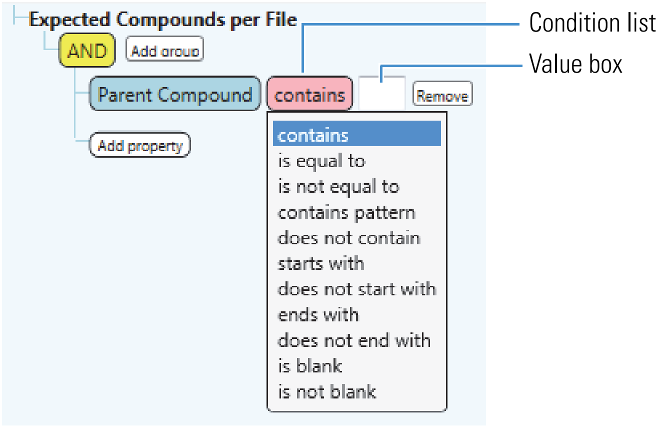
   - For the Checked property, select a condition.

     This figure shows the condition list for the Checked property.



   - For a non-numeric property, such as Parent Compound, select a condition and type a value in the value box if applicable.

This figure shows the condition list for non-numeric properties.



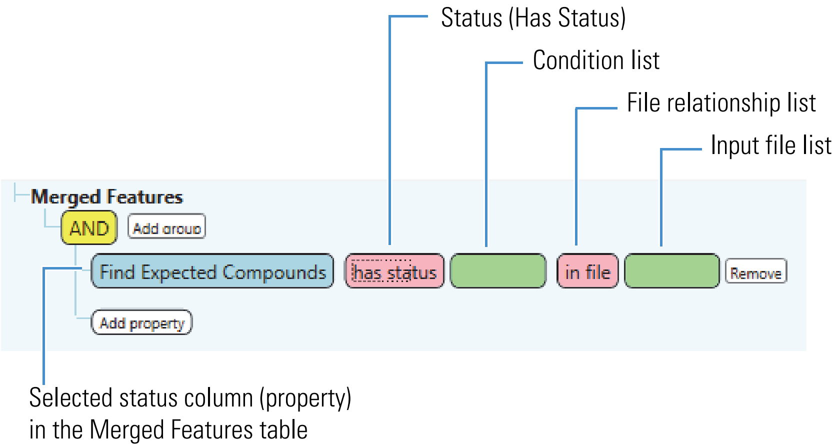
- For a status property, see the next procedure "To set up filters for the status columns."

❖ To set up filters for the status columns

1. If the Result Filters view is not open, open it.
2. Select one of these tables: **Merged Features** or **Compounds**.
3. Select a status property; for example, for the Merged Features table, select **Find Expected Compounds**.

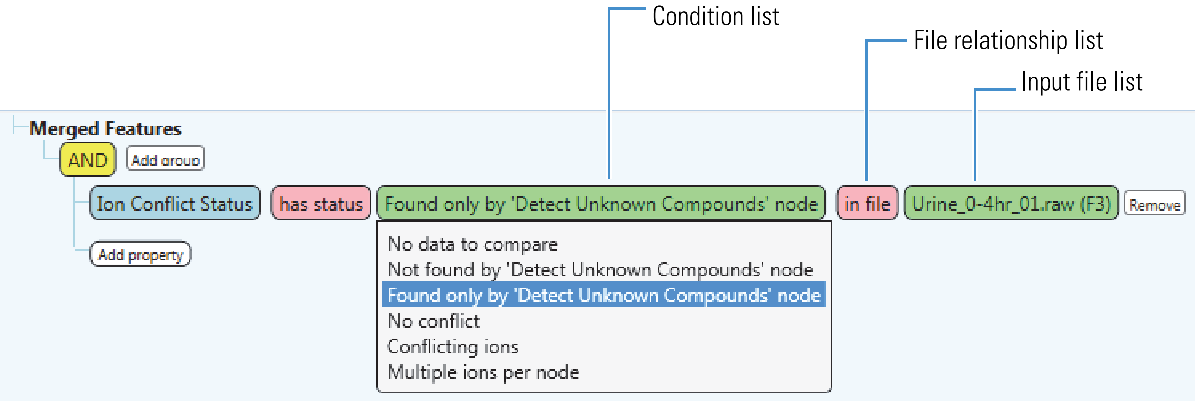
   From left to right, the following items appear:

   - A (pink) list with one selection: Has Status
   - A (green) condition list with no selection
   - A (pink) file relationship list with the selection of In File
   - A (green) input file list with no selection

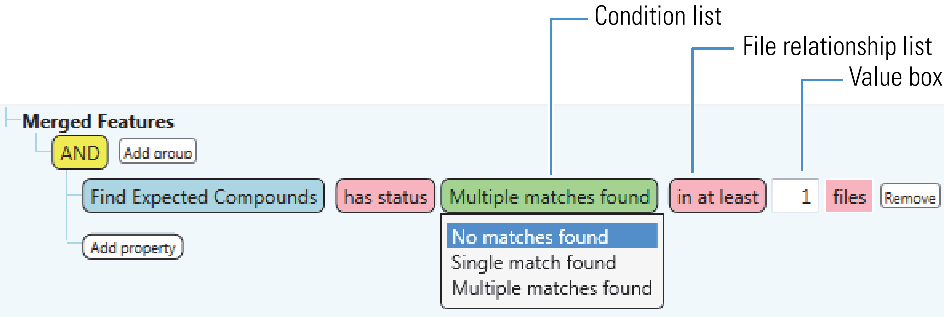


The input file list changes to a value box when you select anything other than In File in the file relationship list:

- If you select In File, select the file of interest in the input file list.



- If you select a file relationship that requires additional input, a value box appears.



4. Select a status condition for the selected property (table column).

Ion Conflict Status	Find Expected Compounds, Detect Compounds, or Custom Explanations
No Data to Compare	No Matches Found
No Conflict	Single Match Found
Conflicting Ions	Multiple Matches Found
Multiple Ions Per Node	–
Not Found by Detect Unknown Compounds node	–
Found Only By Detect Unknown Compounds node	–

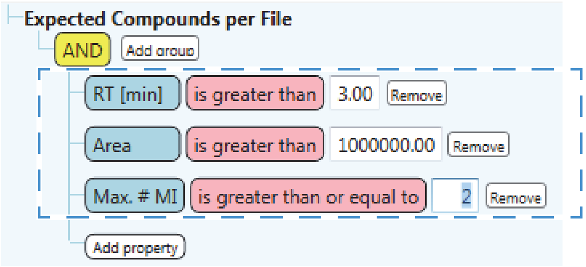
5. Select a file relationship and enter a value or select a file.

❖ 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. 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 up 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 the Expected Compounds per File 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 at least two or more matching isotopes were found in the MS scans that make up the peak's data points.



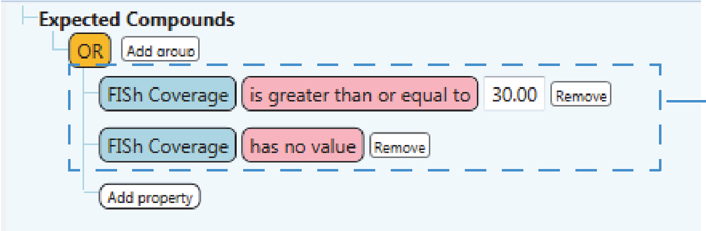
Three properties connected to an AND conjunction

❖ 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.

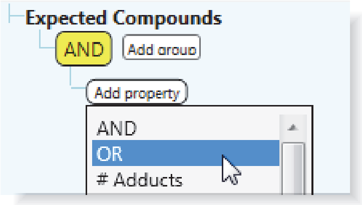
   This figure shows a filter set that uses two properties conjoined with an OR conjunction. When you apply this filter set to the data in the Expected Compounds table, those rows that meet at least one of the conditions remain—that is, you see the rows where the FISh coverage value is greater than or equal to 30 or where the FISh coverage column has no reported value.



Two properties connected to an OR conjunction

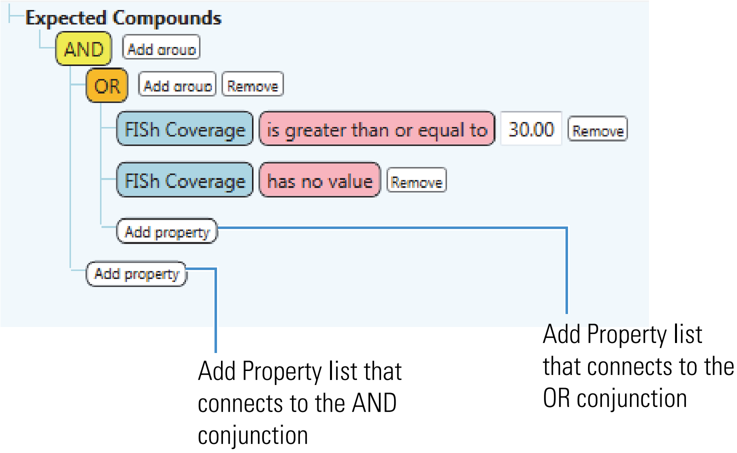
❖ To create a filter set using both the AND and the OR logical conjunctions

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. (The FISh scoring algorithm does not calculate scores for AIF 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.

This figure shows a result filter that keeps chromatographic peaks that meet the following conditions:

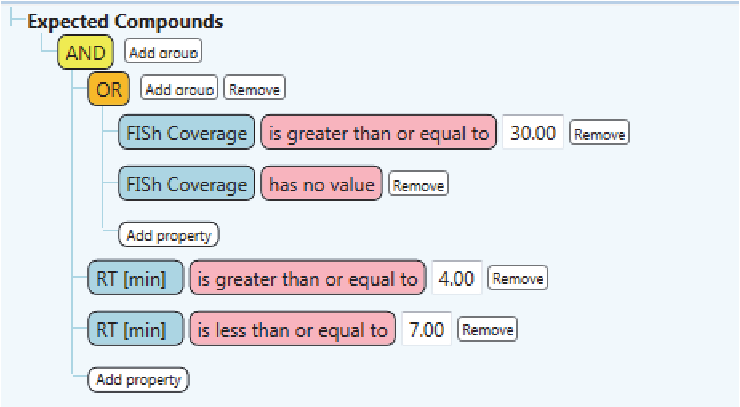
- A FISh Coverage score that meets one of these conditions:
  - A FISh Coverage score that is greater than or equal to 30

  –or–

  - No FISh Coverage score

–and–

- A Retention Time from 4 to 7 minutes



Expected Compounds

AND

OR

FISh Coverage is greater than or equal to 30.00

FISh Coverage has no value

RT [min] is greater than or equal to 4.00

RT [min] is less than or equal to 7.00

❖ To apply the filter conditions in the current filter set

Click **Apply Filters**.

❖ To save a filter to a file

1. Click **Save** or **Save As**.
2. Browse to the location where you want to store the file, name the file, and click **Save**.

   The application saves the file as a FILTERSET file type.

❖ To load a saved filter set

1. Click **Load**.

   The Load Filter Set dialog box opens.

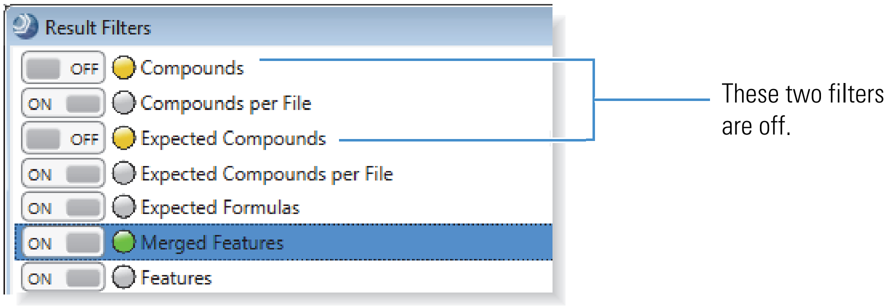
2. Browse to the appropriate folder and select the filter set of interest.
3. Click **Open**.

   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.

❖ To turn off the filter conditions for a specific table

In the left pane of the Result Filters view, click **ON** to the left of the table name.

The indicator icon to the left of the table name turns from green to yellow, and the button displays OFF.



Result Filters
OFF ● Compounds
ON ○ Compounds per File
OFF ● Expected Compounds
ON ○ Expected Compounds per File
ON ○ Expected Formulas
ON ● Merged Features
ON ○ Features

These two filters are off.

❖ To clear the filter conditions for a specific table

1. In the left pane of the Result Filters view, select the table.
2. Click **Clear**.

❖ To clear all of the filters conditions in a filter set

Click **Clear All**.

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 31 describes the panes and buttons in the Result Filters view.

Table 31. 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 "To set up filter conditions" on page 163.
AND or OR	Specifies the logical connection between properties or groups.
Add Group	Adds a group.

Table 31. Result Filters panes and buttons (Sheet 2 of 2)

Feature	Description
Add Property	Adds a property.
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 settings in the file with the current filter conditions in the Result Filters window.
Save As	Opens the Save Filter dialog box where you can define the file name and select a folder for a FILTERSET file.
Clear All	Clears all of the filter conditions for the current filter set.
Clear	Clears the current filter condition.
Apply Filters	Applies all of the filter conditions for the current filter set.

Viewing the Result Summary

In the Summaries view, you can view the following summaries:

- Workflow Summary
- Processing Messages Summary
- Filter Summary
- Study Summary
- Grouping & Ratios Summary

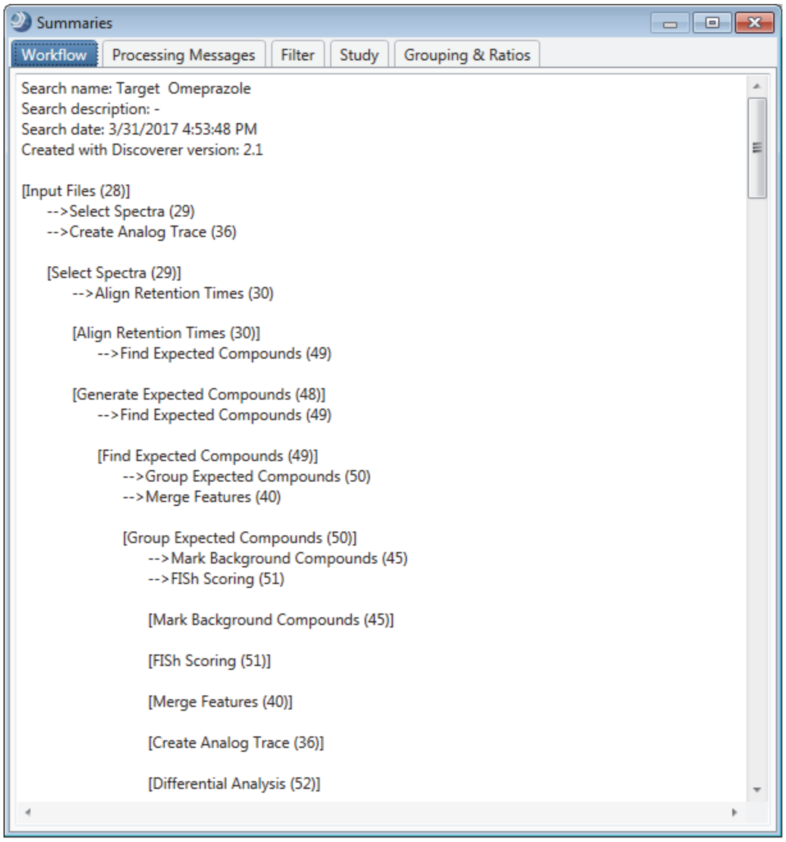
❖ To open the Summaries view

1. Open the result file of interest (see "To open a result file from the application window" on page 142).

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 63).

Figure 63. Summaries view



```
Search name: Target  Omeprazole
Search description: -
Search date: 3/31/2017 4:53:48 PM
Created with Discoverer version: 2.1

[Input Files (28)]
    -->Select Spectra (29)
    -->Create Analog Trace (36)

    [Select Spectra (29)]
        -->Align Retention Times (30)

        [Align Retention Times (30)]
            -->Find Expected Compounds (49)

        [Generate Expected Compounds (48)]
            -->Find Expected Compounds (49)

            [Find Expected Compounds (49)]
                -->Group Expected Compounds (50)
                -->Merge Features (40)

                [Group Expected Compounds (50)]
                    -->Mark Background Compounds (45)
                    -->FISh Scoring (51)

                    [Mark Background Compounds (45)]

                    [FISh Scoring (51)]

                    [Merge Features (40)]

                    [Create Analog Trace (36)]

                    [Differential Analysis (52)]
```

Workflow Summary

To view the processing workflow 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 5, “Creating and Editing Processing Workflows.” For information about selecting one of the defined workflows, see “Nomenclature for the Defined Processing Workflows” on page 36.

Processing Messages Summary

To view a summary of the processes 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 "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162).

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:

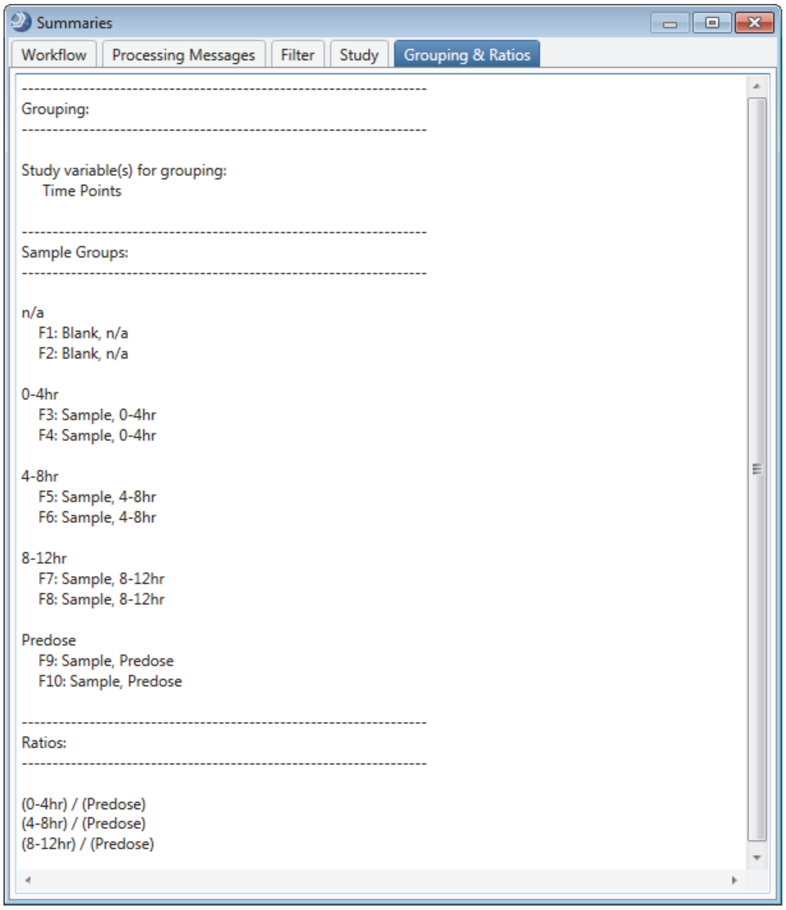
- Name and creation date of the study
- Directory location of the study
- Study factors and their values
- Sample names (Xcalibur RAW files) and their directory location

Grouping & Ratios Summary

To view a summary of the sample groups and ratios for the analysis, open the Grouping & Ratios page.

Figure 64 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 64. Grouping & Ratios Summary page



```
----------------------------------------------------------------
Grouping:
----------------------------------------------------------------

Study variable(s) for grouping:
    Time Points

----------------------------------------------------------------
Sample Groups:
----------------------------------------------------------------

n/a
   F1: Blank, n/a
   F2: Blank, n/a

0-4hr
   F3: Sample, 0-4hr
   F4: Sample, 0-4hr

4-8hr
   F5: Sample, 4-8hr
   F6: Sample, 4-8hr

8-12hr
   F7: Sample, 8-12hr
   F8: Sample, 8-12hr

Predose
   F9: Sample, Predose
   F10: Sample, Predose

----------------------------------------------------------------
Ratios:
----------------------------------------------------------------

(0-4hr) / (Predose)
(4-8hr) / (Predose)
(8-12hr) / (Predose)
```

Exporting the Tabular Results 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
- Exporting the Result Table Contents to a Spreadsheet or Text File
- Exporting an Xcalibur Inclusion or Exclusion List
- Exporting the Contents of the Compounds Table to TraceFinder

Shortcut Menu Commands for the Result Tables

Table 32 describes the shortcut menu commands for the result tables.

Table 32. Shortcut menu commands for the result tables (Sheet 1 of 3)

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 "To copy a single row to the Clipboard" on page 538).
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 (see "To copy table cells to the Clipboard" on page 537). 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 a column moves it to the left of the Checked column (see "Freezing Table Columns" on page 536).
Export > As Plain Text	Exports the data to a comma-separated values file (see "To export the contents of a result table to a text file" on page 179).
Export > As Excel	Exports the data to an Excel™ spreadsheet file (see "To export the contents of a result table to a spreadsheet file" on page 177).
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 selected row's check box.
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.

Table 32. Shortcut menu commands for the result tables (Sheet 2 of 3)

Command	Description
Expected Compounds and Compounds tables	
Edit Compound Annotation	If the table does not already include the Name and FISh Coverage columns, adds these columns and 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.
Clear Compound Annotation	Removes the custom annotation.
Export > Export to Xcalibur 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 (see "Exporting an Xcalibur Inclusion or Exclusion List" on page 179). The information includes the *m/z* value of the monoisotopic ion and the start and stop times for the chromatographic peak.
Export > Single Compound to an Existing mzVault Library	Exports a selected compound to an existing mzVault library.
Export > Compounds to a New mzVault Library	Exports the selected compounds to a new mzVault library.
Compounds table	
Export > Export to TraceFinder	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 "Exporting the Contents of the Compounds Table to TraceFinder" on page 182).
Structure Proposals table (related to the Compounds and Expected Compounds tables)	
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. 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.

Table 32. Shortcut menu commands for the result tables (Sheet 3 of 3)

Command	Description
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.
Structure Proposals > Use as Compound Annotation	Replaces the annotations in the selected row of the Compounds or Expected Compounds table with the annotations in the current row of the Structure Proposals table.
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. 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.

Exporting the Result Table Contents to a Spreadsheet or Text File

You can export the contents of any of the result tables to a spreadsheet file or a text file.

Follow these procedures as needed:

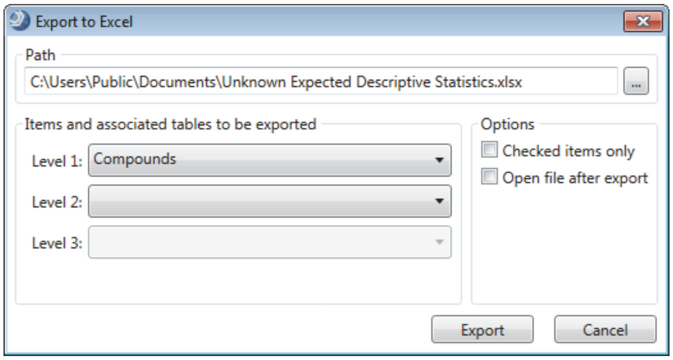
- To export the contents of a result table to a spreadsheet file
- To export the contents of a result table to a text file

❖ 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 > Export to Excel**.

   The Export to Excel dialog box opens (Figure 65). The default storage path is C:\Users\Public\Documents*result file name*. The default selection in the Level 1 box is the name of the active result table.

Figure 65. Export to Excel dialog box with the Compounds table selected



Path: C:\Users\Public\Documents\Unknown Expected Descriptive Statistics.xlsx

Level 1: Compounds

Level 2:

Level 3:

☐ Checked items only

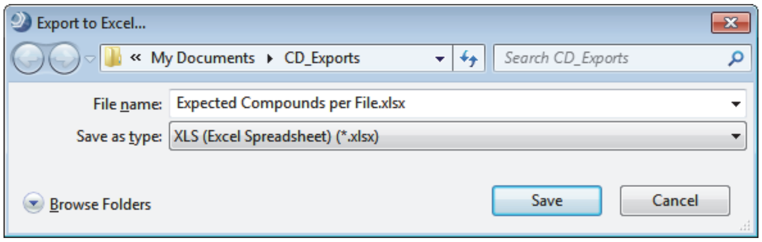
☐ Open file after export

2. If necessary, select a different result table from the Level 1 list.

   The list includes all the main tables in the result file.

3. Click the browse icon next to the Path box.

   A second Export to Excel dialog box (where you specify the location and file name for the file) opens in front of the first Export to Excel dialog box.



« My Documents ▸ CD_Exports

File name: Expected Compounds per File.xlsx

Save as type: XLS (Excel Spreadsheet) (*.xlsx)

4. Browse to the folder where you want to store the file.

   By default, the File Name box displays the name of the result table that you are exporting.

5. Overwrite or rename the file as appropriate, select the spreadsheet type (**XLS** or **Microsoft Excel File**), and click **Save**.

6. In the Export to Excel dialog box (for selecting the table rows to be exported), select related tables from the Level 2 and Level 3 lists as appropriate.

7. In the Options area, make the following selections:

   - To export only those rows that are checked in the result table or tables, select the **Checked Items Only** check box. Otherwise, leave the check box clear to export all of the table rows.

   - To automatically open the newly created spreadsheet after you export it, select the **Open File After Export** check box.

8. Click **Export** to export the data to a spreadsheet.

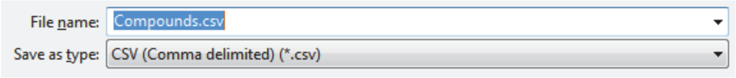
   When the export is finished, you receive a confirmation message with the file's location.

9. At the prompt, click **OK**.

❖ 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 > Export to Text File**.

   The Export to CSV File dialog box opens. The File Name box displays the name of the selected result table.



File name: Compounds.csv
Save as type: CSV (Comma delimited) (*.csv)

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.

Exporting an Xcalibur Inclusion or Exclusion List

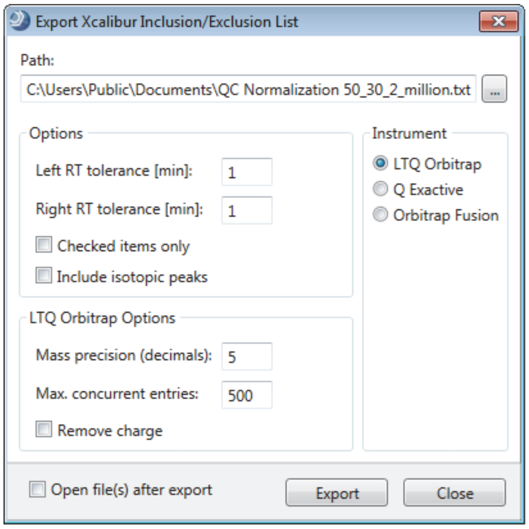
You can export the contents of the Compounds table or the Expected Compounds table to an Xcalibur Inclusion/Exclusion list, and then import this list into an instrument method that controls your Thermo Scientific mass spectrometer.

❖ To export an Xcalibur inclusion or exclusion list

1. Right-click the Compounds table or the Expected Compounds table and choose **Export > Export to Xcalibur Inclusion/Exclusion List**.

   The Export Xcalibur Inclusion/Exclusion List dialog box opens (Figure 66).

Figure 66. Export Xcalibur Inclusion/Exclusion List dialog box



Export Xcalibur Inclusion/Exclusion List

Path: C:\Users\Public\Documents\QC Normalization 50_30_2_million.txt

Options
Left RT tolerance [min]: 1
Right RT tolerance [min]: 1
☐ Checked items only
☐ Include isotopic peaks

Instrument
● LTQ Orbitrap
○ Q Exactive
○ Orbitrap Fusion

LTQ Orbitrap Options
Mass precision (decimals): 5
Max. concurrent entries: 500
☐ Remove charge

☐ Open file(s) after export

2. Make the appropriate selections and entries (Table 33).

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 33 describes the parameters in the Export to Xcalibur Exclusion List dialog box.

Table 33. Export to Xcalibur Inclusion/Exclusion List dialog box parameters (Sheet 1 of 3)

<table>
<tr><th>Parameter</th><th>Description</th></tr>
<tr><td>Path</td><td>Specifies the file name and directory path of the text file that contains the inclusion/exclusion list for your Xcalibur instrument method.</td></tr>
<tr><td colspan="2">Options</td></tr>
<tr><td colspan="2">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</td></tr>
<tr><td>Left RT Tolerance [min]</td><td>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</td></tr>
<tr><td>Right RT Tolerance [min]</td><td>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</td></tr>
</table>

Table 33. Export to Xcalibur Inclusion/Exclusion List dialog box parameters (Sheet 2 of 3)

Parameter	Description
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
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.

Table 33. Export to Xcalibur Inclusion/Exclusion List dialog box parameters (Sheet 3 of 3)

Parameter	Description
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.

Exporting the Contents of the Compounds Table to TraceFinder

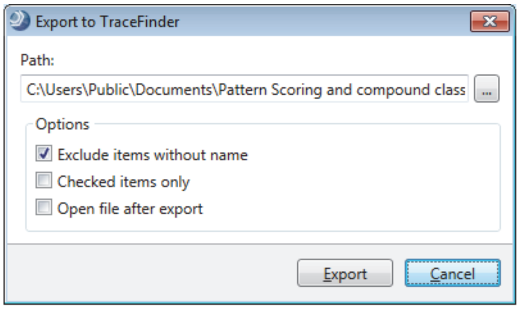
You can export the contents of the Compounds table to a CSV file that the TraceFinder application can use for data processing.

❖ 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 you selected. The default file name is the name of the active result file.

   Figure 67. Export to TraceFinder dialog box

   Path: C:\Users\Public\Documents\Pattern Scoring and compound class

   ☑ Exclude items without name
   ☐ Checked items only
   ☐ Open file after export

2. Select the folder where you want to store the file.

3. Do the following as needed:

   - 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**.

Exporting Spectral Data to a New or Existing mzVault Library

To export spectral data to a new or existing mzVault Library file, see these topics:

- Adding a Compound to an Existing mzVault Library
- Creating a New mzVault Library

Adding a Compound to an Existing mzVault Library

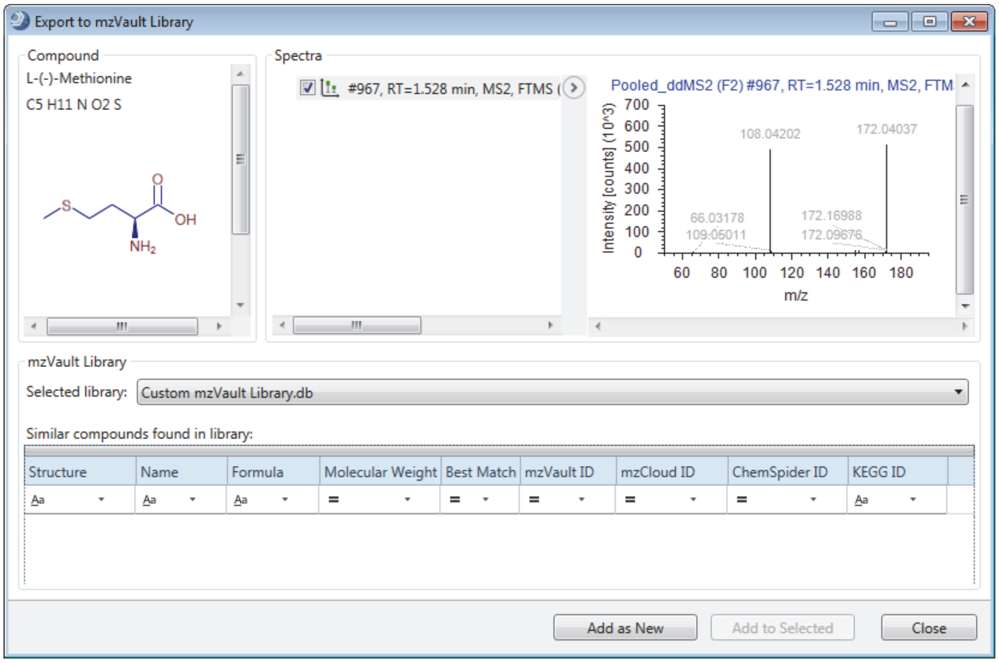
From a Compounds or Expected Compounds result table, use the Export > Single Compound to an Existing mzVault Library shortcut menu command to export a selected compound to an existing mzVault library.

❖ To add a compound to an existing mzVault Library

1. Open a result file (see "Opening, Closing, and Updating Result Files" on page 142).
2. Click the **Compounds** tab or the **Expected Compounds** tab.
3. Right-click a compound in the table and choose **Export > Single Compound to an Existing mzVault Library**.

   The Export to mzVault Library dialog box opens (Figure 68). Its Spectra view displays the available fragmentation spectra for the selected compound.

Figure 68. Export to mzVault Library dialog box populated with a Compounds table compound



Compound: L-(-)-Methionine
C5 H11 N O2 S

☑ #967, RT=1.528 min, MS2, FTMS (

Pooled_ddMS2 (F2) #967, RT=1.528 min, MS2, FTM

Selected library: Custom mzVault Library.db

Similar compounds found in library:

Structure	Name	Formula	Molecular Weight	Best Match	mzVault ID	mzCloud ID	ChemSpider ID	KEGG ID

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.

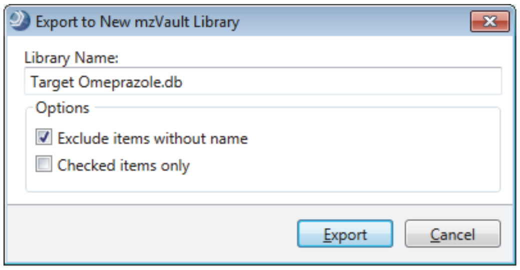
Creating a New mzVault Library

From a Compounds or Expected Compounds result 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 "Opening, Closing, and Updating Result Files" on page 142).
2. Click the **Compounds** tab or the **Expected Compounds** tab.
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 > Compounds to a New 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.



Library Name: Target Omeprazole.db

Options
☑ Exclude items without name
☐ Checked items only

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.

Tip To modify the library with the mzVault 2.1 application, export the library to another folder. Then, use the Replace command to replace the existing library with the modified library.

Copying or Saving Graphical Views for Publication

You can copy the contents of a graphical view (see "Working with the Graphical Result Views" on page 187) to the Clipboard as editable text or 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.

Table 34 lists the shortcut menu commands for copying data to the Clipboard or an external file.

Table 34. 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
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)

Table 34. 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
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

7

Working with the Graphical Result Views

To work with the graphical views that are available when a result page is active, see these topics.

Contents

For information about using the Result Filters view, see "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162. For information about viewing a summary of the analysis parameters for a result file, see "Viewing the Result Summary" on page 171.

Working with the Chromatograms View

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 35).

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.

You can display chromatogram traces (a plot of intensity versus time) by selecting a row in any of these tables: Compounds, Compounds per File, Expected Compounds, Expected Compounds per File, Expected Formulas, Merged Features, Expected Features, FISh Trace Fragments, Specialized Traces, or Manual Peaks.

Follow these procedures as needed:

- To view a chromatogram
- To apply a shortcut menu command
- To add a plot in the Chromatograms view
- To overlay multiple chromatograms in one chromatogram plot
- To change the grouping of the chromatogram traces
- To hide the chromatogram trace or traces for a study variable value
- To update all the plots in the Chromatograms view simultaneously
- To integrate chromatographic peaks manually

❖ To view a chromatogram

1. 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.

2. 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.

  Depending on the nodes in the processing workflow, the Specialized Traces table can contain the following traces:

  - A Create Mass Trace node can generate these traces: an extracted ion (mass range) chromatogram (XIC), a base peak chromatogram (BPC), or a total ion chromatogram (TIC).
  - A Create Analog Trace node can generate these traces: 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.
  - A Create Pattern Trace node generates a TIC trace by summing the intensities of the mass spectral peaks (across the entire scan) that match the user-defined isotope pattern.

  - A Create FISh Trace node generates the following:
    - A summed FISh trace of all the matching fragment ion scans (DDF or AIF) 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.

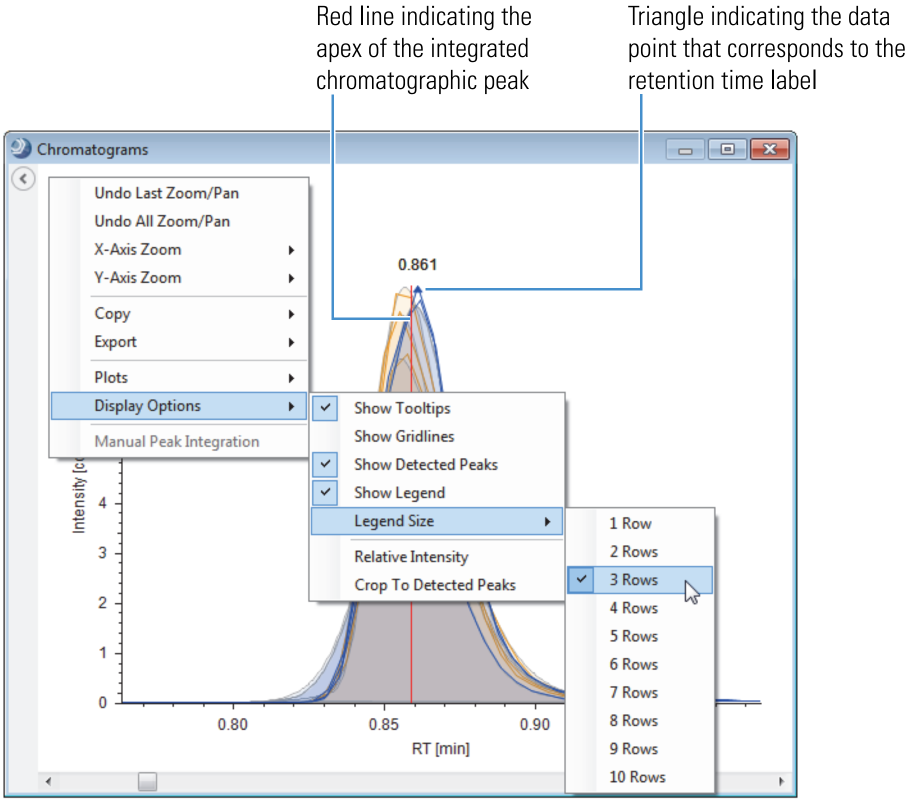
> **Tip** By default, the Filled Gaps table is hidden. To display this table, open the Select Visible Tables dialog box, select the **Filled Gaps** check box, and click **OK**. For more information, see "Filled Gaps Table" on page 304.

3. 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**.

4. 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 (Figure 69).

   In Figure 69, 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 69. Chromatograms view showing the shortcut menu



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.

❖ To apply a shortcut menu command

Right-click the Chromatograms view and choose a command from the shortcut menu.

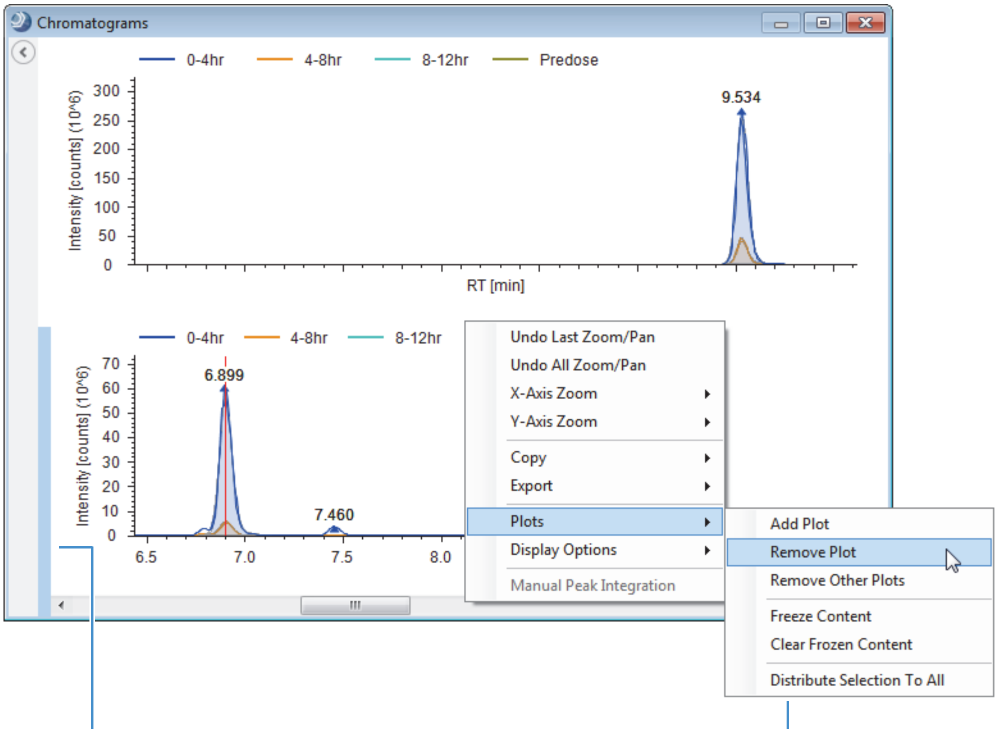
❖ To add a plot in the Chromatograms view

Right-click the Chromatograms view and choose **Plots > Add Plot**.

The new plot appears below the original plot. Only the screen size of your computer monitor limits the maximum number of plots that you can add to the Chromatograms view. When you exceed the maximum number of plots, the plots disappear from the view.

In a Chromatograms view with more than one plot, a light blue bar on the left border highlights the active plot (Figure 70). If you right-click the Chromatograms view and choose Plots > Remove Plot, the application removes the active plot.

Figure 70. Chromatograms view with two plots



Light blue bar on the left border of the active plot

Plots shortcut menu

To overlay multiple chromatograms in one chromatogram plot

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.

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.

To hide the chromatogram trace or traces for a study variable value

Under Filter By, clear the check box for the study variable value.

To update all the plots in the Chromatograms view simultaneously

1. Add two or more plots to the Chromatograms view.
2. 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.

To integrate chromatographic peaks manually

1. Open the Chromatograms view.
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.

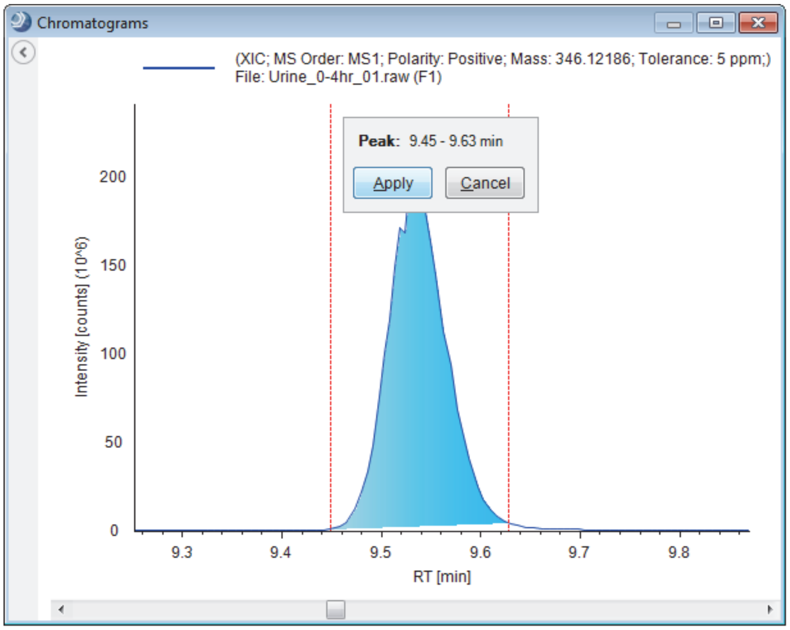
4. Drag one line to the beginning of the chromatographic peak and the other line to the end of the chromatographic peak.

   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 71).

Figure 71. Manually integrated chromatographic peak



(XIC; MS Order: MS1; Polarity: Positive; Mass: 346.12186; Tolerance: 5 ppm;)
File: Urine_0-4hr_01.raw (F1)

Peak: 9.45 - 9.63 min

6. To add the manual peak to the Manual Peaks table, either click **Apply**, or 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.

Table 35 describes the shortcut menu commands for the Chromatograms view.

Table 35. Shortcut menu commands for the Chromatograms view (Sheet 1 of 4)

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.

Table 35. Shortcut menu commands for the Chromatograms view (Sheet 2 of 4)

Command	Description
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.
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.

Table 35. Shortcut menu commands for the Chromatograms view (Sheet 3 of 4)

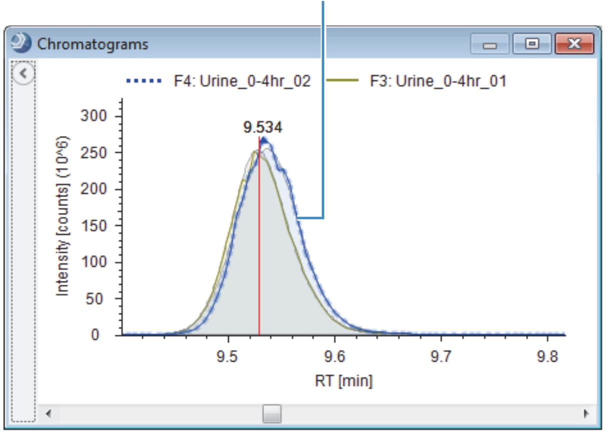
Command	Description
Plots > Add Plot	Adds an empty, active plot to the Chromatograms view. Only the screen size limits the maximum number of displayed plots. When you reach the screen's limit, the Chromatograms view appears to be empty and the following message appears: Not enough space for drawing chart properly.
Plots > Remove Plot	Removes the active plot, which has a gray border. Adding more than one plot activates this command.
Plots > Remove Other Plots	Removes all of the plots in the Chromatograms view. Adding more than one plot to the Chromatograms view activates this command.
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.  Frozen peak with dashes
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.

Table 35. Shortcut menu commands for the Chromatograms view (Sheet 4 of 4)

Command	Description
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 • Chemical formula of the peak component • Molecular weight of the peak component • Selected retention time, in minutes • Intensity, in counts, of the selected point on the chromatogram trace • File name of the input file
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
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 "To integrate chromatographic peaks manually" on page 192). Selecting a trace in the Specialized Traces table activates this command.

Table 36 describes the traces that you can display in the Chromatograms view.

Table 36. Chromatograms view traces

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.
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.

Working with the Mass Spectrum View

The Mass Spectrum view displays the spectral tree of a selected component in the result table. When you open a result file, the Mass Spectrum view is empty.

The Chromatograms view and the Mass Spectrum view are interactive. Double-clicking a time point in the Chromatograms view displays the mass spectral tree and closest full scan for that time point. When you apply the Undo All Zoom/Pan command to the Chromatograms view (which displays the entire chromatographic run), you can double-click time points in the Chromatograms view and move up or down the rows of the active result table and display updated scans in the Mass Spectrum view.

The following topics describe the Mass Spectrum view panes and shortcut menu:

- Spectral Tree Pane
- MS1 Spectrum with Isotope Pattern Matching for Compounds with Predicted Formulas
- Mass Spectrum View Shortcut Menu Commands

Follow these procedures as needed:

- To display a mass spectrum
- To zoom in or out on the *x axis of the Mass Spectrum view*
- To open the shortcut menu for the Mass Spectrum view
- To view the matching fragment structures predicted by the FISh Scoring node for expected compounds
- To create a mirror plot
- To search the mzCloud database for a matching fragmentation spectrum

❖ To display a mass spectrum

Select a row in one of these tables:

- Compounds Table
- Compounds per File Table
- Expected Compounds Table
- Expected Compounds per File Table
- Features Table
- Expected Features Table
- mzCloud Results Table
- Structure Proposals Table

The Mass Spectrum view displays the matching spectral tree and a zoomed-in view of the full MS scan.

❖ To zoom in or out on the *x* axis of the Mass Spectrum view

- To zoom in, drag the cursor to the right over the *m/z* range of interest.
- To zoom out, drag the cursor to the left over the *m/z* range of interest.

❖ To open the shortcut menu for the Mass Spectrum view

Right-click the **Mass Spectrum** view.

❖ To view the matching fragment structures predicted by the FISh Scoring node for expected compounds

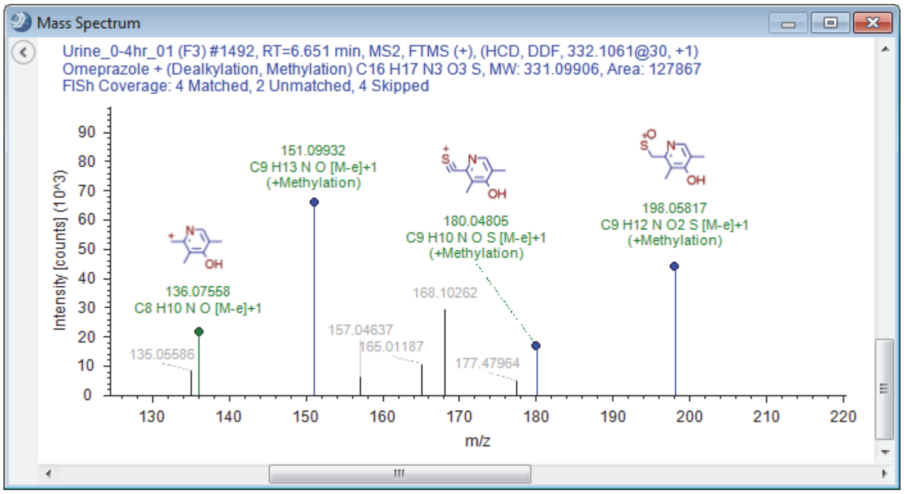
1. Enlarge the view (see "To enlarge a view to fill the screen" on page 150).
2. In the spectral tree, select an MS/MS (labeled MS2) or higher scan.

   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 72 shows a fragmentation spectrum with one direct match and three shifted matches.

Figure 72. Fragmentation spectrum with FISh annotations



Urine_0-4hr_01 (F3) #1492, RT=6.651 min, MS2, FTMS (+), (HCD, DDF, 332.1061@30, +1)
Omeprazole + (Dealkylation, Methylation) C16 H17 N3 O3 S, MW: 331.09906, Area: 127867
FISh Coverage: 4 Matched, 2 Unmatched, 4 Skipped

❖ To create a mirror plot

1. In the spectral tree pane, select the scan that you want to use as a reference scan.
2. Right-click the **Mass Spectrum** view and choose **Use As Reference**.

   > **Note** The Use As Reference command is unavailable when the Show Library Spectra As Reference command is enabled.

3. Select the fragmentation scan that you want to compare.

❖ To search the mzCloud database for a matching fragmentation spectrum

> **Note** The mzCloud database is only compatible 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. In the Spectral Tree pane, select a fragmentation scan.
2. 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.

3. Check the settings and click **OK**.

Spectral Tree Pane

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)

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 (DDF or AIF).

MS1 Spectrum with Isotope Pattern Matching for Compounds with Predicted Formulas

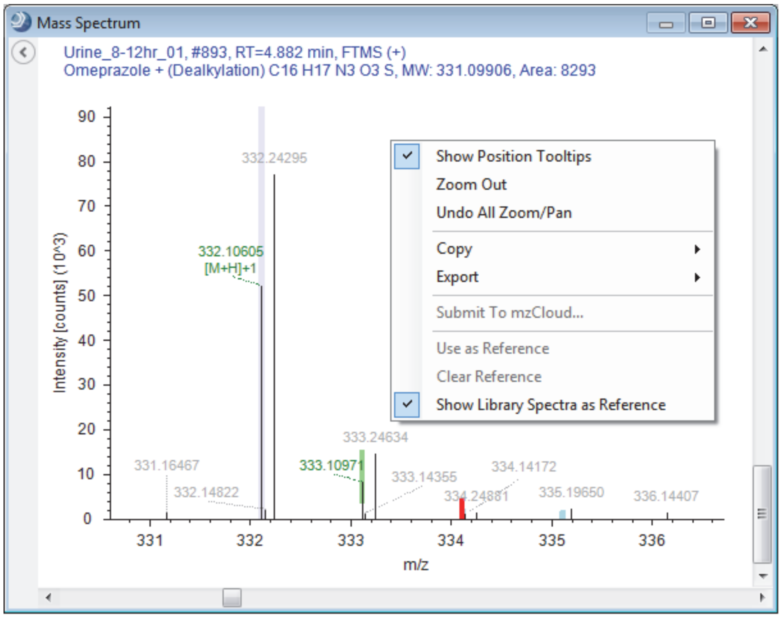
Selecting a row in the following result tables populates the Mass Spectrum view with a spectral tree for the selected retention time in the left pane and the first MS1 scan for the selected retention time in the right pane.

- Expected Compounds
- Expected Compounds per File
- Expected Features
- Compounds

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 (Figure 73 on page 201). 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, 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 73. MS1 scan with color-coded mass spectrum peaks and the shortcut menu



Urine_8-12hr_01, #893, RT=4.882 min, FTMS (+)
Omeprazole + (Dealkylation) C16 H17 N3 O3 S, MW: 331.09906, Area: 8293

Table 37 describes the color coding for the centroids in an MS1 spectrum.

Table 37. Color coding for the centroids in an MS1 spectrum for an expected compound (per file)

Color	Meaning
(🟪) Lavender	The labeled centroid matches the monoisotopic mass of the expected compound ion.
(🟩) Green	The labeled centroid matches the delta mass and the relative intensity of the theoretical isotope pattern 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.
(🟦) Light blue	The expected centroid for this *m/z* value might be missing because its theoretical intensity is at the level of the baseline noise.

The elemental formula for this transformation product (C16 H17 N3 O3 S) yields the following expected isotope pattern.

Mass spectrum peak		Delta mass	Relative intensity
A0	monoisotopic protonated molecule	0	100%
A1	protonated molecule with one ^{13}C	1.00332	18%[a]
A2	protonated molecule with one ^{34}S	1.99583	4.6%[b]
A2	protonated molecule with two ^{13}C	2.00598	2%[c]
A3	protonated molecule with one ^{13}C and one ^{34}S	2.99920	0.8%

[a] Carbon is an X + 1 element. The relative abundance of ^{13}C is 1.1%. The relative intensity of the A1 isotopic peak is approximately equal to $1.1n_c$, where n_c is the number of carbon atoms.

[b] Sulfur is an X + 2 element. The relative abundance of ^{34}S is 4.22%. The relative intensity of the A2 isotopic peak (one ^{34}S) is approximately equal to $4.4n_s$, where n_s is the number of sulfur atoms.

[c] The relative intensity of the A2 isotopic peak (two ^{13}C) is approximately equal to $0.006 \times n_c^2$, where n_c is the number of carbon atoms.

The analysis found the A0 and A1 isotopes. The A2 isotope with one sulfur-34 atom is missing. The expected relative intensity of the A3 isotope falls within the baseline noise.

Mass Spectrum View Shortcut Menu Commands

Table 38 describes the shortcut menu commands for the Mass Spectrum view (Figure 73 on page 201).

Table 38. 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	Zooms out to the full scan range.
Undo All Zoom/Pan	Zooms out to the full scan range.
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.
Submit to mzCloud	Opens the Spectrum Search dialog box for the mzCloud database. Available for an MS/MS data-dependent scan. To set up the mzCloud search options for single scans, see "Specifying the Default mzCloud Mass Tolerance Settings" on page 455. To test your computer's ability to connect to the mzCloud database, see Chapter 15, "Testing Communication to the Online Databases." **IMPORTANT** The mzCloud web application is only compatible with the Internet Explorer™ web browser.
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.

Table 38. Mass Spectrum view shortcut menu commands (Sheet 2 of 2)

Command	Description
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.

Viewing Scatter Plots, Histograms, Bar Graphs, and Pie Charts

Use the Result Charts view to plot the data in a result table. For information about plotting the data, see these topics:

- Scatter Charts
- Histogram Charts
- Bar Charts
- Pie Charts

Follow these procedures as needed.

Note The Zoom Out and Undo All Zoom/Pan commands are available for the Scatter Chart, Histogram Chart, and Bar Chart plots.

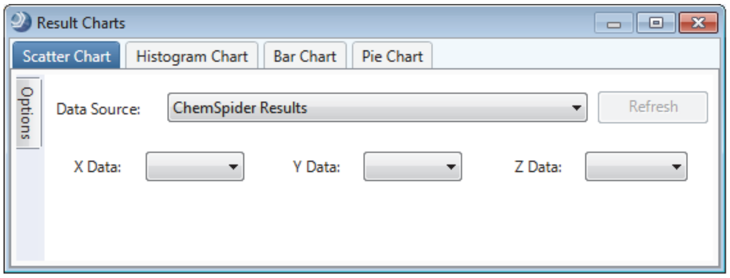
❖ To open the Result Charts view

1. Open a result file (see "To open a result file from the application window" on page 142).
2. In the menu bar, choose **View > Result Charts**.

   By default, the Result Charts view opens as a floating window (Figure 74). You can resize the window, drag the window to another screen, or dock the window. For information about working with floating and docking windows, see "Rearranging the Views on a Result Page" on page 147.

   The Options pane for modifying the appearance of a chart view is a collapsible pane to the left of each chart.

Figure 74. Result Charts view with the collapsed (unpinned) Options pane



❖ To access the shortcut menu for a result chart page

1. Select the variables that you want to plot.
2. Click **Refresh** to plot the data.
3. Right-click the chart to access the shortcut menu for the plot.

❖ To display the Options pane

Point to the vertical Options tab on the left.

❖ To keep the Options pane open

Click the pin icon, ⊣□, in the upper right corner of the Options pane.

❖ To zoom in

Drag the cursor to select the area you want to enlarge in size.

❖ To zoom out (undo the last zoom-in step)

Drag the cursor to the left.

–or–

Right-click the chart and choose **Zoom Out**.

❖ To return to the default magnification

Right-click the chart and choose **Undo All Zoom/Pan**.

Scatter Charts

Use the Scatter Chart plot to determine if there is a linear or logarithmic relationship between two or three variables (columns) in a result table.

For general information about working with the result charts, see “Viewing Scatter Plots, Histograms, Bar Graphs, and Pie Charts” on page 204.

To work with the Scatter Chart plot, see these topics:

- Setting Up a Scatter Chart Plot
- Customizing the Appearance of the Scatter Chart
- Working with the Data Points on the Scatter Chart Plot
- Scatter Chart Parameters and Shortcut Menu Commands

Setting Up a Scatter Chart Plot

To set up a scatter chart plot, follow these procedures:

- To open the Scatter Chart page
- To select the variables and generate the plot

❖ To open the Scatter Chart page

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. You can resize the window, drag the window to another screen, or dock the window. For information about working with floating and docking windows, see Rearranging the Views on a Result Page.

3. Click the **Scatter Chart** tab.

❖ To select the variables and generate the plot

1. In the Data Source list, select one of the available result tables.

   The available selections depend on the workflow nodes in the processing workflow.

2. 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.

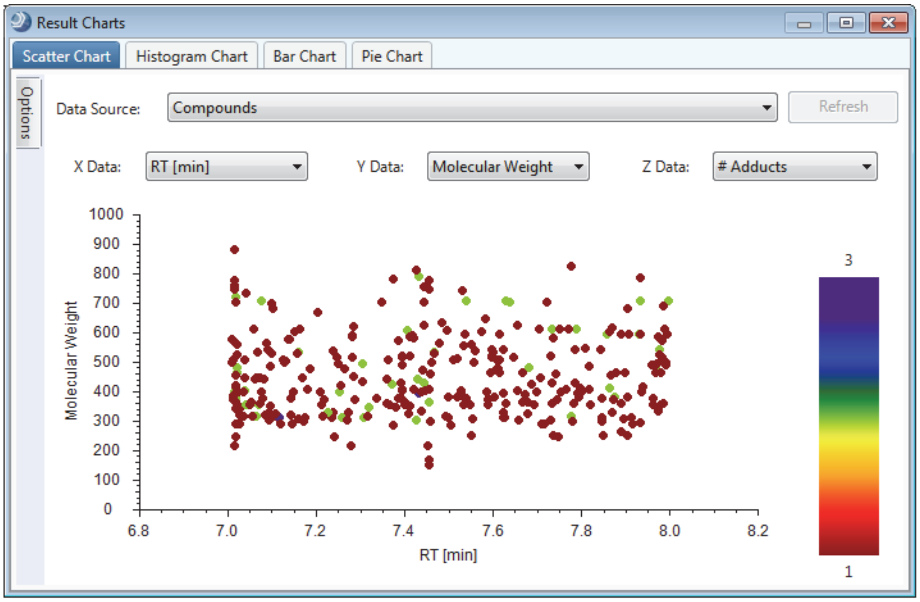
   c. To create a three-dimensional scatter plot, select the variable in the Z Data list that you want to plot against the *z* axis.

      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.

3. 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 75).

Figure 75. Three-dimensional scatter chart



Customizing the Appearance of the Scatter Chart

Follow these procedures to customize the appearance of the scatter chart plot.

❖ To change the scaling, colors, labels, and legends in the display

1. Open the Options pane (see "To display the Options pane" on page 205).
2. 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

1. Open the Options pane (see "To display the Options pane" on page 205).
2. To change the fonts, do one of the following:
   a. Click the expand icon to the left of Axis Scale Font or Axis Title Font.

      A browse icon and a set of font parameters appear.

   b. Make the appropriate selections.

      –or–

      Click the browse icon to open the Font dialog box where you can make your selections.

❖ To return the option settings to the original default settings

In the Options pane, click **Factory Defaults**.

Working with the Data Points on the Scatter Chart Plot

To change the data display, follow these procedures:

- To select the visible data points in the scatter plot
- To undo the selection of the visible data points in the scatter plot
- To select the check box for a single data point in the scatter plot
- To undo the selection of a single data point in the scatter plot
- To copy the scatter plot
- To save the scatter plot as an image file
- To export the data from the scatter plot to a text file
- To interactively filter the scatter plot by using the Result Filters view

❖ To select the visible data points in the scatter plot

1. Zoom in to restrict the view to the area of interest.
2. Right-click the chart and choose **Check All Visible Points.**

   The color and shape of the points change, and the application places a check mark in the result file for all the result items corresponding to the selected data points in the chart. The selections in the Options pane control the appearance of the selected points.

   Conversely, you can place a check mark next to the items in the result file that you want to display in a scatter plot.

❖ To undo the selection of the visible data points in the scatter plot

Right-click the chart and choose **Uncheck Visible Points**.

❖ To select the check box for a single data point in the scatter plot

Right-click the data point in the scatter plot, and choose **Check Point**.

❖ To undo the selection of a single data point in the scatter plot

Right-click the data point of interest in the scatter plot, and choose **Uncheck Point**.

❖ To copy the scatter plot

Right-click the chart and choose **Copy**.

The application places an image file on the Clipboard. You can paste the chart image into another document.

❖ To save the scatter plot as an image file

1. Right-click the graph pane and choose **Save As**.

2. In the Save As dialog box, browse to the location where you want to save the file, and name the file.
3. Click **Save**.

❖ To export the data from the scatter plot to a text file

1. Right-click the graph pane and choose **Save Points As**.
2. In the Save As dialog box, browse to the location where you want to save the file and optionally type a different file name in the File Name box.

   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

3. Click **Save**.

   Exporting data from a scatter plot creates three text files:

   File name Filtered-out Points.txt

   File name Points.txt

   File name Selected Points.txt

❖ 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.

   In the Scatter Chart view, the Refresh button turns orange.

2. Click **Refresh** to refresh the scatter chart plot.

Scatter Chart Parameters and Shortcut Menu Commands

These tables describe parameters and shortcut menu commands for the Scatter Chart page:

- Table 39 describes parameters that are visible in the Scatter Chart page. Use these parameters to set up the scatter plot.
- Table 40 describes the parameters in the Options pane. Use these parameters to customize the appearance of the Scatter Chart page.
- Table 41 describes the shortcut menu commands for the Scatter Chart page. Use these commands to work with the data points in the scatter plot.

Table 39. 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 panel	Use the parameters in this pane to customize the Scatter Chart page. For more information, see Table 40.
Buttons	
Refresh	Refreshes the content of the chart area.

Table 40. Options pane (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.

Table 40. Options pane (Sheet 2 of 2)

Parameter	Description
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.
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.

Table 41. 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	Copies the scatter chart plot as a bitmap (raster) image to the Clipboard.
Copy Points	Copies the data points for the selected variables to the Clipboard.
Save 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.
Save Points As	Opens the Save As dialog box where you can save the data as a plain text file.
Select Item for Point	Highlights the appropriate row in the result table (selected Data Source).

Table 41. Scatter Chart shortcut menu commands (Sheet 2 of 2)

Command	Description
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.
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.

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. Choose **View > Result Charts**.
2. Click the **Histograms Chart** tab.
3. From the Data Source list, select the variable (result table column) that you want to plot.
4. Click **Refresh**.

❖ To change the appearance of the histogram

1. Open the Options pane (see “To display the Options pane” on page 205).
2. 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.
3. (Optional) 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.

❖ To return the settings to the original default settings

In the Options pane, click **Factory Defaults**.

❖ To copy an image of the histogram to the Clipboard

1. Right-click the chart and choose **Copy**.
2. Paste the contents of the chart into another document.

   An image of the histogram appears in the document.

❖ To save a histogram as an image

1. Right-click the chart and choose **Save As**.
2. In the Save As dialog box, browse to the location where you want to save the file, name the file, and select the image file type.

   Selections: EMF, PNG, GIF, JPG, TIF, or BMP
3. Click **Save**.

❖ To copy the points in a histogram as text

1. Right-click the chart and choose **Copy Data**.
2. Paste the points in the chart into another document.

   The data points appear as editable text in the document.

❖ To save the data from the histogram in a text file

1. Right-click the chart and choose **Save Data As**.
2. In the Save As dialog box, browse to the location where you want to export the data and name the file.

   The Save As Type list displays the one available selection: Plain Text File (*.txt).
3. Click **Save**.

   A text file appears in the selected folder. The text file contains the data range describing the histogram column and the count values for the target and excluded items, if they are selected.

Table 42 describes the parameters for the Histogram Chart page.

Table 42. Histogram Chart parameters (Sheet 1 of 5)

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.
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.

Table 42. Histogram Chart parameters (Sheet 2 of 5)

Parameters	Description
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.
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. • Embross: Displays the columns or bars as three-dimensional rectangles. • LightToDark: Displays the columns or bars as shaded rectangles.
Column Width	Specifies the relative width of the columns as a fraction 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

Table 42. Histogram Chart parameters (Sheet 3 of 5)

Parameters	Description
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.
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 needed 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.

Table 42. Histogram Chart parameters (Sheet 4 of 5)

Parameters	Description
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.
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 42. Histogram Chart parameters (Sheet 5 of 5)

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.

❖ To return the settings to the original default settings

In the Options pane, click **Factory Defaults**.

❖ To copy a bar chart in an image format

1. Right-click the chart and choose **Copy**.
2. Paste the contents into another document.

   The contents appear as an image of the bar chart in the document.

❖ To save a bar chart in an image format

1. Right-click the chart and choose **Save As**.
2. In the Save As dialog box, browse to the location where you want to save the file and name the file.
3. Click **Save**.

   The application creates a text file containing an image of the bar chart.

❖ To copy the points in a bar chart as text

1. Right-click the chart and choose **Copy Data**.
2. Paste the points in the chart into another document.

   The contents appear as text in the document.

❖ To save the data from the bar chart in a text file

1. In the graph pane, right-click and choose **Save Data As**.
2. In the Save As dialog box, browse to the location where you want to export the data and name the file.
3. Select **Plain Text File (*.txt)** in the File Type box if it is not already selected.
4. Click **Save**.

   The application creates a file containing the category description and the count of items per category.

Table 43 describes the parameters on the Bar Chart page of the Result Charts view.

Table 43. Bar Chart parameters (Sheet 1 of 4)

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.

Table 43. Bar Chart parameters (Sheet 2 of 4)

Command or option	Description
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
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.

Table 43. Bar Chart parameters (Sheet 3 of 4)

Command or option	Description
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. • Embross: Displays the columns or bars as three-dimensional rectangles. • LightToDark: Displays the columns or bars as shaded rectangles.
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.
Column Label	Specifies the font of the column labels that appear on top of the bars in the bar chart. Default: 8-point Arial

Table 43. Bar Chart parameters (Sheet 4 of 4)

Command or option	Description
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 open the Pie Chart page of the Result Charts view

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.

❖ To return the settings to the original default settings

In the Options pane, click **Factory Defaults**.

❖ To copy a pie or doughnut chart in an image format

1. Right-click the chart and choose **Copy**.
2. Paste the contents of the chart into another document.

    The contents appear as an image of the chart in the document.

❖ To save a pie or doughnut chart in an image format

1. Right-click the chart and choose **Save As**.
2. In the Save As dialog box, browse to the location where you want to save the file and name the file.
3. Click **Save**.

    The application creates a file containing an image of the pie or doughnut chart.

❖ To copy the points in a pie or doughnut chart as text

1. Right-click the chart and choose **Copy Data**.
2. Paste the points of the chart into another document.

    The contents appear as text in the document.

❖ To save the data from the pie or doughnut chart in a text file

1. In the graph pane, right-click and choose **Save as Text**.
2. In the Save As dialog box, browse to the location where you want to export the data and name the file.
3. Select **Plain Text File (*.txt)** in the File Type box if it is not already selected.
4. Click **Save**.

   The application creates a text file containing the category description and the count of items per category.

Table 44 describes the parameters on the Pie Chart page of the Result Charts view.

Table 44. 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.
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.

Table 44. Pie Chart page parameters (Sheet 2 of 3)

Command or Option	Description
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.
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

Table 44. Pie Chart page parameters (Sheet 3 of 3)

Command or Option	Description
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.

Working with the 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.

For a single compound, you can select to view either a box-and-whisker plot or a trendline plot. For multiple compounds, you can only view a set of trendline plots.

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.

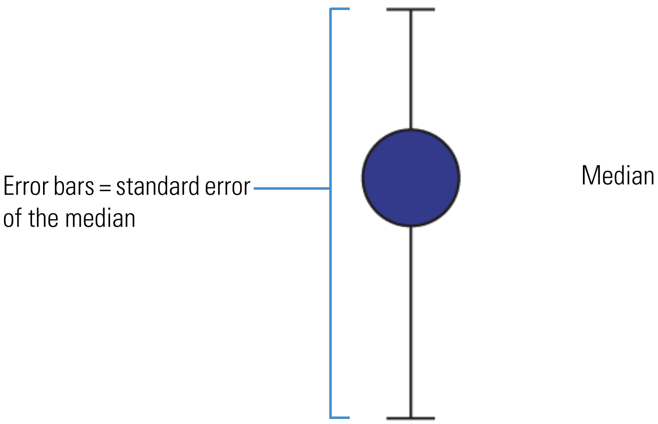
The box-and-whisker plot requires a minimum of two data points to plot the box for a sample group. It does not plot sample groups that include only one data point. If none of the sample groups includes the minimum number of data points, the following text appears in the chart area: No results available to plot.

The Trend Chart can plot the data from rows in these result tables: Compounds, Expected Compounds, and Merged Features. For a single compound, the chart can plot the data as a trendline or 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.

By default, the trendline 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 (Figure 76). 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 76. 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 (Figure 77). The application uses the following equations to calculate the upper and lower whiskers:

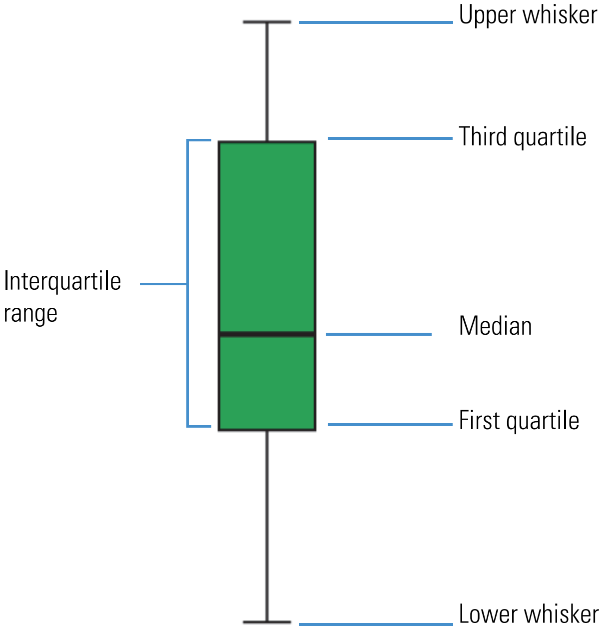
$$\text{Interquartile range (IQR)} = \text{Quartile 3 (Q3)} - \text{Quartile 1 (Q1)}$$

$$\text{Upper whisker} = \text{Q3} + \text{IQR} \times 1.5$$

$$\text{Lower whisker} = \text{Q1} - \text{IQR} \times 1.5$$

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 77. 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.

Follow these procedures as needed:

- To open the Trend Chart view
- To compare the peak areas for compounds in each sample group
- To change the sort order for a Box Whisker chart or a Trendline chart
- To plot the peak areas for multiple compounds
- To change the hierarchy of a variable used for grouping
- To view error bars for each data point in a trendline chart

❖ 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 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.

❖ To compare the peak areas for compounds in each sample group

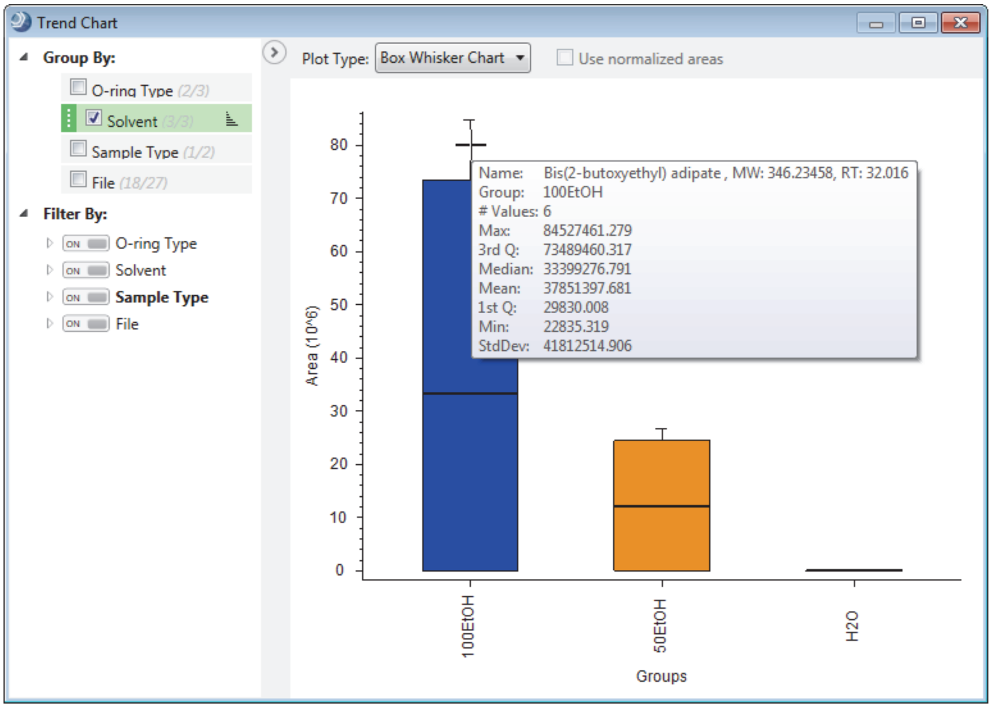
1. Open the Trend Chart view.
2. Select one row (one component or one feature) in the Compounds table, Expected Compounds table, or Merged Features table.
3. Under Group By, select the appropriate check boxes to define the sample groups.
4. Right-click the graph area and choose **Show Legend**.

   The legend displays the sample group colors.
5. 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 78 shows a box-and-whisker plot. Placing the cross-hair cursor on a box or whisker opens a ToolTip with descriptive statistics.

Figure 78. Box-and-whisker plot for one compound



Group By:
☐ O-ring Type (2/3)
☑ Solvent (3/3)
☐ Sample Type (1/2)
☐ File (18/27)

Plot Type: Box Whisker Chart ☐ Use normalized areas

Name: Bis(2-butoxyethyl) adipate , MW: 346.23458, RT: 32.016
Group: 100EtOH
Values: 6
Max: 84527461.279
3rd Q: 73489460.317
Median: 33399276.791
Mean: 37851397.681
1st Q: 29830.008
Min: 22835.319
StdDev: 41812514.906

❖ To change the sort order for a Box Whisker chart or a Trendline chart

Under Group By in the left pane, 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 *x*-axis labels (Figure 79).

Figure 79. Trend chart with compounds grouped by solvent and sorted in ascending or descending order

Sorted in ascending order

Sorted in descending order

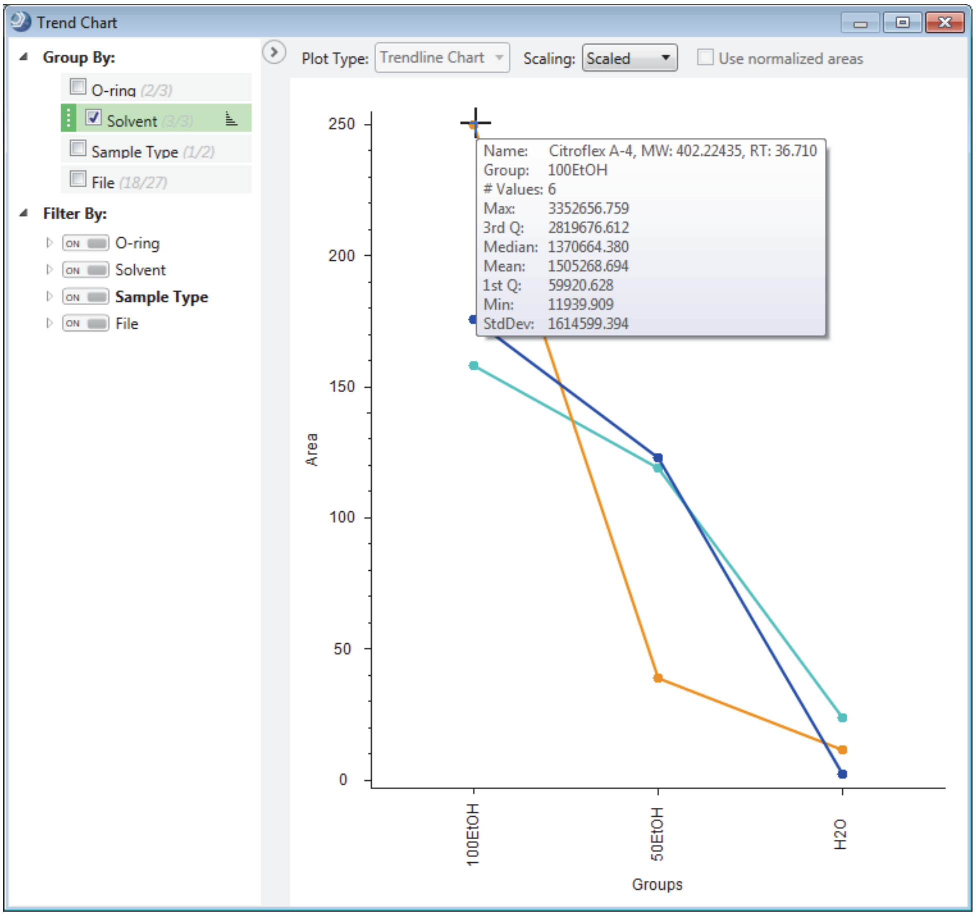
❖ To plot the peak areas for multiple compounds

Press the CTRL key and select rows in the result table, 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 80 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 80. Trendline chart with three compounds



Plot Type: Trendline Chart
Scaling: Scaled
☐ Use normalized areas

Name: Citroflex A-4, MW: 402.22435, RT: 36.710
Group: 100EtOH
Values: 6
Max: 3352656.759
3rd Q: 2819676.612
Median: 1370664.380
Mean: 1505268.694
1st Q: 59920.628
Min: 11939.909
StdDev: 1614599.394

❖ To change the hierarchy of a variable used for grouping

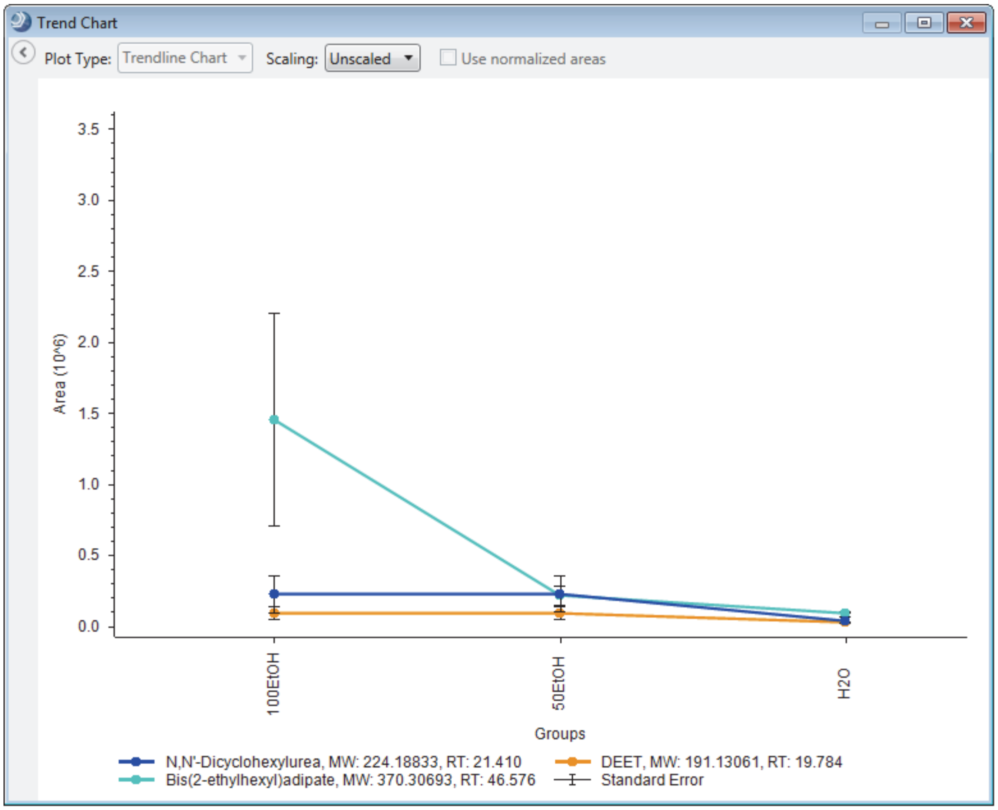
Use the handle (⋮) next to the variable (see "To change the hierarchy of the study variables" on page 77).

❖ To view error bars for each data point in a trendline chart

1. In the Scaling list, 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 81).

Figure 81. Trendline chart with error bars



Plot Type: Trendline Chart

Scaling: Unscaled

☐ Use normalized areas

Table 45 describes the parameters in the Trend Chart view.

Table 45. Trend Chart 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 includes the Normalize Areas node.

Working with the 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.

Follow these procedures as needed:

- To open the Principal Component Analysis view
- To set up the plot
- To interpret the scores plot
- To interpret the loadings plot
- To select the corresponding compound in the result table
- To interpret the variance plot

❖ To open the Principal Component Analysis view

1. Open a result file of interest.

   The result file must contain the results of a targeted analysis with grouped compounds, an untargeted analysis with grouped compounds, or a combined targeted and untargeted analysis with merged features.

2. From the menu bar, choose **View > Principal Component Analysis**.

   If the result file contains a Compounds result table, the view opens with the Compounds table selected as the data source.

❖ To set up the plot

1. In the Data Source list, select the **Compounds**, **Expected Compounds**, or **Merged Features** table as appropriate for the data set.
2. 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.

3. If the data points differ by several orders of magnitude, select the **Center and Scale** check box.

4. If the processing workflow included the Normalize Areas node, select the **Use Normalized Areas** check box as appropriate.
5. To display a legend at the bottom of the plot, right-click the plot and choose **Show Legend**.
6. 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**.
7. To remove points from the plot, clear the check boxes under Filter By as appropriate.

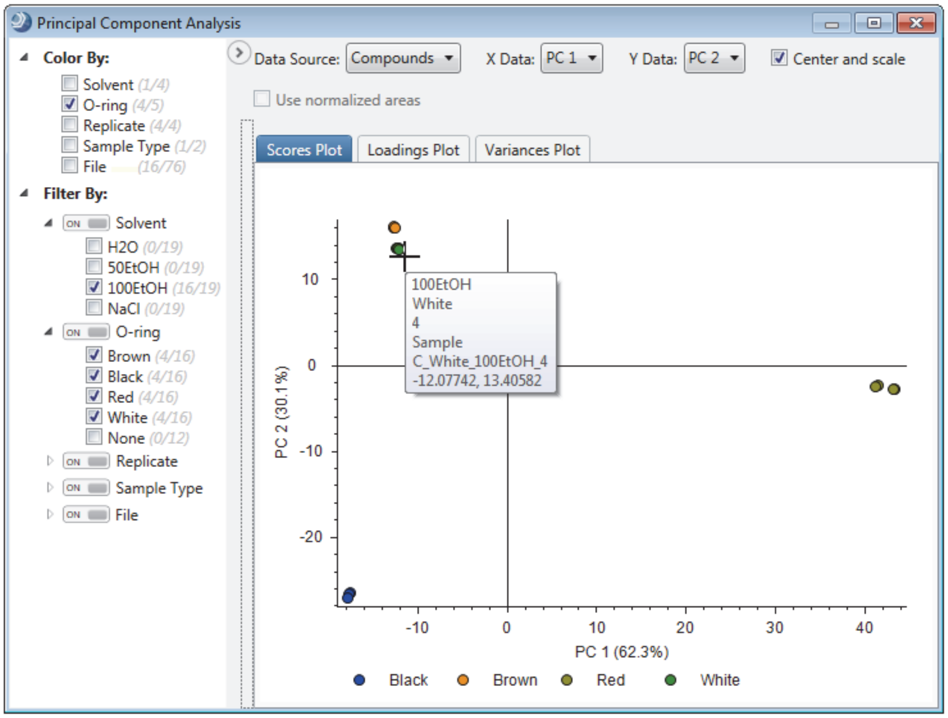
   Using the new population, the application recalculates the principal components, including their contribution to the variance, and shifts the coordinates of the remaining data points.

❖ To interpret the scores plot

1. Use the scores plot to interpret the relationship among the sample groups. Sample groups that are near each other are similar.
2. 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.
3. Place the cross-hair cursor on a data point to view its coordinates.

   Figure 82 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, whereas 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 82. Scores plot for four o-ring types (white, brown, red, and black)



Principal Component Analysis

Color By:

- ☐ Solvent (1/4)
- ☑ O-ring (4/5)
- ☐ Replicate (4/4)
- ☐ Sample Type (1/2)
- ☐ File (16/76)

Filter By:

- ON Solvent
  - ☐ H2O (0/19)
  - ☐ 50EtOH (0/19)
  - ☑ 100EtOH (16/19)
  - ☐ NaCl (0/19)
- ON O-ring
  - ☑ Brown (4/16)
  - ☑ Black (4/16)
  - ☑ Red (4/16)
  - ☑ White (4/16)
  - ☐ None (0/12)
- ON Replicate
- ON Sample Type
- ON File

Data Source: Compounds   X Data: PC 1   Y Data: PC 2   ☑ Center and scale

☐ Use normalized areas

100EtOH
White
4
Sample
C_White_100EtOH_4
-12.07742, 13.40582

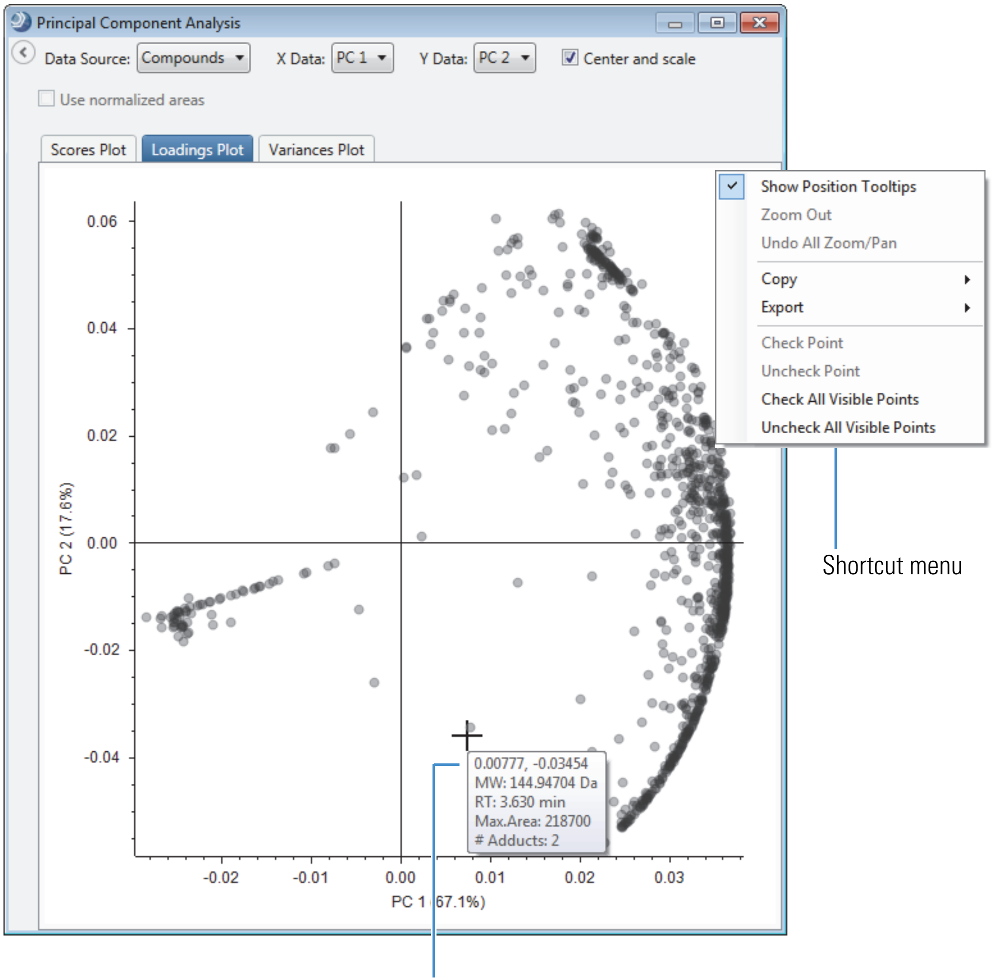
❖ To interpret the loadings plot

1. Use the loadings plot to interpret the relationship among the variables.

   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 with the following information about the compound: the principal component coordinates, molecular weight, retention time, maximum peak area, and number of adduct ions (Figure 83).

Figure 83. Loadings plot with its shortcut menu displayed



Data Source: Compounds

X Data: PC 1

Y Data: PC 2

☑ Center and scale

☐ Use normalized areas

0.00777, -0.03454
MW: 144.94704 Da
RT: 3.630 min
Max.Area: 218700
Adducts: 2

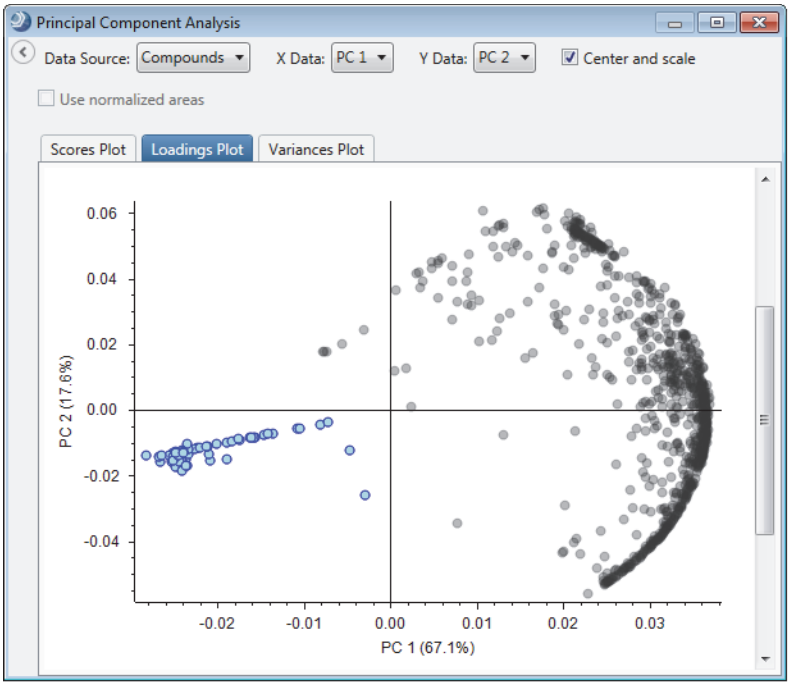
Shortcut menu

ToolTip

3. To export the information for data points to a spreadsheet file, do the following:
   a. Drag the cursor across a rectangular area of the plot to zoom in on that area.
   b. Right-click the plot and choose **Check All Visible Points**.

      The selected points change color (Figure 84).

Figure 84. Loadings plot with checked points shown in blue



Data Source: Compounds X Data: PC 1 Y Data: PC 2 ☑ Center and scale

☐ Use normalized areas

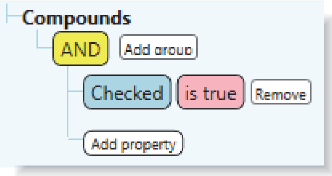
c. To export the checked table rows to a spreadsheet, see “To export the contents of a result table to a spreadsheet file” on page 177.

4. To set up a result filter that displays only the checked points in the Compounds table, do the following:

   a. From the menu bar, choose **View > Result Filters**.

      The Result Filters dialog box opens.

   b. Set up the following filter and click **Apply Filters**.



> **Note** You can view the filtered data points in the volcano plot (Differential Analysis view) where they appear in a color that is not listed in the legend.

   c. To remove the filtering, click **Clear All**, and then click **Apply Filters**.

5. To clear the selected check boxes in the result table, right-click the result table and choose **Uncheck All > In This Table**.

❖ To select the corresponding compound in the result table

Double-click a data point of interest in the loadings plot.

❖ To interpret the variance plot

Use the variance plot to determine the relative differentiation between sample groups.

For example, Figure 85 shows the variance plot for the compounds leached from red o-rings soaked in water or an aqueous solution of sodium chloride. Figure 86 shows the variance plot for the same type of o-rings soaked 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 85. Water versus an aqueous solution of sodium chloride (extraction strength)

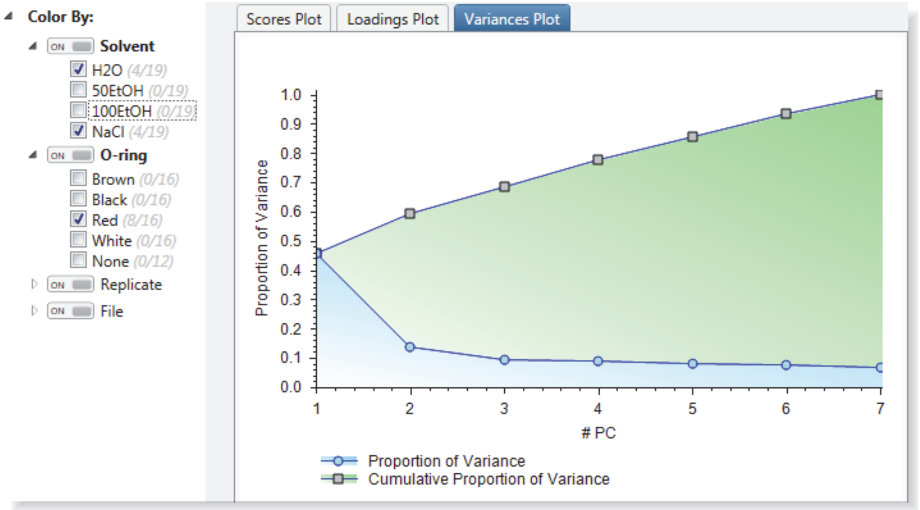


Figure 86. Water versus ethanol (extraction strength)

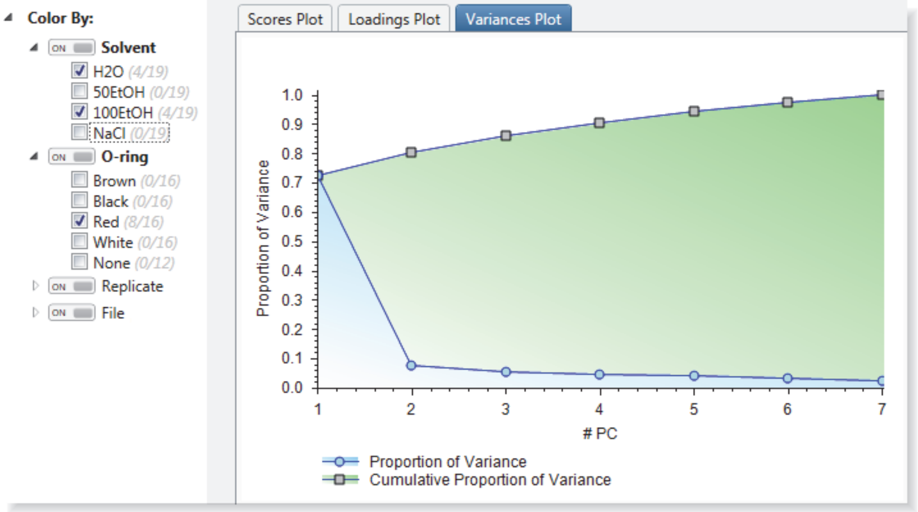


Table 46 describes the parameters in the Principal Component Analysis view.

Table 46. 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.

Working with the Descriptive Statistics View

Use the Descriptive Statistics view to visually compare the statistics of the peak areas for all compounds currently displayed in the Compounds table or the Expected Compounds table as a box-and-whisker plot.

A box-and-whisker plot displays the data for a variable as a rectangular box with a set of whiskers at each end (Figure 87). 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:

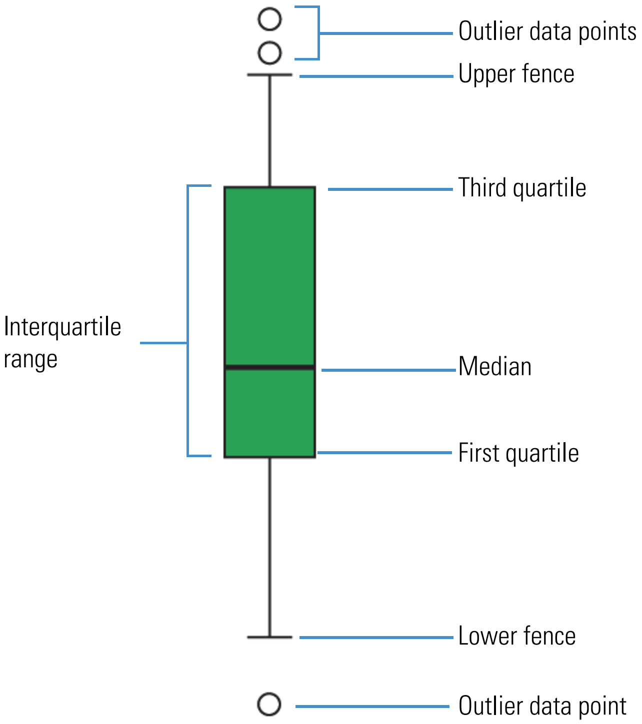
Interquartile range (IQR) = Quartile 3 (Q3) – Quartile 1 (Q1)

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 87. 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 "Copying or Saving Graphical Views for Publication" on page 185.

Follow these procedures as needed:

- To copy or save the data as an image
- To copy or save the data as editable text

- To view the table row for an outlier data point
- To select the check box for an outlier data point
- To select the check boxes for all of the visible data points
- To export the outlier data points to a spreadsheet

❖ To 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.

❖ To 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.

❖ To view the table row for an outlier data point

In the plot, double-click the data point.

❖ To 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.

❖ To select the check boxes for all of the visible data points

Right-click the plot and choose **Check All Visible Points**.

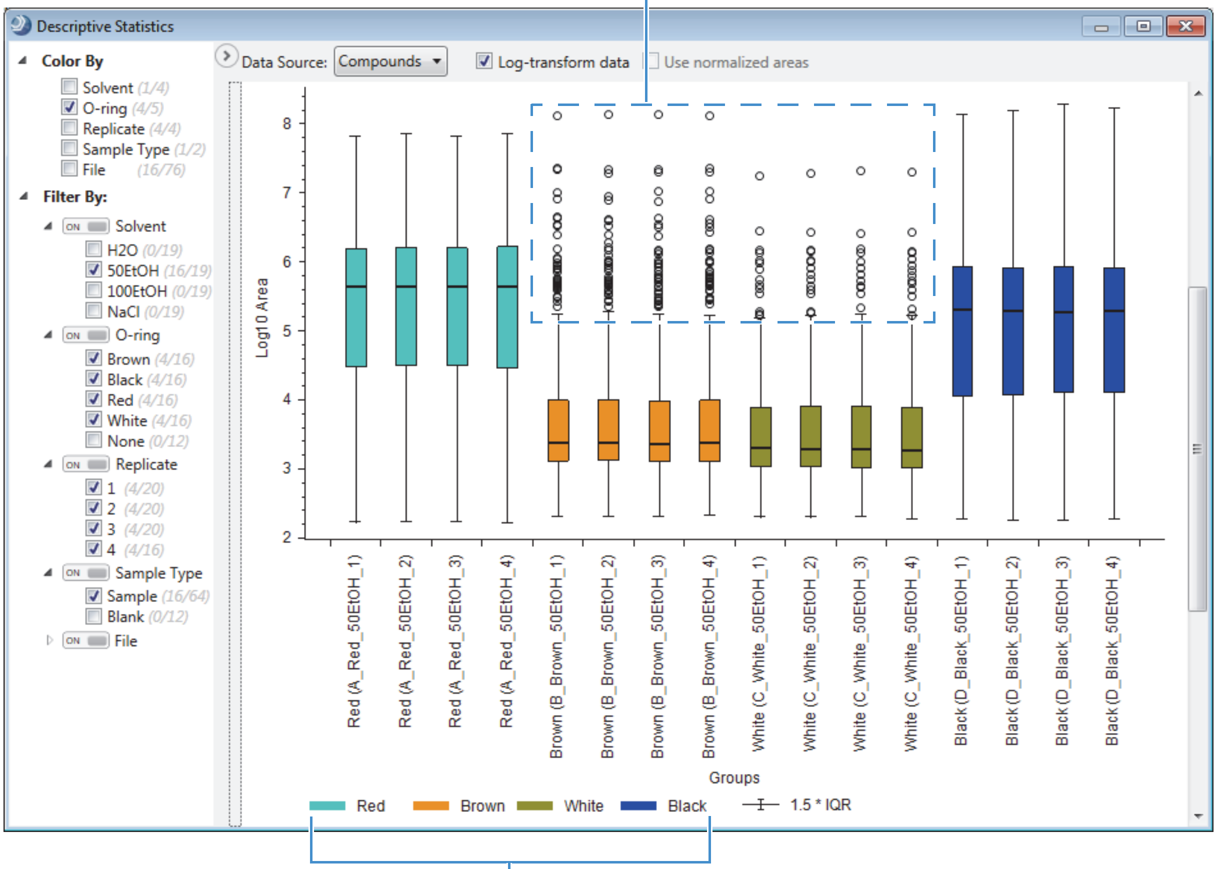
❖ To export the outlier data points to a spreadsheet

1. In the view, zoom in on the outlier points so that they are the only visible points on the screen.

   Figure 88 shows a box-and-whisker plot for the chromatographic peak areas of compounds that leach out of four different o-ring types. The compounds leached from the red and black o-rings show more variation; however, the peak areas for all of the these compounds fall within the lower and upper fences. The compounds leached from the brown and white o-rings show less variation (in peak area); however, the peak areas for numerous compounds fall outside the upper fences.

Figure 88. Box-and-whisker plot for the leachable compounds in four types of o-rings

Compounds with chromatographic peak areas that are greater than the upper fences for the brown and white o-rings



Descriptive Statistics

Color By
- ☐ Solvent (1/4)
- ☑ O-ring (4/5)
- ☐ Replicate (4/4)
- ☐ Sample Type (1/2)
- ☐ File (16/76)

Filter By:
- ON Solvent
  - ☐ H2O (0/19)
  - ☑ 50EtOH (16/19)
  - ☐ 100EtOH (0/19)
  - ☐ NaCl (0/19)
- ON O-ring
  - ☑ Brown (4/16)
  - ☑ Black (4/16)
  - ☑ Red (4/16)
  - ☑ White (4/16)
  - ☐ None (0/12)
- ON Replicate
  - ☑ 1 (4/20)
  - ☑ 2 (4/20)
  - ☑ 3 (4/20)
  - ☑ 4 (4/16)
- ON Sample Type
  - ☑ Sample (16/64)
  - ☐ Blank (0/12)
- ON File

Data Source: Compounds ☑ Log-transform data ☐ Use normalized areas

Four o-ring types

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 47 describes the components of the Descriptive Statistics view.

Table 47. Descriptive Statistics view parameters (Sheet 1 of 2)

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.

Table 47. Descriptive Statistics view parameters (Sheet 2 of 2)

Parameter	Description
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.

Viewing a Volcano Plot and Running a New Differential Analysis

Use the Differential Analysis view to view a volcano plot of the differential analysis performed during data processing or to run a new differential analysis.

Follow these procedures as needed:

- To open the Differential Analysis view and review the initial analysis
- To change the analysis displayed in the volcano plot
- To run a new differential analysis

❖ To open the Differential Analysis view and review the initial analysis

1. Open the result file of interest.
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 ($-\log_{10} 0 = \text{Infinity}$, $-\log_{10} 1 = 0$).

3. To show the legend, right-click the plot and choose **Show Legend**.

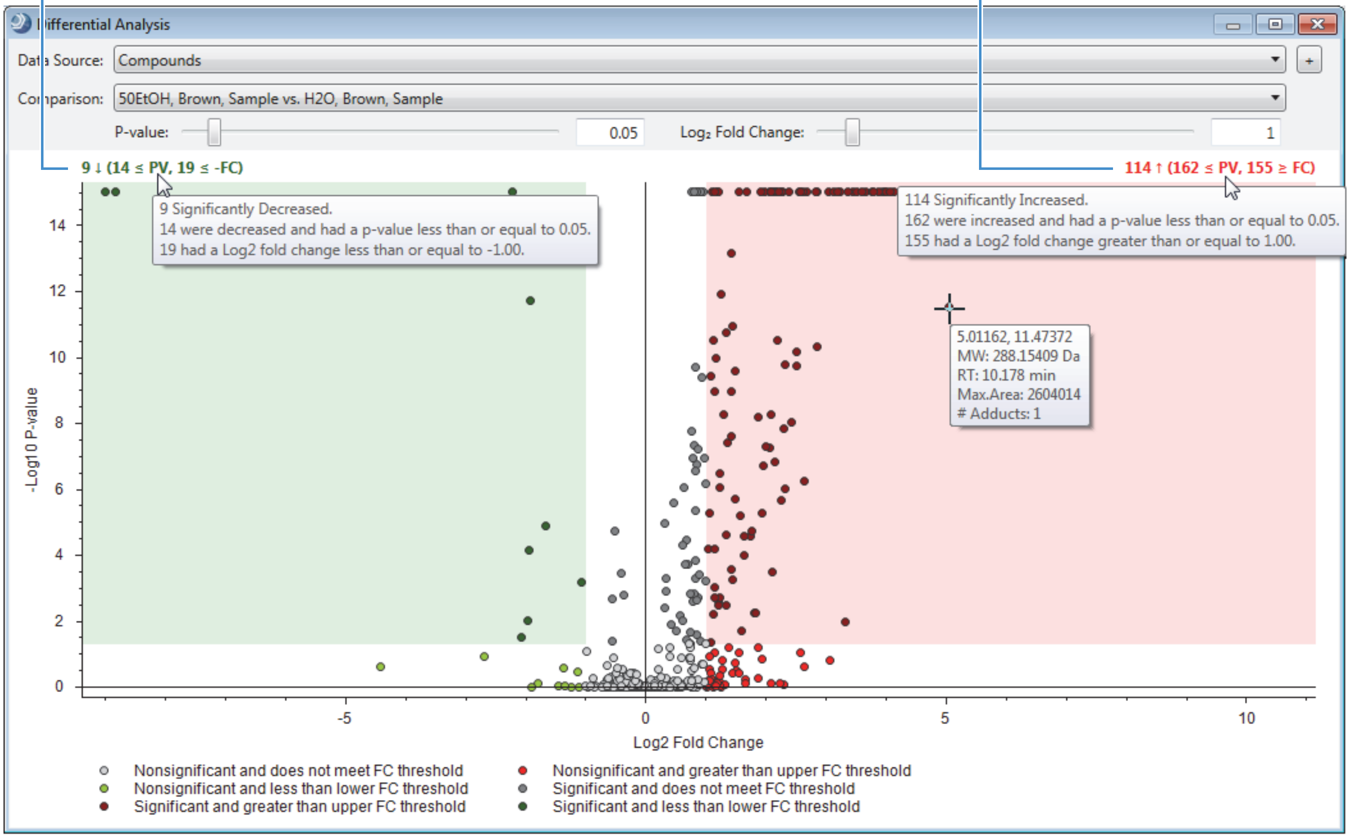
   The data points are color-coded, as defined by the legend.

   Figure 89 shows a comparison between two extraction solvents—water and an aqueous solution of 50% ethanol.

Figure 89. Differential Analysis view with the analysis run during data processing

Analysis summary for the negative fold changes (down-regulated compounds)

Analysis summary for the positive fold changes (up-regulated compounds)



Differential Analysis

Data Source: Compounds

Comparison: 50EtOH, Brown, Sample vs. H2O, Brown, Sample

P-value: 0.05

Log₂ Fold Change: 1

9 ↓ (14 ≤ PV, 19 ≤ -FC)

9 Significantly Decreased.
14 were decreased and had a p-value less than or equal to 0.05.
19 had a Log2 fold change less than or equal to -1.00.

114 ↑ (162 ≤ PV, 155 ≥ FC)

114 Significantly Increased.
162 were increased and had a p-value less than or equal to 0.05.
155 had a Log2 fold change greater than or equal to 1.00.

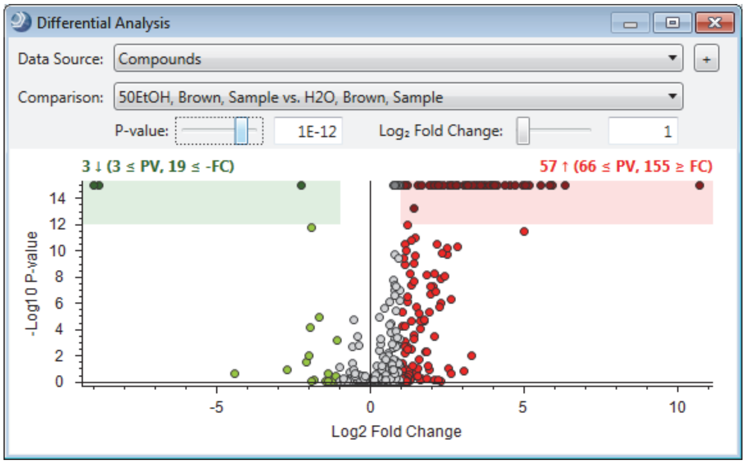
5.01162, 11.47372
MW: 288.15409 Da
RT: 10.178 min
Max.Area: 2604014
Adducts: 1

❖ 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 90 shows the effect of changing the p-value setting.

Figure 90. P-value decreased from 0.05 to 1E–12



Differential Analysis

Data Source: Compounds

Comparison: 50EtOH, Brown, Sample vs. H2O, Brown, Sample

P-value: 1E-12

Log₂ Fold Change: 1

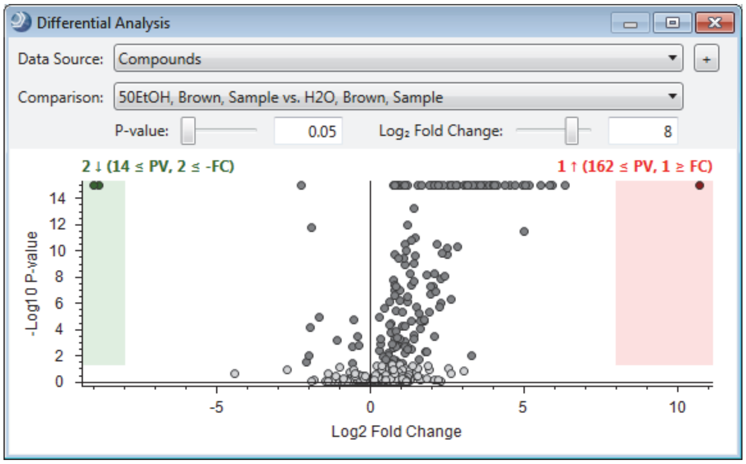
3 ↓ (3 ≤ PV, 19 ≤ -FC)

57 ↑ (66 ≤ PV, 155 ≥ FC)

- Change the fold change setting by dragging the slider. This changes the *x*-axis range of the shaded areas.

Figure 91 shows the effect of changing the Log_2 Fold Change setting.

Figure 91. Fold change increased from 1 to 8



Differential Analysis

Data Source: Compounds

Comparison: 50EtOH, Brown, Sample vs. H2O, Brown, Sample

P-value: 0.05

Log₂ Fold Change: 8

2 ↓ (14 ≤ PV, 2 ≤ -FC)

1 ↑ (162 ≤ PV, 1 ≥ FC)

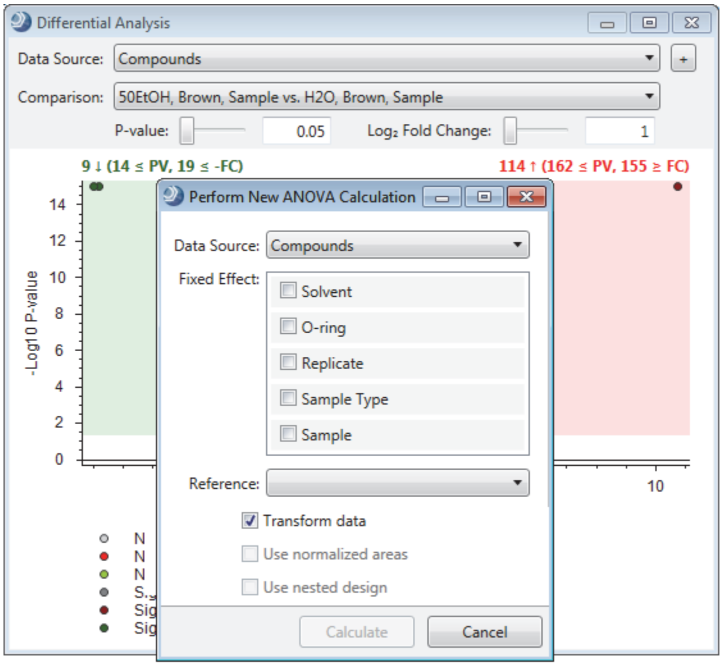
❖ To run a new differential analysis

> **Note** 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.

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 92).

Figure 92. Perform New ANOVA Calculation dialog box



Data Source: Compounds

Comparison: 50EtOH, Brown, Sample vs. H2O, Brown, Sample

P-value: 0.05 Log₂ Fold Change: 1

Perform New ANOVA Calculation

Data Source: Compounds

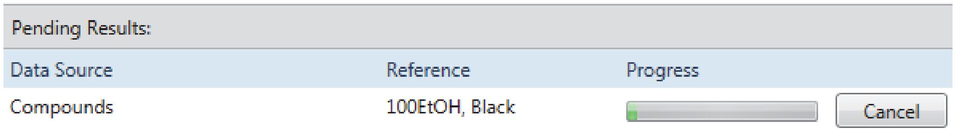
Fixed Effect:
☐ Solvent
☐ O-ring
☐ Replicate
☐ Sample Type
☐ Sample

Reference:

☑ Transform data
☐ Use normalized areas
☐ Use nested design

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.



Pending Results:

Data Source	Reference	Progress
Compounds	100EtOH, Black	

   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.

Table 48 describes the parameters in the Differential Analysis view.

Table 48. 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 ($-\log_{10} 0.05 = 1.3$)
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.

Table 48. Differential Analysis view parameters (Sheet 2 of 2)

Parameter	Description
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 49 describes the shortcut menu commands for the Differential Analysis view.

Table 49. 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.
Copy and Export commands	See “Copying or Saving Graphical Views for Publication” on page 185.
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 (the Compounds table or the Expected Compounds table). 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.

Table 49. Shortcut menu commands for the Differential Analysis view (Sheet 2 of 2)

Command	Description
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.

Working with the 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.

❖ To open the Partial Least Squares–Discriminant Analysis view

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.

❖ To determine a set of compounds that you can use to discriminate the experimental variables by

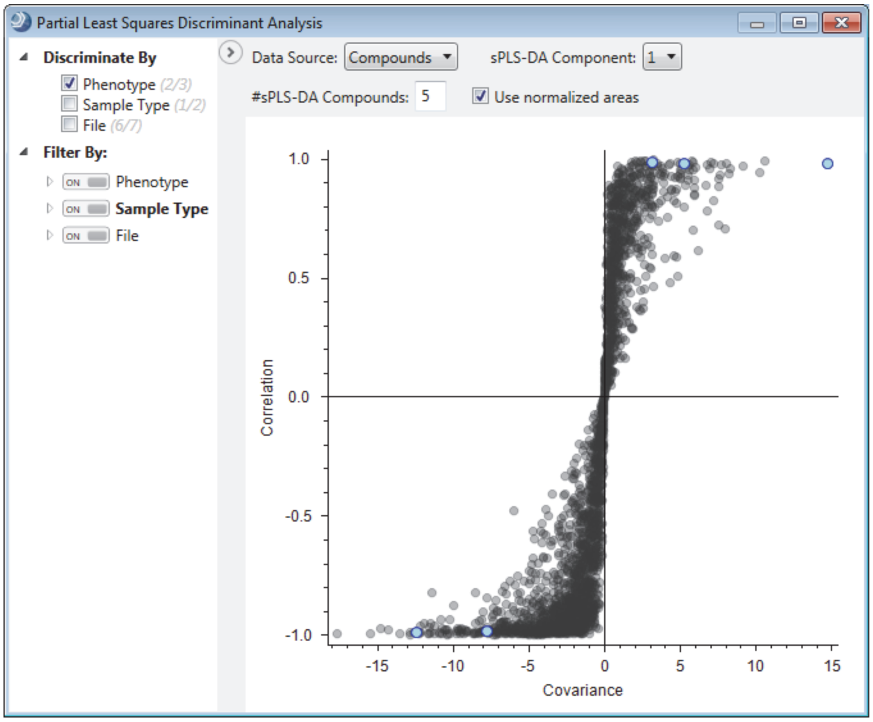
1. In the collapsible pane on the left, under Discriminate By, select the study factors that you want to discriminate by.
2. On the right above the plot, in the Data Source list, select the data source.
3. In the #sPLS-DA Compounds box, type the number of compounds that you want to use to differentiate the selected study factors.
4. To update the plot, click anywhere in the plot.

   The orange circles represent the discriminating compounds.

5. 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 93).

Figure 93. PLS-DA view with five checked discriminating compounds



Partial Least Squares Discriminant Analysis

Discriminate By
☑ Phenotype (2/3)
☐ Sample Type (1/2)
☐ File (6/7)

Filter By:
ON Phenotype
ON **Sample Type**
ON File

Data Source: Compounds
sPLS-DA Component: 1
#sPLS-DA Compounds: 5
☑ Use normalized areas

6. 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.

Table 50 describes the parameters in the Partial Least Squares - Discriminant Analysis view.

Table 50. Partial Least Squares - Discriminant Analysis view parameters

Parameter	Description
Data Source	Specifies the result table for the source data. Selections: Compounds 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.

Viewing KEGG Pathways

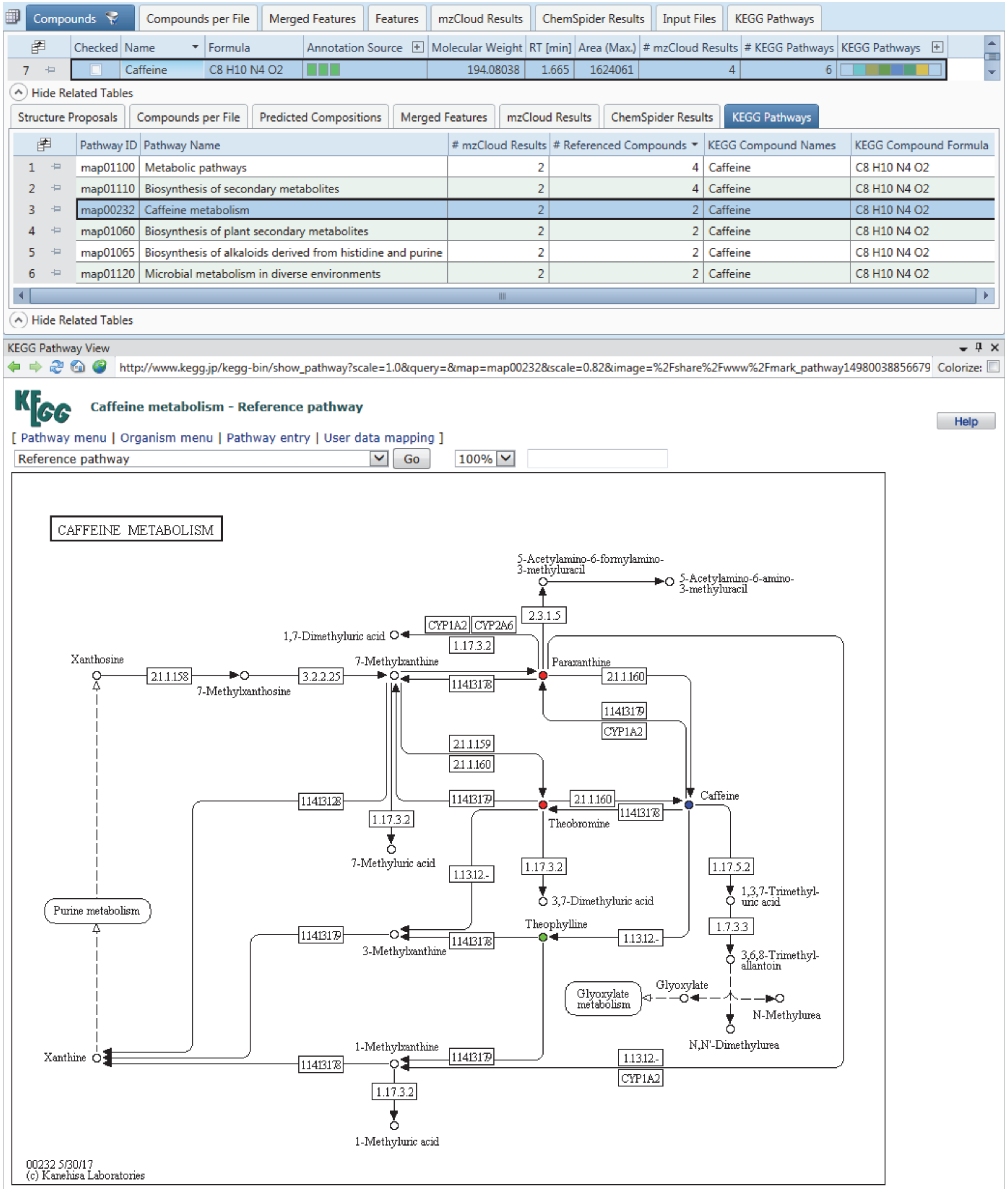
Use the KEGG Pathways view to view the reaction pathway of a detected compound in a KEGG pathway.

❖ To view the KEGG pathways for a compound in the Compounds table

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. 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 94 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 94. Caffeine metabolism pathway where caffeine appears as a blue circle



	Checked	Name	Formula	Annotation Source	Molecular Weight	RT [min]	Area (Max.)	# mzCloud Results	# KEGG Pathways	KEGG Pathways
7	☐	Caffeine	C8 H10 N4 O2	🟩🟩🟩	194.08038	1.665	1624061	4	6	

	Pathway ID	Pathway Name	# mzCloud Results	# Referenced Compounds	KEGG Compound Names	KEGG Compound Formula
1	map01100	Metabolic pathways	2	4	Caffeine	C8 H10 N4 O2
2	map01110	Biosynthesis of secondary metabolites	2	4	Caffeine	C8 H10 N4 O2
3	map00232	Caffeine metabolism	2	2	Caffeine	C8 H10 N4 O2
4	map01060	Biosynthesis of plant secondary metabolites	2	2	Caffeine	C8 H10 N4 O2
5	map01065	Biosynthesis of alkaloids derived from histidine and purine	2	2	Caffeine	C8 H10 N4 O2
6	map01120	Microbial metabolism in diverse environments	2	2	Caffeine	C8 H10 N4 O2

http://www.kegg.jp/kegg-bin/show_pathway?scale=1.0&query=&map=map00232&scale=0.82&image=%2Fshare%2Fwww%2Fmark_pathway14980038856679 Colorize: ☐

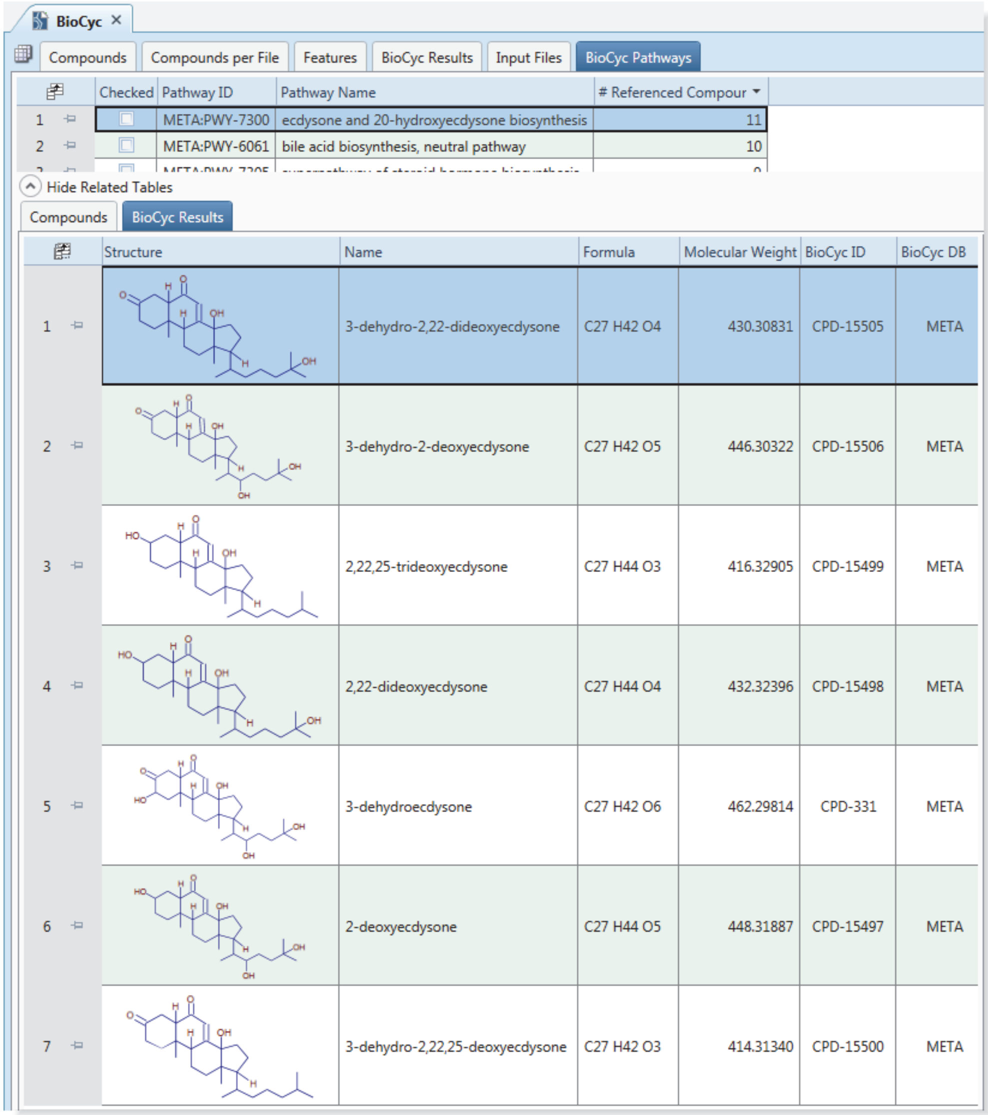
Viewing BioCyc Pathways

When the result file's processing workflow includes the Map to BioCyc Pathways Node, use the BioCyc Pathways view to view 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 panel, 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 95).

Figure 95. BioCyc Results table for the selected pathway



	Checked	Pathway ID	Pathway Name	# Referenced Compour
1	☐	META:PWY-7300	ecdysone and 20-hydroxyecdysone biosynthesis	11
2	☐	META:PWY-6061	bile acid biosynthesis, neutral pathway	10

	Structure	Name	Formula	Molecular Weight	BioCyc ID	BioCyc DB
1		3-dehydro-2,22-dideoxyecdysone	C27 H42 O4	430.30831	CPD-15505	META
2		3-dehydro-2-deoxyecdysone	C27 H42 O5	446.30322	CPD-15506	META
3		2,22,25-trideoxyecdysone	C27 H44 O3	416.32905	CPD-15499	META
4		2,22-dideoxyecdysone	C27 H44 O4	432.32396	CPD-15498	META
5		3-dehydroecdysone	C27 H42 O6	462.29814	CPD-331	META
6		2-deoxyecdysone	C27 H44 O5	448.31887	CPD-15497	META
7		3-dehydro-2,22,25-deoxyecdysone	C27 H42 O3	414.31340	CPD-15500	META

7. From the menu bar, choose **View > BioCyc Pathways**.

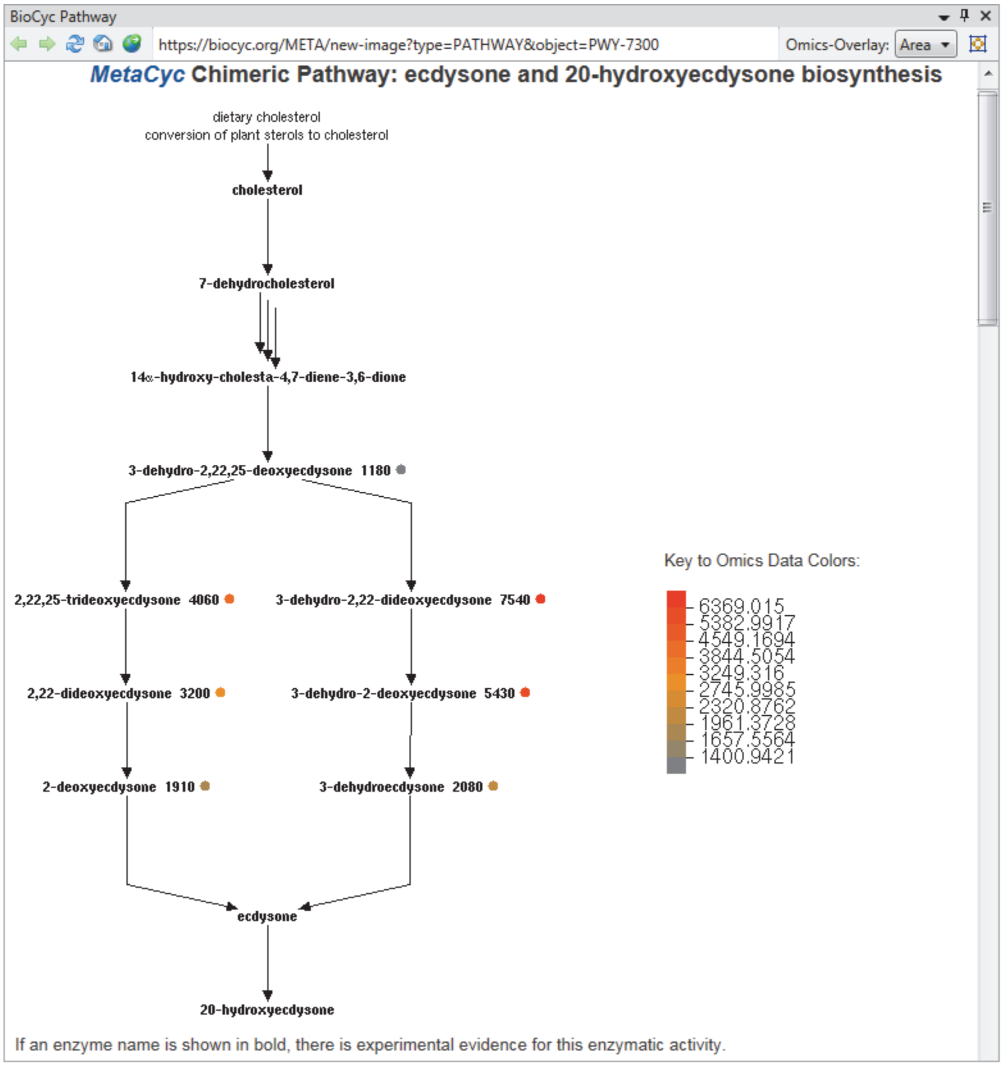
   The BioCyc Pathways view opens to the right of the result tables.

8. In the upper right corner of the view, click the **Fit Pathway to Browser** icon, ⊡.

9. In the Omics-Overlay list (to the left of the icon), select **Area**.

   Figure 96 shows a BioCyc pathway with an Area overlay.

Figure 96. BioCyc Pathways view with an Area overlay



https://biocyc.org/META/new-image?type=PATHWAY&object=PWY-7300

Omics-Overlay: Area

If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

Viewing Metabolika Pathways

Use the Metabolika Pathways view to view 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 panel, 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.

Viewing the Corrected Retention Times of the Alignment Features

When the result file's processing workflow 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.

❖ To open the Retention Time Correction view

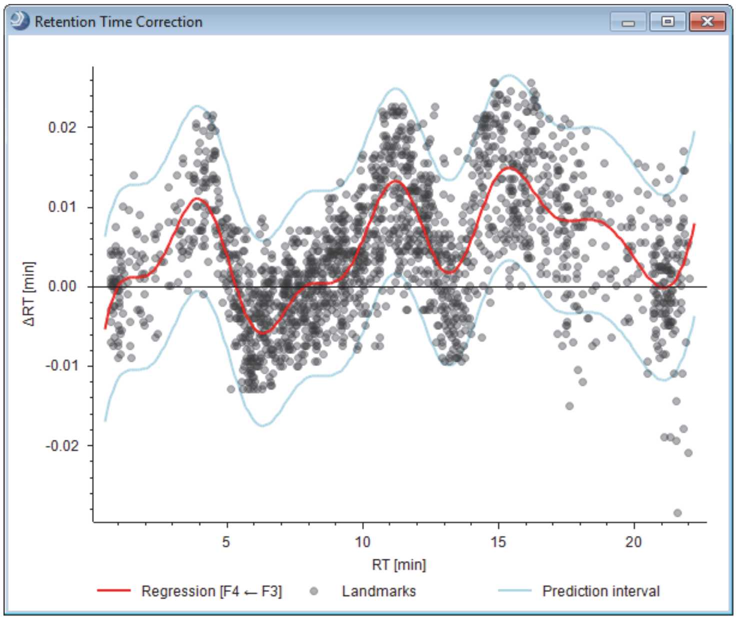
1. Open a result file for an analysis with multiple input files.
2. In the menu bar, choose **View > Retention Time Corrections**.

   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 needed:

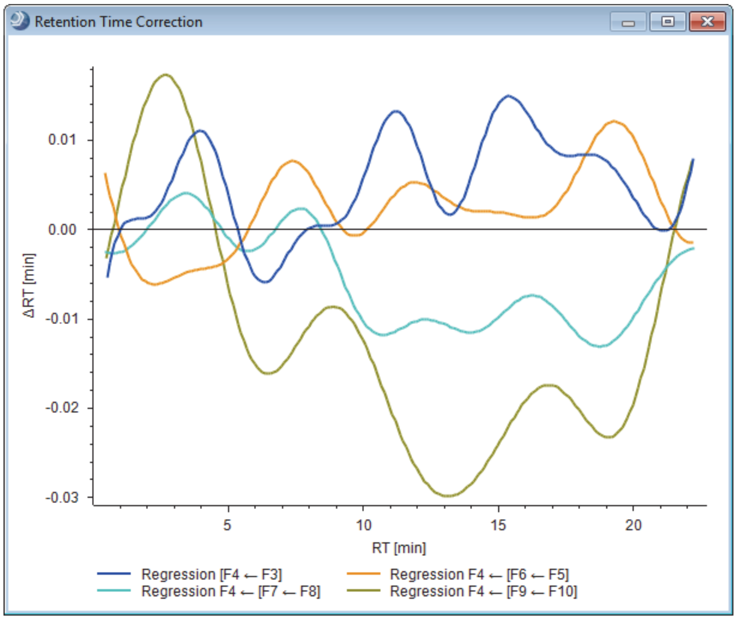
   - To view the regression curve for one input file as well as the prediction interval for the file's landmark features, select one input file (Figure 97).

Figure 97. 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 98).

Figure 98. Retention Time Correction view with regression curves for multiple input files



Viewing the QC-Based Compound Area Correction Curves

When the result file's processing workflow includes the Normalize Areas 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 detected compound in the Compounds Table across the input files.

For information about acquiring a set of raw data files with interspersed quality control samples, setting up the batch normalization criteria in the (post-acquisition) processing workflow, and setting up the Region and Language settings for the processing computer, see "Quality Control Samples for Batch Normalization" on page 39.

❖ To open the Compound Area Correction view

1. Open a result file for an analysis with batch normalization—that is, and analysis that includes QC samples and a processing workflow with the Normalize Areas node.
2. In the Compounds table, select one or more compounds.
3. From the menu bar, choose **View > Compound Area Corrections**.

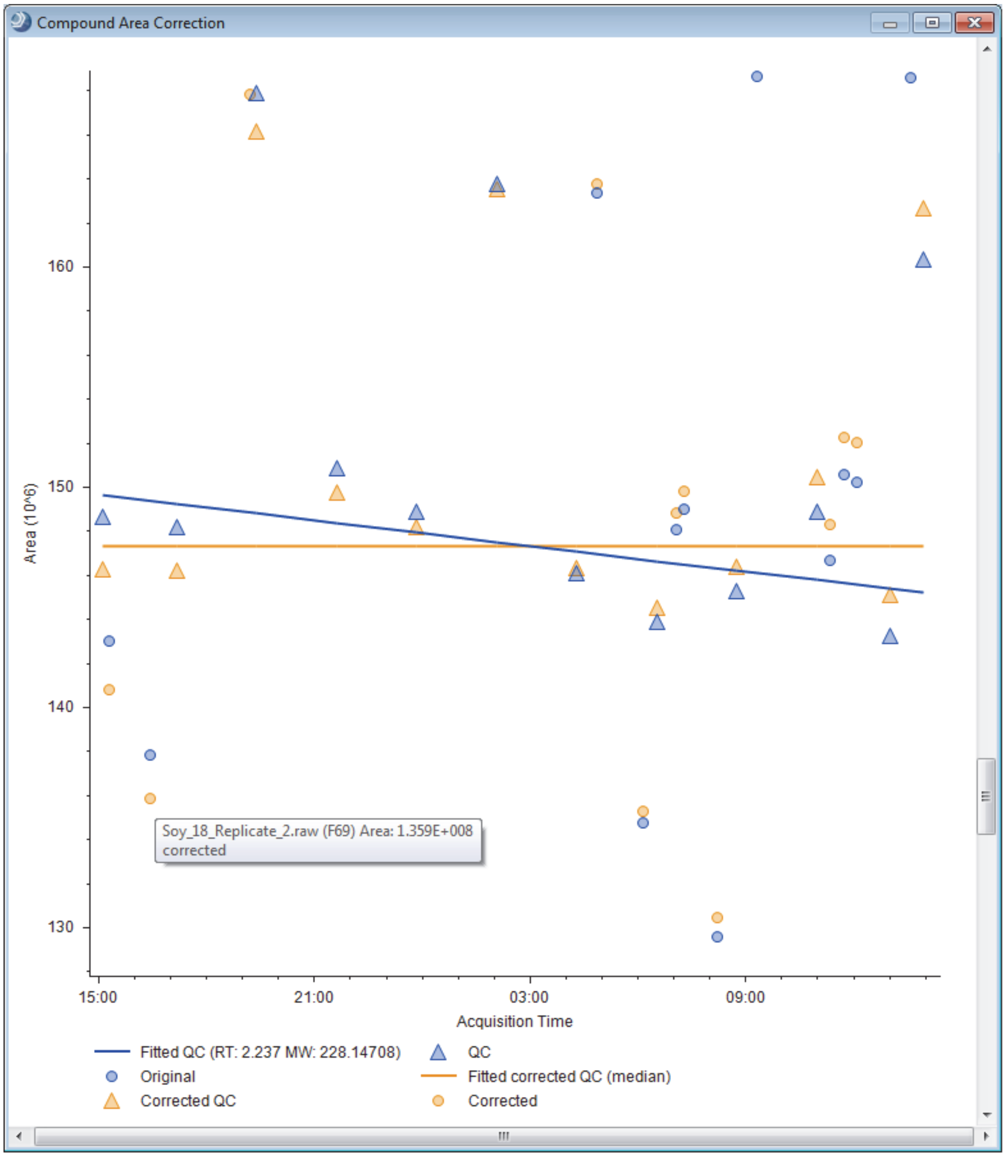
   In the default layout, the Compound Area Correction view opens to the right of the tabbed result tables. The Compound Area Correction view displays a scatter plot of the areas for the selected compound on the *y* axis against the acquisition time for each input file on the *x* axis.

   Figure 99 shows the Compound Area Corrections view for the compound selected in the Compounds table, with the following legend:

   - Blue triangles represent the original compound areas for the QC samples.
   - Orange triangles represent the corrected compound areas for the QC samples.
   - Blue circles represent the original compound areas for the non-QC samples.
   - Orange circles represent the corrected compound areas for the non-QC samples.
   - The blue line is the regression curve for the original compound areas in the QC samples.
   - The orange line is the regression curve for the corrected compound areas in the QC samples.

   Pointing to a circle or triangle displays a ToolTip with the input file name, the compound area, and the status—original or corrected.

Figure 99. Compound Area Corrections view for a selected compound



Viewing the FISh Scoring Queue

Use the FISh Scoring Queue view to view the progress of FISh scoring.

❖ To open 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:

   a. Do one of the following for compounds with assigned structures:

      - In the Compounds table or the Expected Compounds table, right-click a compound and choose **Apply FISh Scoring**.

      - In any of the following 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**.

      The Settings dialog box opens.

   b. In the Settings dialog box, make the appropriate selections and click **OK**.

   –or–

   a. Do one of the following for compounds without assigned structures:

      - In the Compounds table or the Expected Compounds table, right-click a compound and choose **Edit Compound Annotations**.

      - In a Structure Proposals table, double-click a compound.

      The Compound Annotation Editor dialog box opens.

   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**.

Running a Hierarchical Clustering Analysis

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 dendogram.

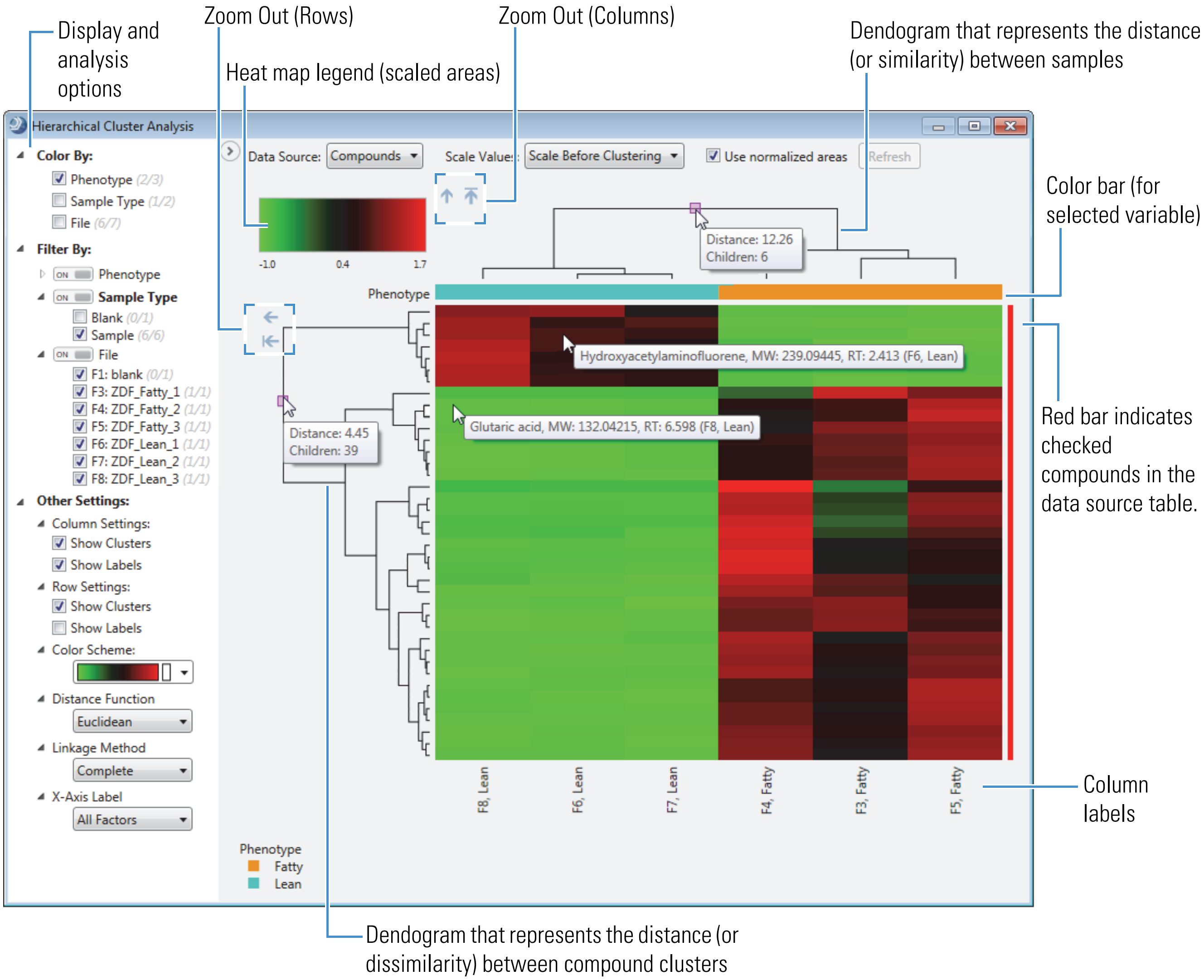
Figure 100 shows the results of a hierarchical cluster analysis for compounds detected in samples from six ZDF rats (phenotypes: Fatty and Lean).

The dendogram 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 dendogram 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 dendogram 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 100. Hierarchical cluster analysis for the compounds detected in six samples



Color By:
☑ Phenotype (2/3)
☐ Sample Type (1/2)
☐ File (6/7)

Filter By:
ON Phenotype
ON Sample Type
☐ Blank (0/1)
☑ Sample (6/6)
ON File
☑ F1: blank (0/1)
☑ F3: ZDF_Fatty_1 (1/1)
☑ F4: ZDF_Fatty_2 (1/1)
☑ F5: ZDF_Fatty_3 (1/1)
☑ F6: ZDF_Lean_1 (1/1)
☑ F7: ZDF_Lean_2 (1/1)
☑ F8: ZDF_Lean_3 (1/1)

Other Settings:
Column Settings:
☑ Show Clusters
☑ Show Labels
Row Settings:
☑ Show Clusters
☐ Show Labels
Color Scheme:
Distance Function: Euclidean
Linkage Method: Complete
X-Axis Label: All Factors

Data Source: Compounds
Scale Values: Scale Before Clustering
☑ Use normalized areas
Refresh

Distance: 12.26
Children: 6

Hydroxyacetylaminofluorene, MW: 239.09445, RT: 2.413 (F6, Lean)

Glutaric acid, MW: 132.04215, RT: 6.598 (F8, Lean)

Distance: 4.45
Children: 39

To determine how to cluster the data, the application provides a choice of commonly used distance functions and linkage methods (see Table 52 and Table 53).

Note The Heat Map supports clustering for 2 to 2000 compounds.

Follow these procedures as needed:

- To set up the hierarchical clustering analysis and display the results
- To enlarge the heat map
- To zoom in on an area of the heat map
- To zoom out of an enlarged area of the heat map
- To view information about a heat map cell
- To view the distance value for a dendogram node

❖ To set up the hierarchical clustering analysis and display the results

1. Filter the result table that you want to use as the data source. The analysis only uses the 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 dendogram above the heat map and sample labels below the heat map.

   Row Settings: Show Clusters—Displays a dendogram 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 52).
    - Under Linkage Method, select how the analysis performs the clustering analysis (Table 53).
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**.

❖ To 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.

❖ To zoom in on an area of the heat map

Drag the pointer across the rectangular area of the heat map.

❖ To zoom out of an enlarged area of the heat map

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**.

–or–

Use 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.

❖ To 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).

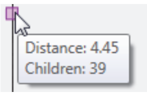
Uric acid, MW: 168.02814, RT: 1.136 (F4, Fatty)

❖ To view the distance value for a dendogram node

Point to the node.

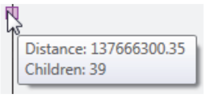
The ToolTip displays the distance value.

- For an analysis where the chromatographic peak areas are scaled before clustering, the distance values are scaled.



Distance: 4.45
Children: 39

- For an analysis where the chromatographic peaks areas are not scaled or are scaled after clustering, the distance values are not scaled.



Distance: 137666300.35
Children: 39

Table 51 describes the parameters in the Hierarchical Clustering Analysis view.

Table 51. 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 51. 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 dendogram 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 dendogram 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 dendogram 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 dendogram for the samples above the heat map; that is, this selection displays the dendogram 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 dendogram 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 51. Hierarchical Clustering Analysis view parameters (Sheet 3 of 3)

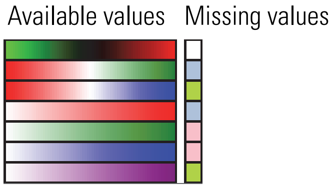
Parameter	Description
Color Schemes	Specifies the color scheme for the heat map. Default: Available values  and Missing values ☐ Selection: 
Distance Function	Specifies the distance function to use for calculating the distance between data points (see Table 52). Default: Euclidean
Linkage Method	Specifies the method to use for hierarchical clustering (see Table 53). 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 52. 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. Note, however, that the effect of outliers is dampened, since they 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 52. 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 does not take the square root.

Table 53. 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.

Running an mzLogic Analysis

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 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**.

❖ 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 form mzCloud area, the matching portions of the similar structures are highlighted in blue.

Table 54. mzLogic Analysis view parameters (Sheet 1 of 2)

Parameter	Description
ChemSpider	Opens the ChemSpider Search dialog box (see "Finding a Structure in the ChemSpider Database" on page 433).
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
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.

Table 54. mzLogic Analysis view parameters (Sheet 2 of 2)

Parameter	Description
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 Selections: mzCloud Match, Forward Coverage, or Reverse Coverage

Working with the Isotopologues Distribution Chart

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

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.

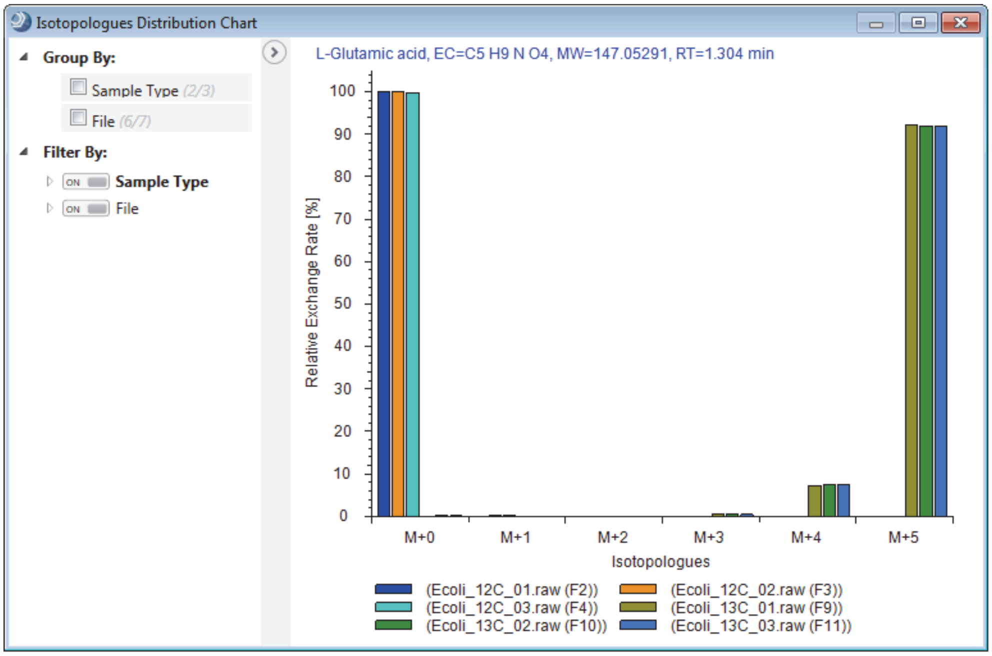
   –or–

   - 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 101). The bars are colorized by input file.

Figure 101. Isotopologues Distribution Chart with no grouping selected

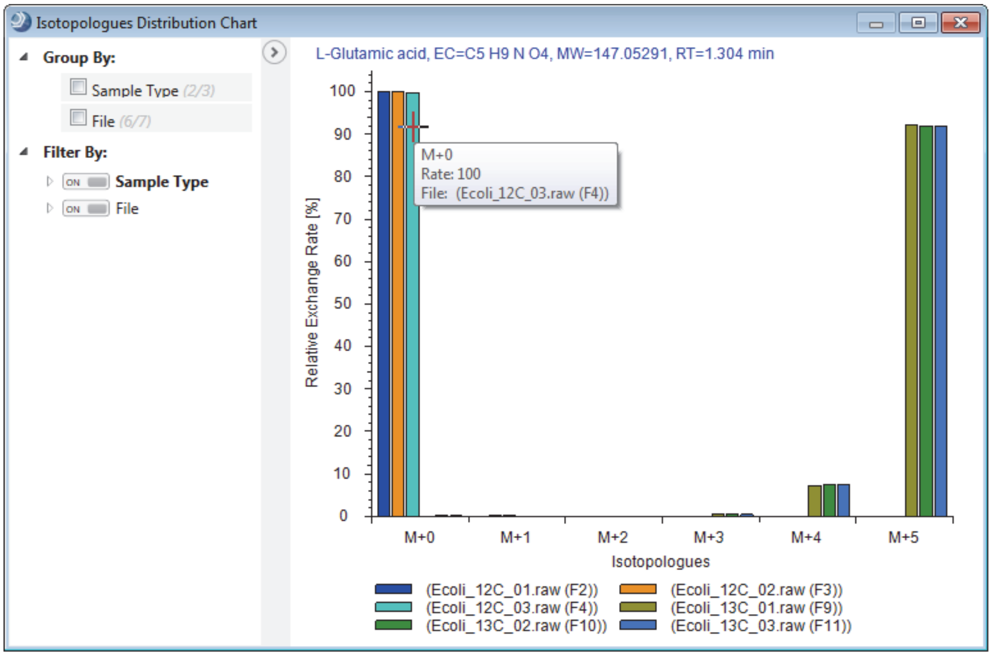


❖ To display a ToolTip for a bar

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 102. Isotopologues Distribution Chart with a Tooltip



Group By:

☐ Sample Type (2/3)

☐ File (6/7)

Filter By:

ON **Sample Type**

ON File

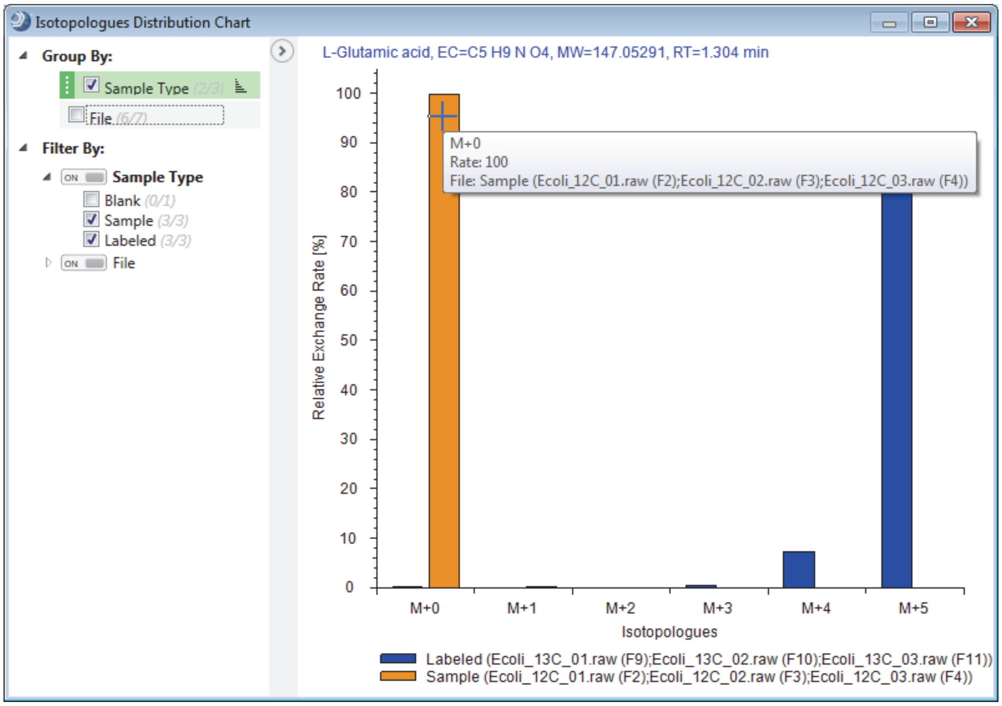
❖ To group the isotopologues by input file

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 103).

Figure 103. Isotopologues grouped by sample type



Isotopologues Distribution Chart

Group By:

☑ Sample Type (2/3)

☐ File (6/7)

Filter By:

ON Sample Type

☐ Blank (0/1)

☑ Sample (3/3)

☑ Labeled (3/3)

ON File

Reviewing the Tabular Result Data

For information about the tabular data in the result files, see these topics.

Contents

For general information about opening result files and working with the result tables, see Chapter 6, "Reviewing the Analysis Results."

Common Result Tables

You can run a targeted analysis that finds expected compounds, an untargeted analysis that detects unknown compounds, or both types of analyses with the Compound Discoverer application.

For information about the result tables that are independent of the analysis type, see these topics:

- Adducts Table (hidden)
- Chromatogram Peaks Table
- File Alignments Table
- FISh Trace Fragments Table

- Input Files Table
- Manual Peaks Table
- Merged Features Table
- Specialized Traces Table
- Structure Proposals Table (related to the Compounds and Expected Compounds tables)

Adducts Table

Use the Adducts table to view the list of adducts in the Adducts library. By default, the Adducts table is hidden (see "Showing or Hiding Result Tables" on page 153).

Chromatogram Peaks Table

Use the Chromatogram Peaks table to view information about the quality of the chromatographic peak for the detected or expected feature. The Chromatogram Peaks table is related to the Features and Expected Features tables.

Table 55 describes the columns in the Chromatogram Peaks table.

Table 55. 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. A clear check box equals False. A selected check box equals True.
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 55. Chromatogram Peaks table (Sheet 2 of 2)

Column	Description
Isotope Number (hidden)	(For chromatographic peaks detected by the Detect Compounds node) 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) 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. If even 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 peak's width and symmetry.

File Alignments Table

Use the File Alignments table to check the alignment process for each input file.

The Align Retention Times Node creates the File Alignments table.

Table 56 describes the columns in the File Alignments table.

Table 56. File Alignments table

Column	Description
Study File ID	Displays the study file ID 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 of the sample being used as a reference.
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.
#Landmarks	Displays the number of features that the analysis used to align the specified file to the reference file.
Alignment Details	Displays additional information about the alignment.
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 structure 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.

Table 57 describes the columns in the FISh Trace Fragments table.

Table 57. 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. A clear check box equals False. A selected check box equals True.
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 ion’s mass-to-charge ratio.
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 of the input file (see “Removing Input Files or Updating Their Location” on page 87.
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, use the related File Alignments Table to check the chromatographic alignment of the features in the input files.

❖ To check the chromatographic alignment of the input files

1. Click the **Input Files** tab.
2. Select a row (input file).
3. Click **Hide Related Tables** below the main tables.
4. Click the **File Alignments** tab.

5. From the menu bar, choose **View > Retention Time Corrections**.

   The Retention Time Corrections view displays the regression curve for the selected input file.

Table 58 describes the information displayed in the Input Files table.

Table 58. Input Files table

Column	Description
Study File ID	Displays the identification number assigned by the Compound Discoverer application.
File Name	Displays the file name of the input file.
Creation Date	Displays the acquisition time stamp from the data system.
RT Range [min]	Displays the data acquisition time for the raw data file.
Instrument Name	Displays the mass spectrometer type used to acquire the raw data file.
Software Revision	Displays the software version of the instrument control software used to acquire the raw data file.
Instrument Hardware (hidden)	Displays the hardware version of the Thermo Scientific mass spectrometer or analog detector used to acquire the raw data file.
Ref. File ID	Displays the reference file that the retention time alignment algorithm used to align the landmark features.
Sample Type	Displays the sample type (see "Selecting the Sample Types" on page 65).
Study Factors	Displays the study factor value (item) (see "Assigning or Selecting the Study Factor Values" on page 64).

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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 "To integrate chromatographic peaks manually" on page 192).

Table 59 describes the columns in the Manual Peaks table.

Table 59. 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 of the input file (see "Removing Input Files or Updating Their Location" on page 87).

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. Figure 10 on page 30 shows the hierarchy of the result tables for a targeted analysis, and Figure 12 on page 34 shows the hierarchy of the result tables for an untargeted analysis.

Tip When you add the Merge Features node to the processing workflow, the application automatically connects the Find Expected Compounds node and the Detect Compounds node to it. The Merge Features node consolidates the chromatographic peaks detected by these two nodes.

Table 60 describes the columns in the Merged Features table.

Table 60. 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. A clear check box equals False. A selected check box equals True.
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	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	Missing unknown component—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	No data to compare—The related node did not detect this ion.
(🟥) Red	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 60. 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
(🟥) Red	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
(🟥) Red	Multiple matches found
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" on page 324.	
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 "To integrate chromatographic peaks manually" on page 192.

For information about the Chromatograms view, see "Working with the Chromatograms View" on page 188.

❖ To view a trace in the Chromatograms view

Select the trace of interest in the Specialized Traces table.

Table 61 describes the columns in the Specialized Traces table.

Table 61. 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. A clear check box equals False. A selected check box equals True.
Study File ID	Displays the study file ID of the input file (see "Removing Input Files or Updating Their Location" on page 87.
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.

Structure Proposals Table

Use the Structure Proposals table to store custom structure proposals for the selected compound or expected compound in the result file.

For information about adding structure proposals to the table, see "Adding and Deleting Proposed Structures for a Compound" on page 158.

Table 62 describes the columns in the Structure Proposals table.

Table 62. 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. A clear check box equals False. A selected check box equals True.
Structure	Displays the structure of the compound (see “Modifying Result File Layouts” on page 145).
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 Targeted Compounds and Proposed Structures” on page 41).
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 Table
- Expected Formulas Table
- Merged Features 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. The compounds are grouped by formula, molecular weight, and retention time.

The Group Expected Compounds Node adds the Expected Compounds table to the result file. The Descriptive Statistics post-processing node adds the descriptive statistics columns, and the Differential Analysis post-processing node adds the differential analysis columns (Ratio, Log2 Fold Change, P-value, and Adjusted P-value).

Table 63 describes the columns in the Expected Compounds table.

Table 63. Expected Compounds 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. A clear check box equals False. A selected check box equals True.
Structure (hidden)	Displays the structure of the compound if available.
Name	Displays the user-specified compound name. To populate this cell, you can type a name or use the Edit Compound Annotation command.
Parent Compound	Displays the selected compound for each Generate Expected Compounds node that you connected to the Find Expected Compounds node. Before you can select a specific compound in the Generate Expected Compounds node, you must first add it to the compound library (see "Importing, Exporting, and Deleting Compounds" on page 390).
Formula	Displays the elemental formula of the parent compound and the theoretical formulas for the dealkylation and transformation products.
Molecular Weight	Displays the molecular weight (MW) of the compound calculated from the formula (neutral mass). 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.

Table 63. Expected Compounds table (Sheet 2 of 2)

Column	Description
Composition Change	Displays the composition change caused by any dealkylation or dearylation reaction, any of the user-specified transformation reactions, or both.
RT (min)	Displays the weighted average of the retention times for this chromatographic peak in the input file set.
RT Tolerance (min.)	Displays the retention time tolerance setting in the Group Expected Compounds Node.
FISh Coverage	Displays the FISh coverage score from the FISh Scoring Node (see “FISh Scoring for Targeted Compounds and Proposed Structures” on page 41).
Area (Max.)	Displays the area of the largest chromatographic peak found for this compound (Formula × MW× RT) in the sample set.
#Adducts (hidden)	Displays the number of adducts found for this compound.
#MS2 (hidden)	Displays the number of available MS2 scans for the compound. If the MS2 scans are not from an Identification Only sample, you can view them by selecting the rows in the related Expected Features table.
Area (per input file)	Displays the area for the compound (Formula × MW× RT) in each sample (input file). To display the sample names, click the expand icon to the right of the column heading.

Note See the following topics for information about the differential analysis columns and the hidden descriptive statistics columns.

- See “Descriptive Statistics Columns” on page 327 for information about the following columns: Min. Area, Median Area, Mean Area, Q1 Area, Q3 Area, Area CV%, and Area SD.
- See “Differential Analysis Columns” on page 324 for information about the following columns: Group Areas, Ratio, and Log2 Fold Change.

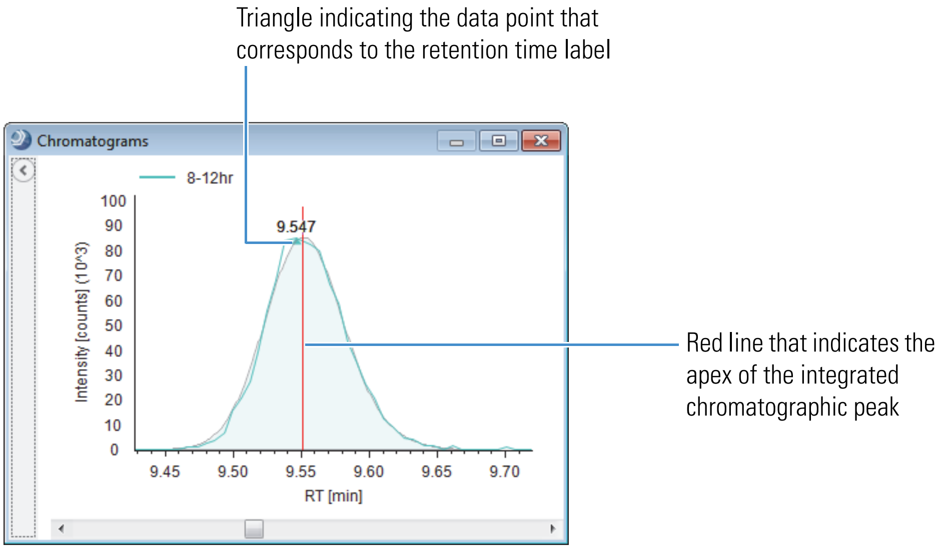
Expected Compounds per File Table

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 (Figure 104). 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. If 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 104. 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 (see Figure 10 on page 30).

Table 64 describes the columns in the Expected Compound per File table. By default, some of these columns are hidden.

Table 64. 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. A clear check box equals False. A selected check box equals True.
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.
Molecular Weight	Displays the molecular weight (MW) of the expected compound.

Table 64. Expected Compounds per File table (Sheet 2 of 3)

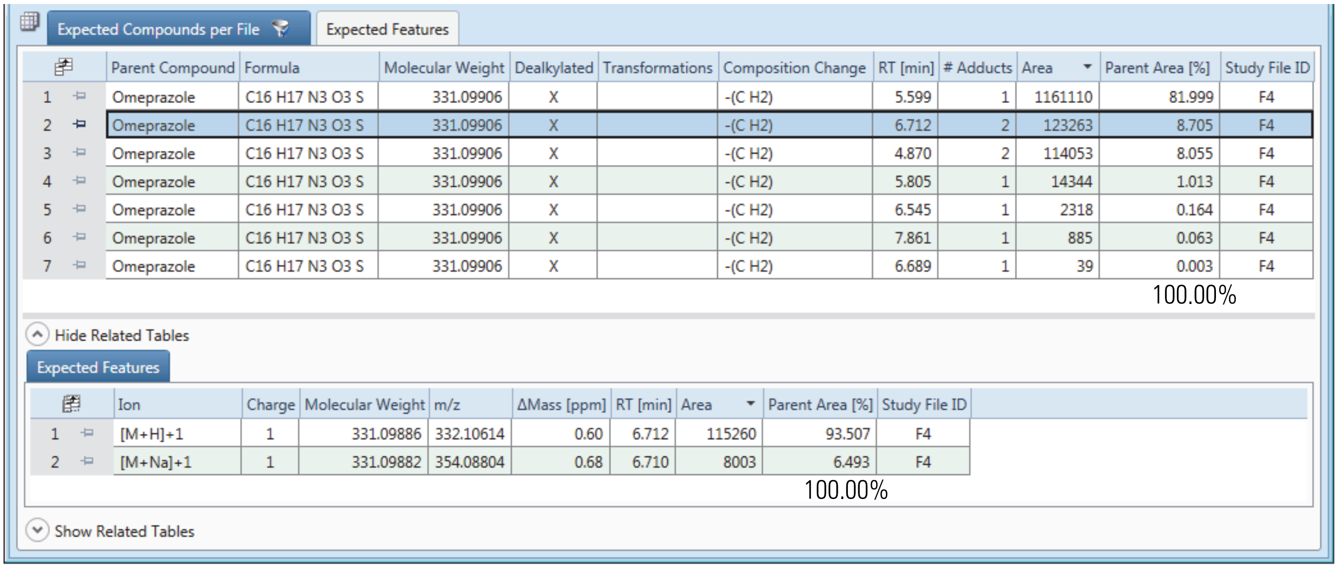
Column	Description
Dealkylated	Displays an X if the parent compound has undergone a dealkylation reaction.
Transformations	Displays the chemical transformations for the expected compound.
Composition Change	Displays the composition change caused by a dealkylation reaction, any of the user-specified transformation 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 only detects 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.

Table 64. Expected Compounds per File table (Sheet 3 of 3)

Column	Description
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). See Figure 105.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID of the input file (see "Removing Input Files or Updating Their Location" on page 87). 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.

Figure 105 shows the relationship between the chromatographic peak area for a component (parent compound, reaction set, formula, MW, and RT) and the total chromatographic peak area for all related components (the same parent compound, reaction steps, formula, and MW). A component and its related components differ only by their retention times.

Figure 105. Chromatographic peaks for the dealkylation product of omeprazole



	Parent Compound	Formula	Molecular Weight	Dealkylated	Transformations	Composition Change	RT [min]	# Adducts	Area	Parent Area [%]	Study File ID
1	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	5.599	1	1161110	81.999	F4
2	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	6.712	2	123263	8.705	F4
3	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	4.870	2	114053	8.055	F4
4	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	5.805	1	14344	1.013	F4
5	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	6.545	1	2318	0.164	F4
6	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	7.861	1	885	0.063	F4
7	Omeprazole	C16 H17 N3 O3 S	331.09906	X		-(C H2)	6.689	1	39	0.003	F4

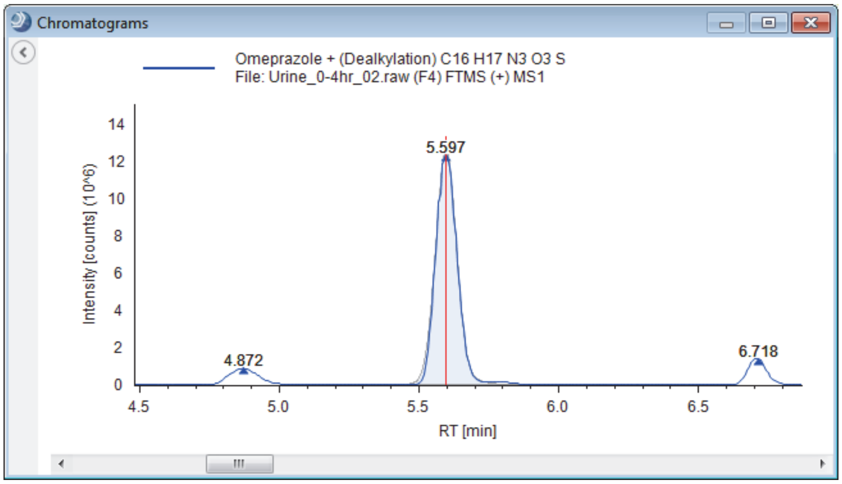
100.00%

	Ion	Charge	Molecular Weight	m/z	ΔMass [ppm]	RT [min]	Area	Parent Area [%]	Study File ID
1	[M+H]+1	1	331.09886	332.10614	0.60	6.712	115260	93.507	F4
2	[M+Na]+1	1	331.09882	354.08804	0.68	6.710	8003	6.493	F4

100.00%

Figure 106 shows the chromatographic peaks for the dealkylation product of omeprazole. By default, the Chromatograms view zooms in on the detected peak for the selected row in the Expected Compounds per File result table. Applying the Undo All Pan/Zoom shortcut menu command displays the entire range of the chromatographic run.

Figure 106. Chromatographic peaks for the dealkylation product of omeprazole



Expected Features Table

Use the Expected Features table to review the expected features (chromatographic peaks with the same *m/z* × RT dimensions) found across the input file set.

The Find Expected Compounds node creates the Expected Features table.

Table 65 describes the columns in the Expected Features table.

Table 65. Expected 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. A clear check box equals False. A selected check box equals True.
Ion	Displays the ionized form of the compound.
Charge	Displays the charge of the ion.
Molecular Weight	Displays the molecular weight of the monoisotopic neutral compound.
m/z	Displays the mass-to-charge ratio of the ion.
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.
RT [min]	Displays the chromatographic retention time of the ion.
FWHM [min]	Displays the width of the chromatographic peak at its half-height in minutes.

Table 65. Expected Features table (Sheet 2 of 2)

Column	Description
SFit [%]	Displays the similarity score between the theoretical and measured isotope patterns as a percentage.
SD	Displays the spectral distance score.
#MI	Displays the number of matched isotopes for the ion.
Intensity	Displays the maximum intensity of all the related peaks per input file.
Area	Displays the summed area of all the related peaks (same expected compound) in the current input file.
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.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID of the input file (see “Removing Input Files or Updating Their Location” on page 87).

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 (see Figure 10 on page 30).

For information about creating a targeted processing workflow, see “Targeted Workflows for Expected Compounds” on page 23.

Table 66 describes the columns in the Expected Formulas table.

Table 66. Expected Formulas 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. A clear check box equals False. A selected check box equals True.
Order (related table)	When you select the Expected Formulas table as a related table for the Transformations table, this column displays the order of the selected transformation.
Parent Compound	Displays the selected compound for each Generate Expected Compounds node that you connected to the Find Expected Compounds node. Before you can select a specific compound in the Generate Expected Compounds node, you must first add it to the compound library (see "Importing, Exporting, and Deleting Compounds" on page 390).
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

The Related Structures table is related to the Expected Features and Expected Compounds per File tables.

❖ 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 67 describes the columns in the Related Structures table.

Table 67. 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. A clear check box equals False. A selected check box equals True.
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 if the parent compound has undergone a dealkylation reaction.
Composition Change	Displays the composition change caused by any dealkylation reaction, any of the user-specified transformation reactions, or both.
Structure	Displays the related structure.

Transformations Table

Use the Transformations table to review the transformations for each formula in the Expected Formulas table. Figure 10 on page 30 shows the relationship between the Expected Formulas table and the Transformations table.

Table 68 describes the columns in the Transformations table.

Table 68. 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. A clear check box equals False. A selected check box equals True.
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 Compound Detection nodes, see these topics, listed in alphabetical order:

- Compounds Table
- Compounds per File Table
- Features Table
- Filled Gaps Table
- Labeled Features Table
- Labeled Compounds per File Table

Compounds Table

Use the Compounds table to review the unknown compounds found across the input file set.

The Group Compounds node creates the Compounds table.

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.

> **Tip** To view the related traces for each XIC trace, do the following:
>
> 1. Select a row in the Compounds table.
> 2. In the first set of related tables, select a row in the Compounds per File table.
> 3. In the second set of related tables, open the Features table.

For information about exporting the compounds as a TXT or CSV file, see "Exporting the Tabular Results to an External File" on page 174. To edit the annotations, see "Editing Compound Annotations" on page 156.

Table 69 describes the columns in the Compounds table, with the additional columns in the related Compounds tables described at the end.

Table 69. Compounds table (Sheet 1 of 8)

Column	Description
Checked	Specifies the rows that you want to display in the result table and in reports after you apply result filters. A clear check box equals False. A selected check box equals True.
Structure (hidden)	Displays the structure of the compound. The structure field is populated if any of the searches returns a structure or you edit the annotations.
Name	When the processing workflow includes a search node, this column displays the compound name from the best match in the searched databases.

Table 69. Compounds table (Sheet 2 of 8)

Column	Description
Formula	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.
Annotation Source	Displays colorized rectangles that represent 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 69. Compounds table (Sheet 3 of 8)

<table>
<tr><th>Column</th><th>Description</th></tr>
<tr><td>FISh Coverage</td><td>Displays the FISh Coverage score for a custom annotation (see “Editing Compound Annotations” on page 156 and “FISh Scoring for Targeted Compounds and Proposed Structures” on page 41).</td></tr>
<tr><td>Molecular Weight</td><td>Displays the molecular weight of the neutral compound.</td></tr>
<tr><td>RT [min]</td><td>Displays the retention time of the chromatographic peak for the compound.</td></tr>
<tr><td>RT Tolerance [min] (hidden)</td><td>Displays the retention time tolerance specified in the Group Compounds node.</td></tr>
<tr><td>Area (Max.)</td><td>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).</td></tr>
<tr><td colspan="2">The Normalize Areas Node and an input file set with QC samples add these columns to the result table: #Usable QC, RSD QC Areas [%], RSD QC Areas [%], QC Fill Status, and Norm. Areas.
For information about the batch normalization process, see “Quality Control Samples for Batch Normalization” on page 39.
To view the area correction for a compound, select the compound and choose **View > Compound Area Correction** (see “Viewing the QC-Based Compound Area Correction Curves” on page 259).</td></tr>
<tr><td># Usable QC</td><td>Displays the number of usable QC samples (see Quality Control Samples for Batch Normalization).</td></tr>
<tr><td>RSD QC Areas [%]</td><td>Displays the relative standard deviation of the peak areas for the compound across the QC samples before area correction.</td></tr>
<tr><td>RSD Corr. QC Areas [%]</td><td>Displays the relative standard deviation of the peak areas for the compound across the QC samples after area correction.</td></tr>
<tr><td>QC Fill Status (hidden)</td><td>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</td></tr>
</table>

Table 69. Compounds table (Sheet 4 of 8)

Column	Description
Norm. Areas	(Normalize Areas node) Displays the normalized peak areas for the compound in each input file.
#ChemSpider Results	(Search ChemSpider Node) 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.
#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.
#Similarity Results (hidden)	Displays the number of similarity results from the Apply mzLogic node.
#mzVault Results	(Search mzVault Node) Displays the number of matching compounds found by the mzVault search for this molecular weight. Use the related mzVault Results Table to investigate the matching compounds.
mzCloud Best Match	(Search mzCloud Node) Displays the best match score from the mzCloud identity search for the compound. Use the related mzCloud Results Table to investigate the matching compounds.
mzCloud Best Sim Match	(Search mzCloud Node) 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. With the factory default setting, this column is the rightmost column in the table. Applying the Identification layout moves this column to the right of the mzCloud Best Match column. Use the related mzCloud Results Table to investigate the matching compounds.

Table 69. Compounds table (Sheet 5 of 8)

Column	Description
#Pathways (for any of the Map to Pathway nodes)	Displays the number of pathways that include the current compound. See Map to Metabolika Pathways Node, Map to BioCyc Pathways Node, or Map to KEGG Pathways Node.
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. See Map to Metabolika Pathways Node, Map to BioCyc Pathways Node, or Map to KEGG Pathways Node.
Mass List Matches	(Search Mass Lists Node) Indicates the match status for each mass list. (🟩) Green—Single match found (🟥) Red—Multiple matches found (⬜) Gray—No matches found Use the related Mass List Search Results Table to investigate the matching compounds.
mzVault Library Matches	(Search mzVault Node) Indicates the match status for each library. (🟩) Green—Single match found (🟥) Red—Multiple matches found (⬜) Gray—No matches found Use the related mzVault Results Table to investigate the matching compounds.
Class Coverage	Displays the class coverage score for the compound. Expand the header to display the names of the compound class libraries.
#Adducts (hidden)	Displays the number of adduct ions that the analysis found for the compound.
Pattern Matches	(Pattern Scoring Node) Displays an orange rectangle when the compound matches the specified isotope pattern. Use the related Matched Patterns Table to investigate the matched isotope pattern.

Table 69. Compounds table (Sheet 6 of 8)

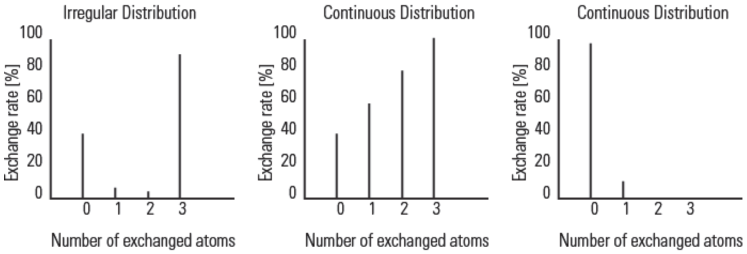
Column	Description
Labeling Status (per file)	The Analyze Labeled Compounds Node evaluates the measured isotope pattern versus the fitted isotope pattern (for the expected isotopologues) to determine the presence of contaminating masses. It also evaluates the distribution of the measured exchange rates for the expected isotopologues. 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.
Avg. Exchange	Average number of atoms exchanged for compound detected in input file.

Table 69. Compounds table (Sheet 7 of 8)

Column	Description
Rel. Exchange [%]	Average exchange relative to the maximum exchange rate. 100 × Average Exchange/Max. Exchange
MS2	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—AIF only—Only AIF scans are available.
Background	(Mark Background Compounds Node–Unknown 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.
Area (one column for each input file) (hidden)	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.
Gap Status (hidden)	(Fill Gaps node) (🟪) Purple—Indicates some missing ions (but not a full gap). (⬜) Gray—Indicates a full gap. (🟩) Green—Indicates a compound without any gap.

Table 69. Compounds table (Sheet 8 of 8)

Column	Description
Note See the following topics for information about the differential analysis columns and the hidden descriptive statistics columns. • See "Descriptive Statistics Columns" on page 327 for information about the following columns: Min. Area, Median Area, Mean Area, Q1 Area, Q3 Area, Area CV%, and Area SD. • See "Differential Analysis Columns" on page 324 for information about the following columns: Group Areas, Ratio, and Log2 Fold Change.	
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	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.
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 the Compounds table that is related to the mzCloud Search Result table.	
Scan Number	Displays the scan number of the scan that matches the reference scan in the mzCloud database.

Compounds per File Table

Use the Compounds per File table to review the compounds detected in each input file.

Table 70 describes the columns in the Compounds per File table.

Table 70. Compounds per File 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. Clear: False Selected: True
Molecular Weight	Displays the molecular weight of the neutral compound.
RT [min]	Displays the retention time at the chromatographic peak apex for the adduct ion that contributes the most area to the chromatographic peak.
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.
Max #MI	Displays the number of matching isotope peaks.
#Adducts	Displays the number of adduct ions.
Area	Displays the chromatographic peak area in counts * minutes.

Features Table

Use the Features table to review the features detected across the input file set.

The Detect Compounds Node adds the Features table to the result file.

Table 71 describes the columns in the Features table.

Table 71. 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. A clear check box equals False. A selected check box equals True.
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.

Table 71. Features table (Sheet 2 of 2)

Column	Description
RT [min]	Displays the retention time in minutes of the chromatographic peak that contains the unknown compound ion.
#MI	Displays the number of matching isotopes for the unknown compound ion.
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.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID of the input file (see "Removing Input Files or Updating Their Location" on page 87).

Filled Gaps Table

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 related to 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**.

The Gap Status column, hidden by default in the Compounds table, identifies the chromatographic peaks that the Fill Gaps node finds as Full Gap or Missing Ion peaks and those that the standard peak detection process finds as No Gap peaks.

Table 72 describes the columns in the Filled Gaps table.

Table 72. Filled Gaps 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. A clear check box equals False. A selected check box equals True.
Ion Description	Displays a description of the adduct where M is the neutral compound.
Charge	Displays the ion's charge.

Table 72. Filled Gaps table (Sheet 2 of 2)

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	The possible states for the chromatographic peak detected or redrawn by the Fill Gaps node are as follows: • (🟩) Green (Filled by Simulated Peak or 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) or the peak was simulated with a Gaussian fit algorithm. • (🟦) Blue (Filled by Spectrum Noise)—The gap was replaced with a chromatographic peak based on the spectrum noise level. • (🟧) Orange (Filled by Matching Ion)—The gap was replaced with a chromatographic peak for a matching ion.
File ID	Displays the integer that the application assigned to the input file.
Study File ID	Displays the study file ID of the input file

Labeled Features Table

Table 73 describes the columns in the Labeled Features table. The labeled features are the labeled adduct ions.

Table 73. 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. A clear check box equals False. A selected check box equals True.
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.
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.

Table 73. Labeled Features table (Sheet 2 of 2)

Column	Description
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 of the input file (see "Removing Input Files or Updating Their Location" on page 87).

Labeled Compounds per File Table

Table 74 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 74. 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. A clear check box equals False. A selected check box equals True.
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.
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.

Table 74. Labeled Compounds per File table (Sheet 2 of 2)

Column	Description
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" on page 300.
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 of the input file (see "Removing Input Files or Updating Their Location" on page 87).

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
- mzVault Results 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 75 describes the columns in the ChemSpider Results table.

Table 75. 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. A clear check box equals False. A selected check box equals True.
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.
#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.
AlogP (hidden)	Displays the AlogP value for the compound. The AlogP value is a measure of the compound’s hydrophobicity, where P is the partition coefficient.
#RSC (hidden)	Displays the number of Royal Society of Chemistry references for the compound.
XlogP (hidden)	Displays the XlogP value for the compound. The XlogP value is a measure of the compounds hydrophobicity, where P is the partition coefficient.
Additional columns in the related ChemSpider Results table	
Compound Match	Indicates the match status between the current item and the assigned compound annotation. For color-coding information, see “Annotation Source” on page 296.

Table 75. ChemSpider Results table (Sheet 2 of 2)

Column	Description
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.

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 76 describes the columns in the Mass List Search Results table.

Table 76. Mass List Search 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. A clear check box equals False. A selected check box equals True.
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 (if available) of the compound in the mass list.
Structure	Displays the structure (if available) of the compound in the mass list.
Name	Displays the name of the compound in the mass list.
Annotation	Displays 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	

Table 76. Mass List Search Results table (Sheet 2 of 2)

Column	Description
Compound Match	Indicates the match status between the current item and the assigned compound annotation. For color-coding information, see "Annotation Source" on page 296.
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.

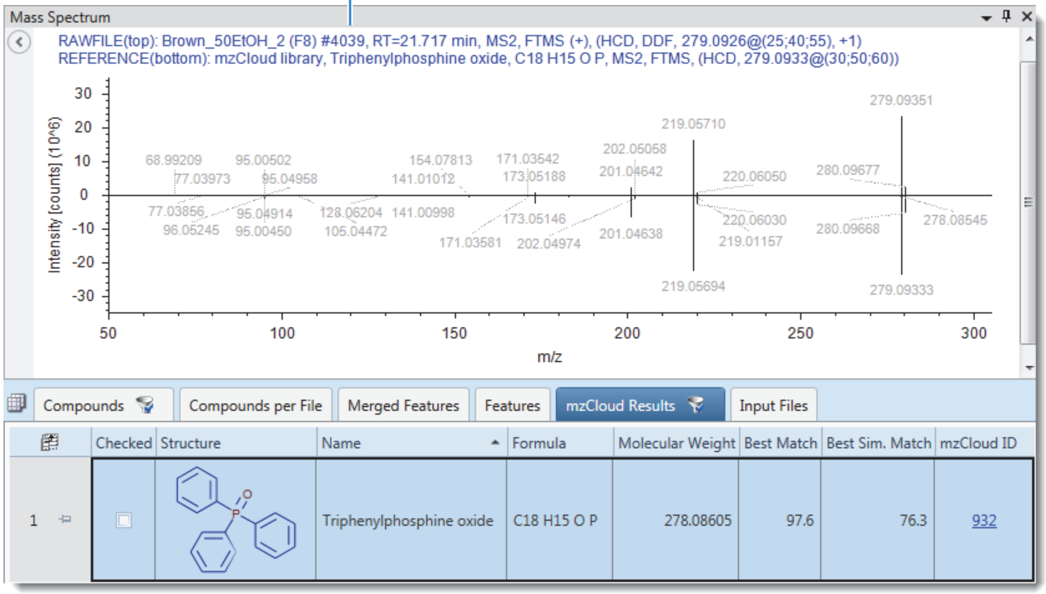
mzCloud Results Table

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. Figure 107 shows the search result for a fragmentation scan acquired with stepped collision energies.

Figure 107. Mass Spectrum view with a mirror plot



Scan information

RAWFILE(top): Brown_50EtOH_2 (F8) #4039, RT=21.717 min, MS2, FTMS (+), (HCD, DDF, 279.0926@(25;40;55), +1)
REFERENCE(bottom): mzCloud library, Triphenylphosphine oxide, C18 H15 O P, MS2, FTMS, (HCD, 279.0933@(30;50;60))

	Checked	Structure	Name	Formula	Molecular Weight	Best Match	Best Sim. Match	mzCloud ID
1	☐		Triphenylphosphine oxide	C18 H15 O P	278.08605	97.6	76.3	932

Table 77 describes the columns in the mzCloud Results table.

Table 77. 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. A clear check box equals False. A selected check box equals True.
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.
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 (0–100%) between the best fragmentation scan for a compound (across the input files) and the matching mzCloud spectrum (mzCloud ID). The related Compounds tables lists the scan number of the best fragmentation scan.
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 number for the matching compound. Clicking this link opens the mzCloud database to the matching compound's reference spectrum.
Name	Displays the mzCloud name for the matching compound.
KEGG ID	Displays the KEGG ID for the compound in the KEGG database.
Compound Classes	Displays the mzCloud compound classes that include the compound.
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 "Annotation Source" on page 296.
Searched with ΔMass [Da]	Displays the maximal difference between the theoretical and measured mass in Da.
Intensity Threshold	Displays the relative intensity threshold for the search spectrum.
ΔMass [Da]	Displays the difference between the theoretical mass of the matching compound and the observed mass of the unknown compound in daltons.

Table 77. mzCloud Results table (Sheet 2 of 2)

Column	Description
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.
Type	Displays the search type: Identify or Similarity.
Scan Number	Displays the scan number from the input files that contains the best matching fragmentation spectrum.
Match	Displays the match value (0–100%) between the specified scan number from the input files and the matching spectrum in the mzCloud database.

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 78 describes the columns in the mzVault Results table.

Table 78. 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. A clear check box equals False. A selected check box equals True.
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 78. 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 "Annotation Source" on page 296.
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.

Predicted Compositions Table

The Predicted Compositions table is related to the Compounds 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 79 describes the columns in the Predicted Compositions result table.

Table 79. Predicted Compositions 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. A clear check box equals False. A selected check box equals True.
Compound Match	Displays whether the predicted composition matches the currently assigned compound annotation. (🟥) Red rectangle—No Match (🟩) Green rectangle—Full Match
Formula	Displays the predicted elemental composition.
Molecular Weight	Displays the molecular weight.
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.
SD (hidden)	Displays the spectral distance score.

Table 79. Predicted Compositions table (Sheet 2 of 2)

Column	Description
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. $\frac{\text{Summed intensity of the matching isotope peaks} \times 100}{\text{Summed intensity of the theoretical isotope pattern}}$ 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.
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. $\frac{\text{Summed intensity of the matching isotope peaks} \times 100}{\text{Summed intensity of all the peaks in the measured pattern}}$ **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.

For more information, see “Viewing BioCyc Pathways” on page 254.

Table 82 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 detected by the untargeted search.

Table 80. BioCyc Pathways 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. A clear check box equals False. A selected check box equals True.
Pathway ID	Displays the identification number of the mapped BioCyc pathway.
Pathway Name	Displays the name of the mapped BioCyc pathway that includes at least one compound in the Compounds table.
#Referenced Compounds	Displays the number of detected compounds that are referenced in the identified BioCyc pathway.
#Identified Compounds	Displays the number of compounds in the referenced pathway that the analysis detected in the input file set. To view the list of detected compounds, select a pathway and open the related BioCyc Results table.
Related BioCyc Pathways table only	
BioCyc Compound IDs	Displays a list of the BioCyc compound IDs in ascending order from left to right.
BioCyc Compound Names (related table)	Displays a list of the BioCyc compound names.
BioCyc Compound Formulas (related table)	Displays a list of the BioCyc compound formulas.

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 81 describes the columns in the BioCyc Results table.

Table 81. BioCyc Results 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. A clear check box equals False. A selected check box equals True.
Compound Match (related table)	Indicates the match status between the current item and the assigned compound annotation. For color-coding information, see "Annotation Source" on page 296.
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.
Max. ΔMass [Da] (related table)	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] (related table)	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.
BioCyc ID (related table)	Displays the BioCyc identification number for the compound.
BioCyc DB (related table)	Displays the name of the BioCyc database that mapped the compound.
mzLogic Score (related table)	Displays the mzLogic score provided by the Apply mzLogic 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 82 describes the columns in the KEGG Pathways table. The KEGG Pathways table lists all the KEGG pathways that include at least one of the compounds detected by the untargeted search.

Table 82. KEGG Pathways 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. A clear check box equals False. A selected check box equals True.
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	Displays the number of detected compounds that are referenced in the identified KEGG pathway.
#Identified Compounds	Displays the number of different KEGG compound IDs.
#mzCloud Results	Displays the number of compounds in the identified KEGG pathway that the mzCloud search identified.
KEGG Compound IDs (related table)	Displays a list of the KEGG compound IDs in ascending order from left to right.
KEGG Compound Names (related table)	Displays a list of the KEGG compound names.
KEGG Compound Formulas (related table)	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 83 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 detected by the untargeted search. The related table displays the search results for the selected compound in the Compounds table.

Table 83. Metabolika Pathways 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. A clear check box equals False. A selected check box equals True.
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.
#Referenced Compounds	Displays the number of detected compounds that are referenced in the identified Metabolika pathway.
#Compounds in Pathway	Displays the total number of compounds in the pathway.
#Identified Compounds	Displays the number of different Metabolika compound IDs.
Metabolika Compound IDs (related table)	Displays a list of the Metabolika compound IDs in ascending order from left to right.
Metabolika Compound Names (related table)	Displays a list of the Metabolika compound names.
Metabolika Compound Formula (related table)	Displays the Metabolika compound formula.

Metabolika Results Table

Use the main Metabolika Results table to review the compounds found in the mapped Metabolika pathways. Use the related Metabolika results table to review the results for a specific compound.

The Map to Metabolika Pathways Node creates the Metabolika Results table.

Table 81 describes the columns in the Metabolika Results table.

Table 84. Metabolika Results 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. A clear check box equals False. A selected check box equals True.
Compound Match (related table)	Displays whether the Metabolika pathway structure is a full or partial match for the selected compound. (🟩)—Full Match (🟧)—Partial Match
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.
Max. ΔMass [Da] (related table)	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] (related table)	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.

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

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.

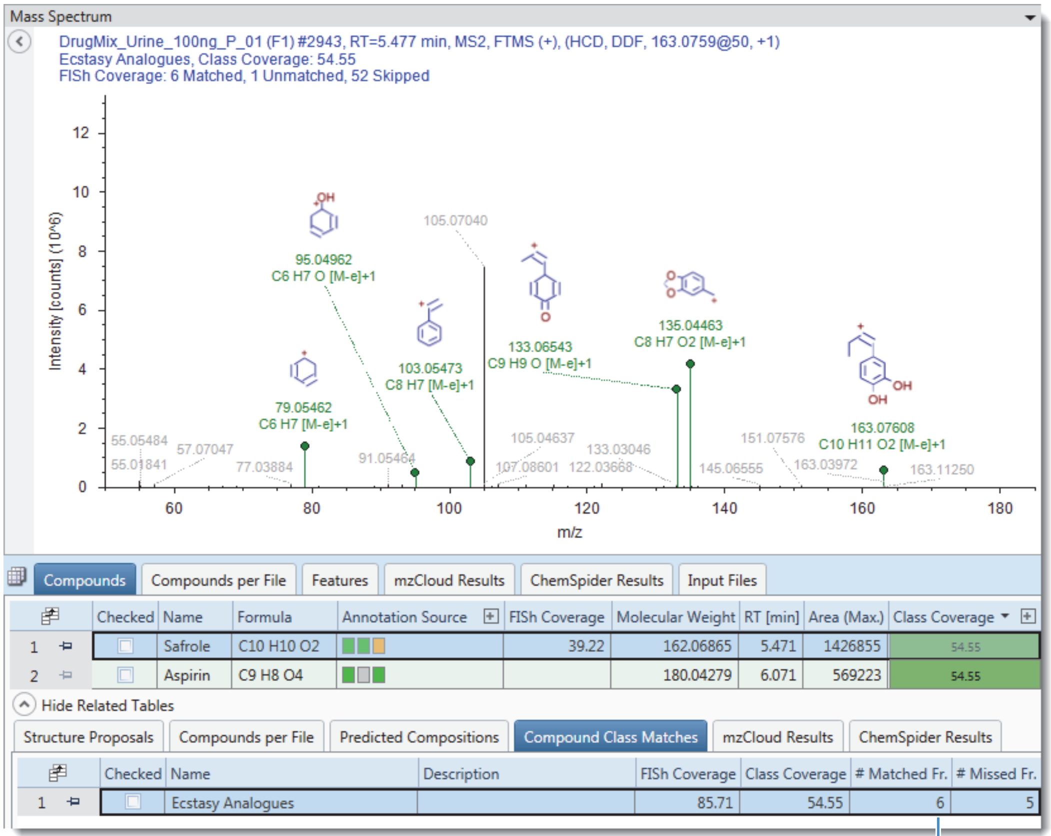
Table 85 describes the columns in the Compound Class Matches table.

Table 85. 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. A clear check box equals False. A selected check box equals True.
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 Targeted Compounds and Proposed Structures" on page 41).
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 108 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 108. Fragmentation scan and compound class match result for a detected compound



DrugMix_Urine_100ng_P_01 (F1) #2943, RT=5.477 min, MS2, FTMS (+), (HCD, DDF, 163.0759@50, +1)
Ecstasy Analogues, Class Coverage: 54.55
FISh Coverage: 6 Matched, 1 Unmatched, 52 Skipped

		Checked	Name	Formula	Annotation Source	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)	Class Coverage
1	⊨	☐	Safrole	C10 H10 O2	🟩🟩🟧	39.22	162.06865	5.471	1426855	54.55
2	⊨	☐	Aspirin	C9 H8 O4	🟩⬜🟩		180.04279	6.071	569223	54.55

		Checked	Name	Description	FISh Coverage	Class Coverage	# Matched Fr.	# Missed Fr.
1	⊨	☐	Ecstasy Analogues		85.71	54.55	6	5

#Matched fragments

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 (see Pattern Scoring Node).

Table 86 describes the columns in the Matched Patterns table.

Table 86. 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. A clear check box equals False. A selected check box equals True.
Name	Displays the name or chemical formula of the compound.

Table 86. 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. $\frac{\text{Summed intensity of the matching isotope peaks} \times 100}{\text{Summed intensity of the theoretical isotope pattern}}$ 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 of the input file (see “Removing Input Files or Updating Their Location” on page 87).

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, and 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 87 describes the columns from a differential analysis.

Table 87. Differential analysis columns (Sheet 1 of 3)

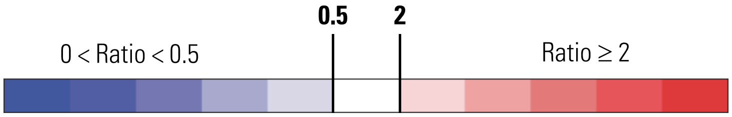
Column	Description
Group Areas	Displays the median chromatographic peak area for the compound in the sample group. To display the group names, click the expand icon to the right of the column heading. When the compound is not found, the cells have a gray background. The Differential Analysis node bins 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: 🟩
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.
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. 

Table 87. Differential analysis columns (Sheet 2 of 3)

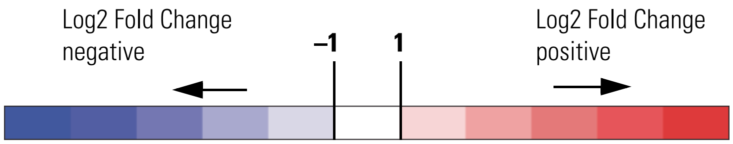
Column	Description
Log2 Fold Change	Displays the fold change (ratio) in the log base 2 scale. A log2 fold change of Infinity has an orange background (Infinity). If the ratio is 0 (0/X) or –Infinity in the Log2 format, the background color is a dark purple (–Infinity). The cells for compounds with log2 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. 
P-value	Displays the p-value for the sample group calculated by running the Tukey HSD test (posthoc) 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.

Table 87. Differential analysis columns (Sheet 3 of 3)

Column	Description
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 88 to the Compounds Table and Expected Compounds Table. The descriptive statistics columns are hidden by default.

Table 88. Descriptive statistics columns (Sheet 1 of 2)

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.

Table 88. Descriptive statistics columns (Sheet 2 of 2)

Column	Description
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.

9

Creating and Printing Reports

This chapter describes how to create, preview, and print reports. You can use the standard report templates provided with the application or you can create your own custom report templates.

Contents

Reporting Workflow

The following flowchart shows the reporting workflow (Figure 109 and Figure 110).

Figure 109. Reporting workflow (page 1)

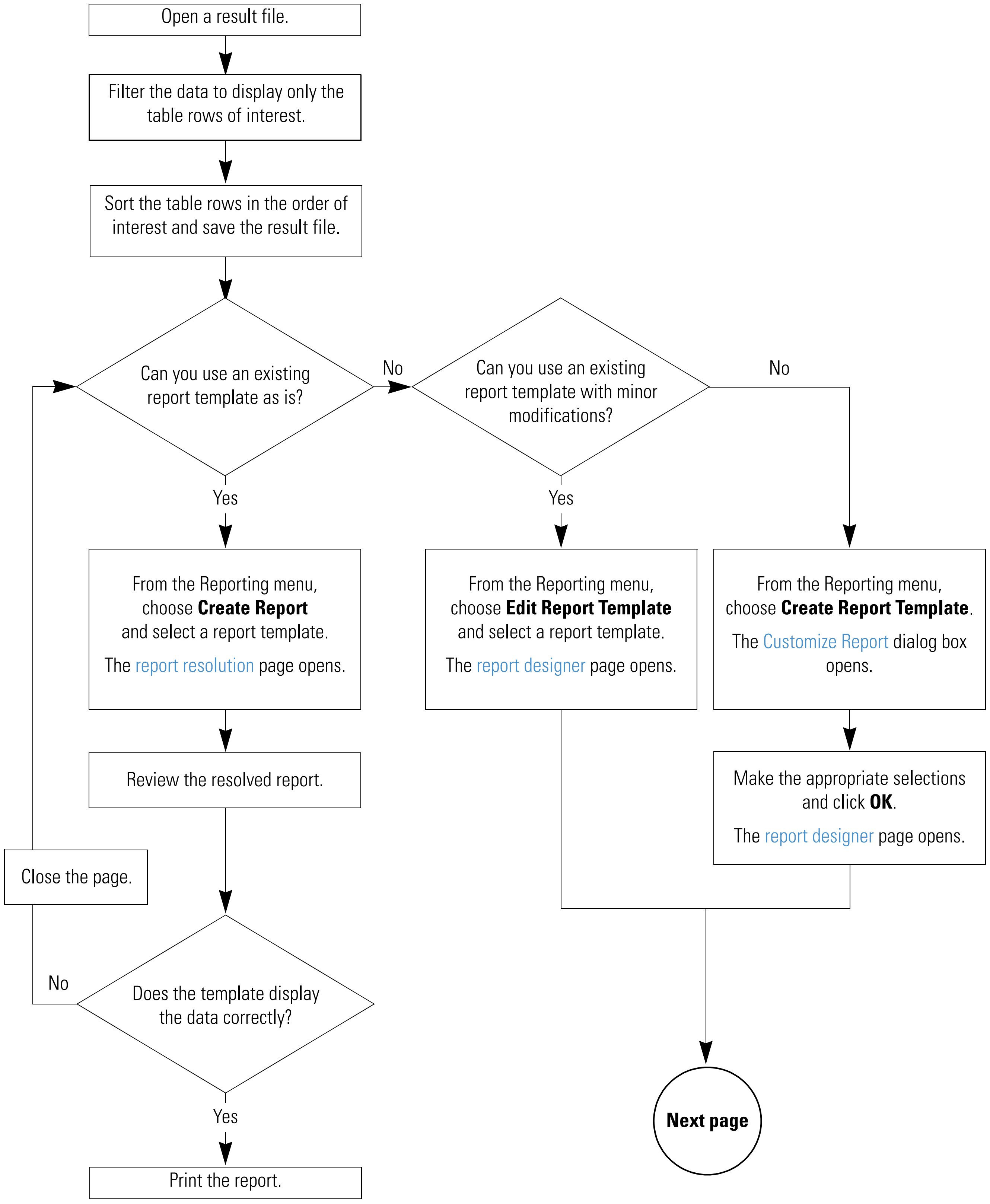
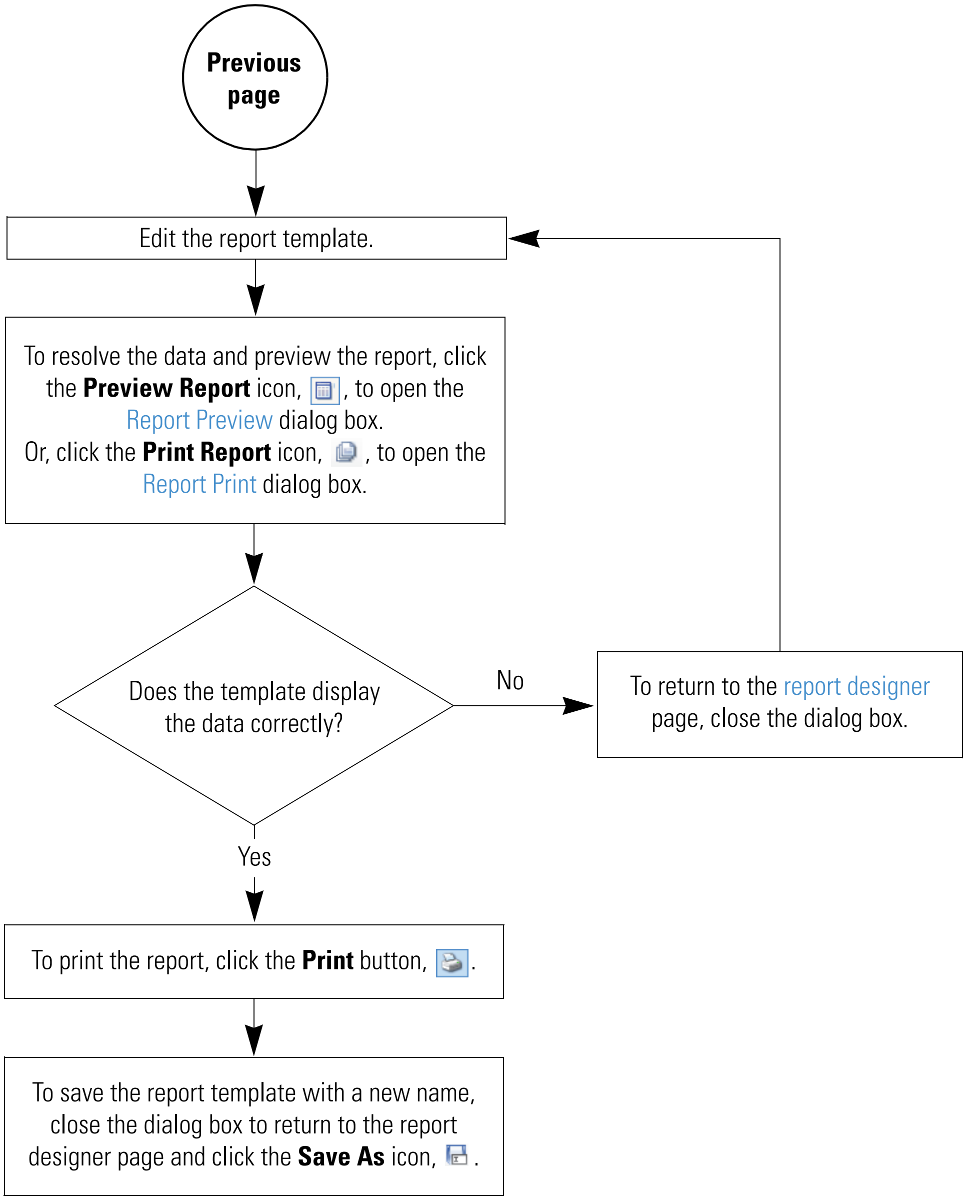


Figure 110. Reporting workflow (page 2)



Generating 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 information about creating new report templates, see “Creating a Report Template with the Customize Report Dialog Box” on page 334.

The application comes with the following eight defined report templates:

- Compounds No Graphs A4.cdReportTemplate
- Compounds with Graphs A4.cdReportTemplate
- Expected Compounds No Graphs.cdReportTemplate
- Expected Compounds per File No Graphs A4.cdReportTemplate
- Expected Compounds per File with Graphs A4.cdReportTemplate
- Expected Compounds w Structures No Graphs
- Expected Compounds w Structures with Graphs A4.cdReportTemplate
- Expected Compounds with Graphs

You can find these report templates in the following folder:

C:\Users\Public\Public Documents\Thermo\Compound Discoverer 3.0\Common Templates\ReportTemplates

❖ To preview and print a report by opening an existing report template

1. Open a result file (see “To open a result file from the application window” on page 142).

   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.

   For information about filtering the data, see “Using Result Filters for Data Reduction and Creating Filter Sets” on page 162.

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.

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

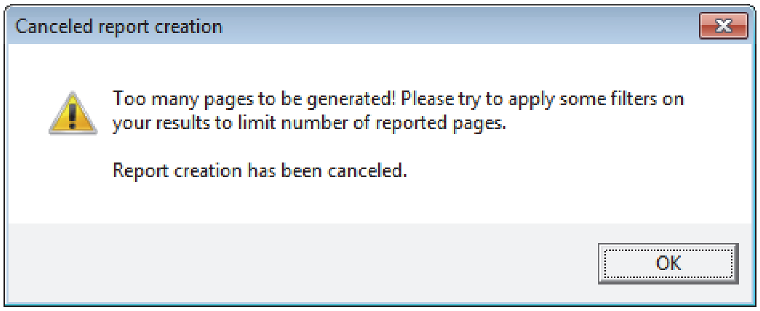
   As the application resolves the data with the report template, the following icon displays the progress.

   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.

   Whether the application displays the pages as it renders them depends on whether the report template contains any ReportInfo items. 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. If the selected template does not contain ReportInfo items, the application displays the pages as it renders them. The standard reports provided with the application do not contain ReportInfo items nor do unedited report templates that you create by using the Customize Report dialog box. For more information about the ReportInfo item, see "ReportInfo" on page 364.

   If the report contains too many pages, the application cancels report generation, and the following message box appears.

   Canceled report creation

   Too many pages to be generated! Please try to apply some filters on your results to limit number of reported pages.

   Report creation has been canceled.

5. Review the contents of the report.

6. On the report resolution page, click the **Print** icon, 🖨, in the toolbar to print the report.

   The Print dialog box opens.

7. 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.

8. If you are not printing on A4 paper, change the printer setting.
9. Click **OK** to print the report.

Creating a Report Template with the Customize Report Dialog Box

This topic describes how to create a new report template by using the Customize Report dialog box where you select the following:

- 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
- Basic appearance of the report, including whether the table columns are displayed from left to right or from top to bottom
- Paper type (PaperKind parameter)
- Page orientation
- Logo image

Tip To quickly select an item in a list in this dialog box, type the first letter of that item.

Once you make these selections and close the Customize Report dialog box, the report designer page opens. Use the report designer page to modify the appearance of the report. For information about using this page, see "Editing an Existing Report Template" on page 344.

To work with the Customize Report dialog box, follow these procedures:

- To open the Customize Report dialog box
- To select the main table
- To select the columns, graphs, and related tables
- To draw a line above the table data
- To transpose the tabular data from columns to rows
- To indent a related table
- To select a color scheme for a report table
- To modify the current color scheme or to add or remove color schemes from the list
- To select the size of the paper
- To select the page orientation

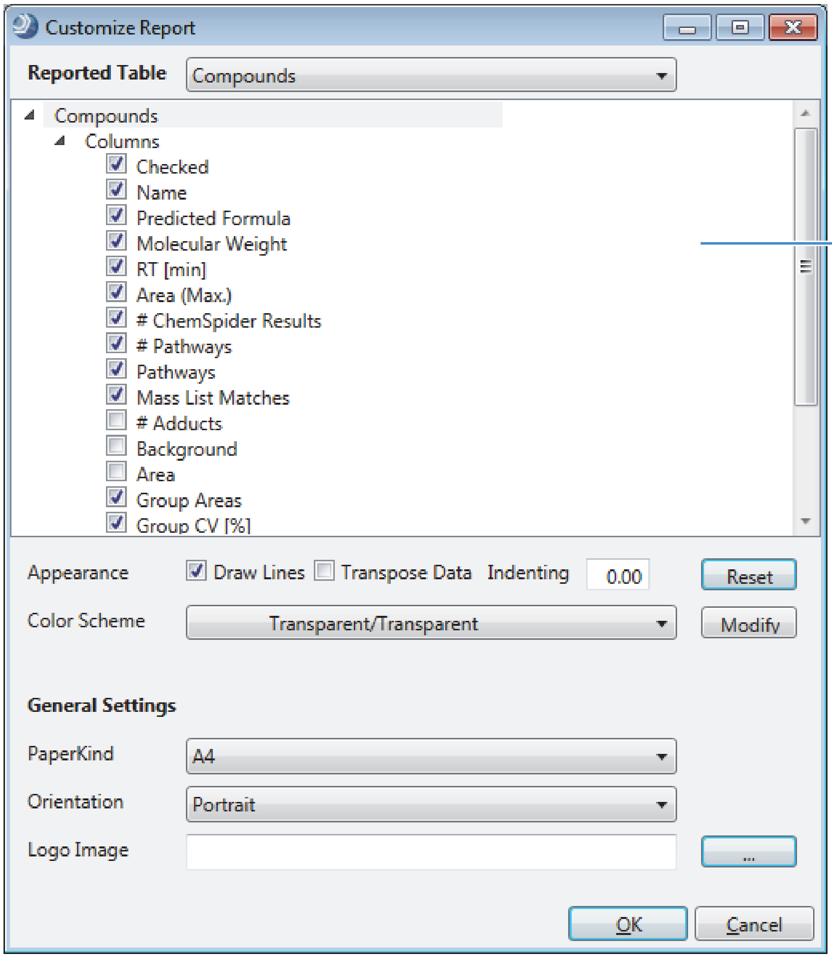
- To select the logo image
- To apply the settings and close the Customize Report dialog box

❖ To open the Customize Report dialog box

1. Open a result file.
2. From the menu bar, choose **Reporting > Create Report Template**, or in the toolbar, click the **Create a New Report Template** icon, .

   The Customize Report dialog box opens (Figure 111).

   Figure 111. Customize Report dialog box



Reported Table Compounds

- Compounds
  - Columns
    - ☑ Checked
    - ☑ Name
    - ☑ Predicted Formula
    - ☑ Molecular Weight
    - ☑ RT [min]
    - ☑ Area (Max.)
    - ☑ # ChemSpider Results
    - ☑ # Pathways
    - ☑ Pathways
    - ☑ Mass List Matches
    - ☐ # Adducts
    - ☐ Background
    - ☐ Area
    - ☑ Group Areas
    - ☑ Group CV [%]

Appearance ☑ Draw Lines ☐ Transpose Data Indenting 0.00

Color Scheme Transparent/Transparent

General Settings

PaperKind A4

Orientation Portrait

Logo Image

List of
data items

❖ To select the main table

In the Reported Table list at the top of the dialog box, select the main result table for the report.

A list of data items for the selected table appears. By default, the list of columns for the main table is open and most of the column check boxes are selected.

❖ To select the columns, graphs, and related tables

1. Under the selected table name, click each expand icon, ▷, to open these sections as needed:
   - Columns
   - Graphs
   - Related Tables
2. 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.

> **Tip** Thermo Fisher Scientific recommends that you select the Max Area (…) and Area Ratio (…) columns. With these selections, the report automatically displays *n* columns of area data, where *n* = the number of input files included in the result file.

❖ To draw a line above the table data

To draw a separator line above the column headers for the tables, 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

❖ To transpose the tabular data from columns to rows

1. In the data item list, select the table that you want to transpose.
   - 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.

   Each time you select a table, the application clears the Transpose Data check box.
2. Select 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	Column 4 label	Column 5 label
Data text box	Data text box	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
Column 4 label	Data text box
Column 5 label	Data text box

❖ To indent a related table

1. Select the related table in the expanded list of data items.
2. 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

❖ To select a color scheme for a report table

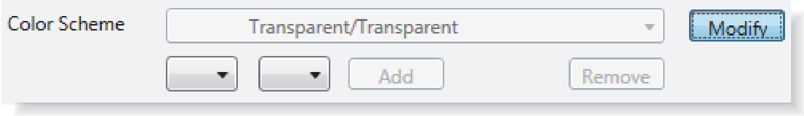
1. In the report item list, select the table of interest, for example, the main table or one of the related tables.
2. In the Color Scheme list, select one of the available color schemes.

   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. To undo the selection, click **Reset**.

❖ To modify the current color scheme or to add or remove color schemes from the list

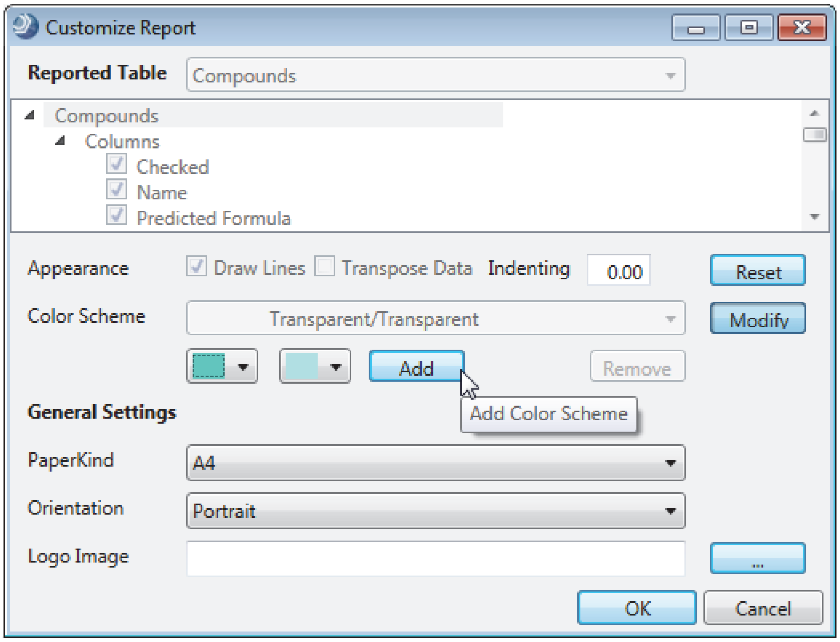
1. Click **Modify**.

   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.



Color Scheme: Transparent/Transparent

2. From the color lists, select one or two background colors, and then click **Add**.



Reported Table: Compounds

- Compounds
  - Columns
    - ☑ Checked
    - ☑ Name
    - ☑ Predicted Formula

Appearance: ☑ Draw Lines ☐ Transpose Data Indenting: 0.00

Color Scheme: Transparent/Transparent

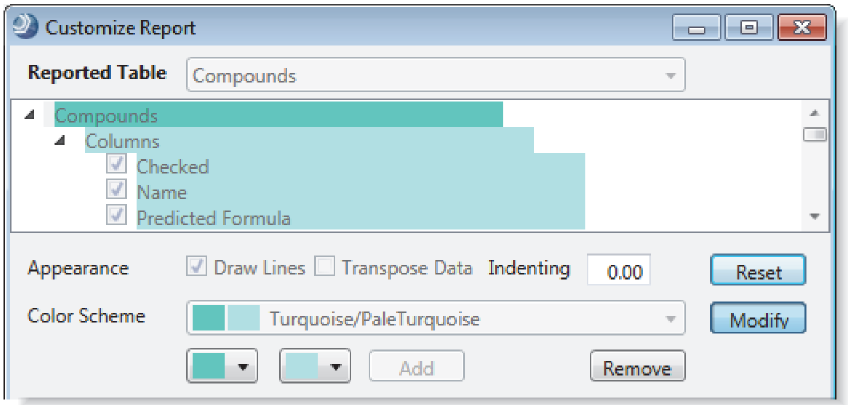
General Settings

PaperKind: A4

Orientation: Portrait

Logo Image:

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 activates the Remove button.



Reported Table: Compounds

- Compounds
  - Columns
    - ☑ Checked
    - ☑ Name
    - ☑ Predicted Formula

Appearance: ☑ Draw Lines ☐ Transpose Data Indenting: 0.00

Color Scheme: Turquoise/PaleTurquoise

> **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 3.0\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.

3. 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.

❖ To select the size of the paper

In the PaperKind list, select the appropriate paper size.

For information about changing the paper size for an existing report template, see "Report Designer Report Template Settings" on page 379.

❖ To select the page orientation

In the Orientation list, select the appropriate page orientation.

For information about changing the paper orientation for an existing report template, see "Report Designer Report Template Settings" on page 379.

❖ To select the logo image

1. Next to the Logo Image box, click the browse icon, ….
2. In the Open Image File dialog box, select the graphic file for the logo and then click **Open**.

❖ To apply the settings and close the Customize Report dialog box

Click **OK**.

Your selections appear on the report designer page.

The tab format for the report designer page is as follows:

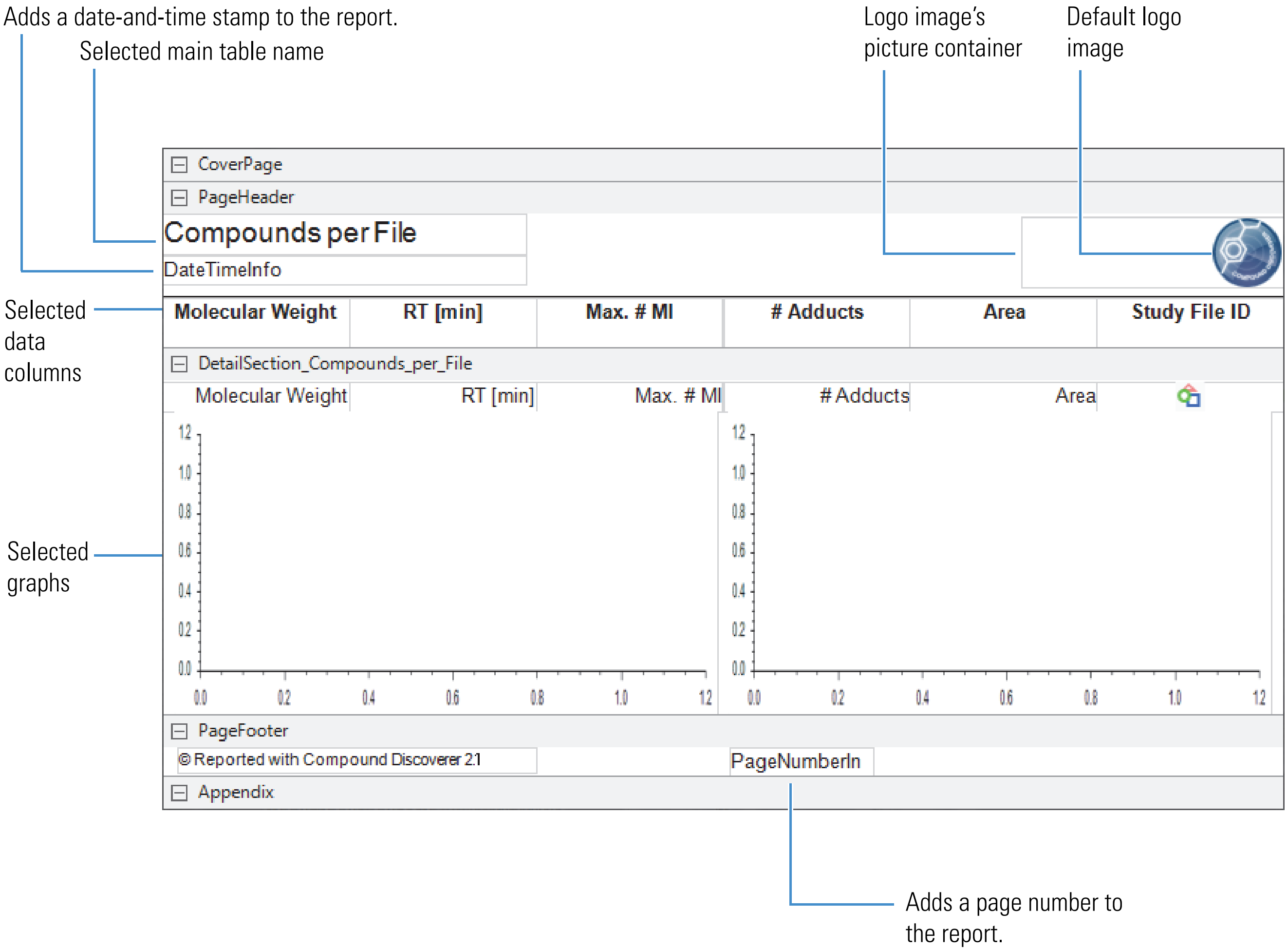
Main Result Table

When you create a report by using the Customize Report dialog box, the application adds the following additional TextBox design items to the report template: DateTimeInfo in the Page Header section and PageNumberInfo in the Page Footer section. For information about editing the date-and-time stamp, see "To change the format of the date-and-time stamp" on page 346.

Figure 112 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 needed (see "To change the logo image" on page 346).

> **Tip** For best results, transpose the data by selecting the Transpose Data check box for result tables with a large number of data columns. Otherwise, you might need to resize the data columns to fit the page.

Figure 112. Report template with data from the Compounds per File table


Adds a date-and-time stamp to the report.

Selected main table name

Logo image's picture container

Default logo image

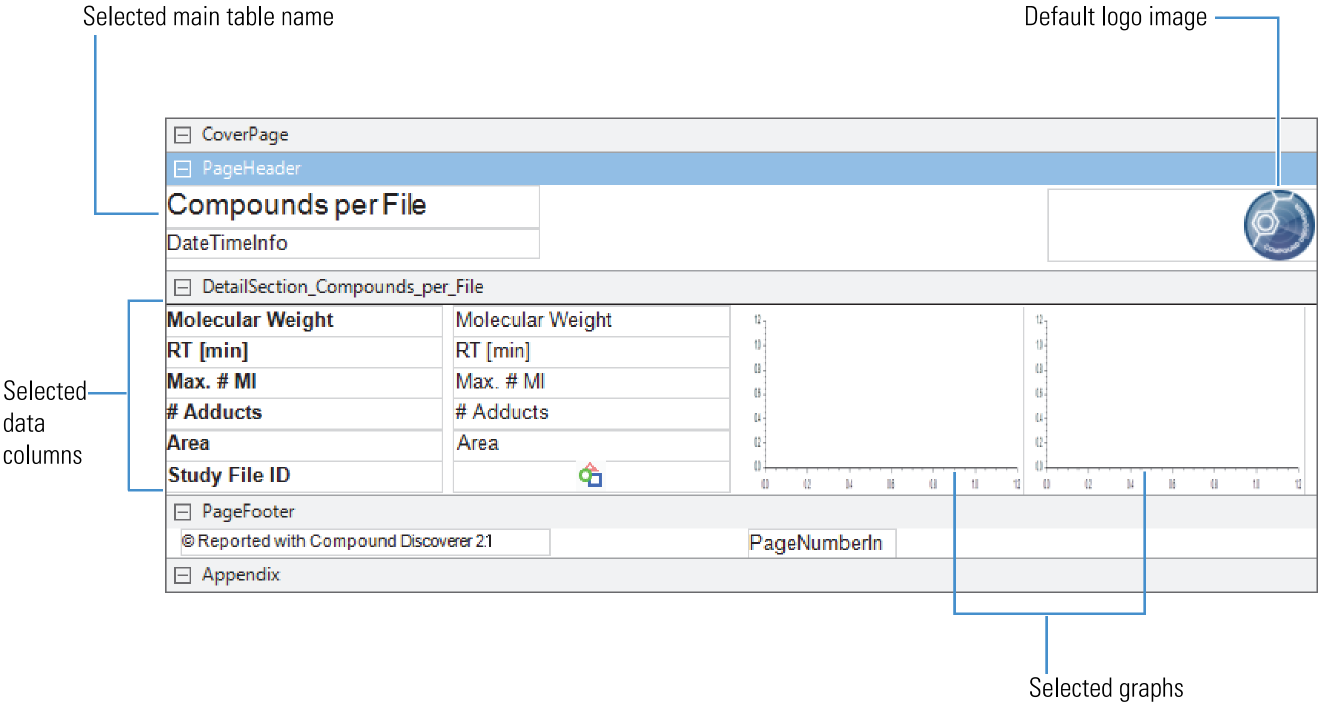
Selected data columns

Selected graphs

Adds a page number to the report.

Figure 112 shows a report template for selected columns in the Compounds per File table and two associated graphs. The table columns are transposed from the original format, which matched the result table, to a two-column format with one column for the column headings and another column for the corresponding data items.

Figure 113. Report template with transposed data from the Compounds per File table



Selected main table name

Default logo image

Selected data columns

Selected graphs

⊟ CoverPage

⊟ PageHeader

Compounds per File

DateTimeInfo

⊟ DetailSection_Compounds_per_File

Molecular Weight	Molecular Weight
RT [min]	RT [min]
Max. # MI	Max. # MI
# Adducts	# Adducts
Area	Area
Study File ID	

⊟ PageFooter

© Reported with Compound Discoverer 2.1

PageNumberIn

⊟ Appendix

For information about adding more design items to the current template, previewing a resolved report, and saving the template, see "Editing an Existing Report Template" on page 344.

Table 89 describes the parameters in the Customize Report dialog box.

Table 89. 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.

Table 89. Customize Report dialog box parameters (Sheet 2 of 3)

Parameter	Description
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.
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 (see "To modify the current color scheme or to add or remove color schemes from the list" on page 338). 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

Table 89. Customize Report dialog box parameters (Sheet 3 of 3)

Parameter	Description
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 (see "Editing an Existing Report Template" on page 344).
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 activates this button. 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.
OK	Applies the selected settings to the new report template.
Cancel	Cancels your selections and closes the dialog box.

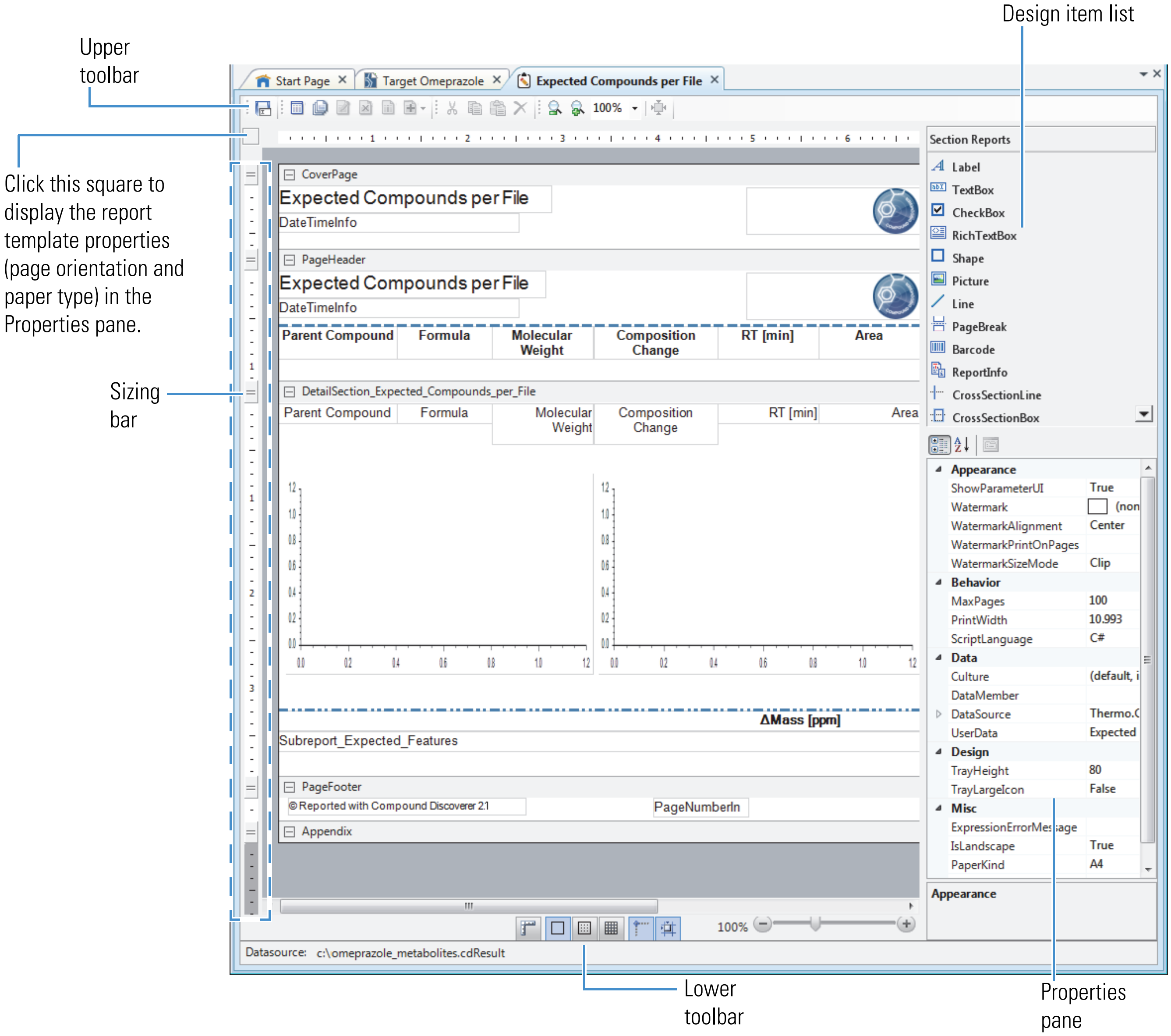
Editing an Existing Report Template

Use the report designer page to modify a report template. The report designer page shows the design items that you selected using the Customize Report dialog box (see "Creating a Report Template with the Customize Report Dialog Box" on page 334) or the items in the existing report template that you selected. Some of the design items appear as containers (a rectangular box) where you can add text, images, or data graphs.

Note You can open more than one report designer page in the application window.

Figure 114 shows the report designer page.

Figure 114. Report designer page



Appearance	
ShowParameterUI	True
Watermark	☐ (non
WatermarkAlignment	Center
WatermarkPrintOnPages	
WatermarkSizeMode	Clip
Behavior	
MaxPages	100
PrintWidth	10.993
ScriptLanguage	C#
Data	
Culture	(default, i
DataMember	
DataSource	Thermo.C
UserData	Expected
Design	
TrayHeight	80
TrayLargeIcon	False
Misc	
ExpressionErrorMessage	
IsLandscape	True
PaperKind	A4

For more information about the features of the report designer page, see these topics:

- Report Designer Workspace Sections and Sizing Bar
- Report Designer Toolbars
- Report Designer Shortcut Menu
- Report Designer Section Reports Pane
- Report Designer Properties Pane
- Report Designer Property Dialog Links
- Report Designer Load File Link
- Report Designer Report Template Settings

To work with the report designer page, follow these procedures as applicable:

- To open the report designer page
- To change the logo image
- To change the format of the date-and-time stamp
- To add a design item to the template that does not extract data from a result file
- To add a main table column to a column set that is arranged from left to right
- To add a main table column to a column set that is vertically arranged
- To add a data graph that is associated with the main table to the template
- To add a column from a related table to the template
- To edit the properties of subreport columns
- To edit a design item by using the mouse
- To modify the properties of a design item by using the Properties pane
- To modify the properties of a design item by using its property dialog box
- To add a page break between reported result table rows
- To save a modified report template with a different name

❖ To open the report designer page

1. Open a result file.
2. From the application window, do one of the following:
   a. Choose **Reporting > Create Report Template** from the menu bar, or click the **Create Report** icon, , in the toolbar.

      The Customize Report dialog box opens.

b. Make the appropriate selections and click **OK**.

The report designer page opens as a tabbed document. The tab format is as follows:

Main Result Table Name

–or–

a. Choose **Reporting > Edit Report Template** from the menu bar, or click the **Edit Report Template** icon, , in the toolbar.

The Open Report Design Template dialog box opens.

b. Select a report template and click **Open**.

The report designer page opens as a tabbed document. The tab format is as follows:

Existing Report Template Name

❖ To change the logo image

1. Select the logo image container on the report designer page.

   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.

2. 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.

   Image System.Drawing.Bitmap ...

   The Open dialog box opens with a setting of All image files for the file type.

3. Browse to the folder where you stored the logo of interest, select the logo, and click **Open**.

   The selected image appears in the container.

4. Modify the Layout properties as appropriate.

❖ To change the format of the date-and-time stamp

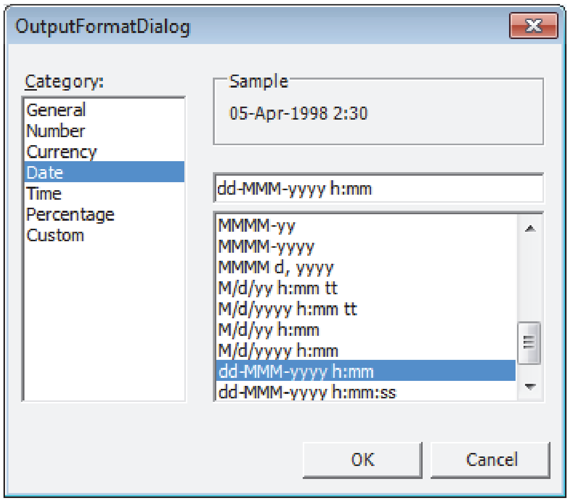
1. On the report designer page, select the **DateTimeInfo** item.

   The properties for this TextBox design item appear in the Properties pane.

2. Under Appearance, click the **OutputFormat** box to make the browse icon appear. Then click the browse icon.

   The OutputFormat dialog box opens (Figure 115).

Figure 115. OutputFormat dialog box



Category: Date

Sample 05-Apr-1998 2:30

dd-MMM-yyyy h:mm

3. Select the format of interest.

4. Click **OK** to accept the setting.

❖ To add a design item to the template that does not extract data from a result file

From the Section Reports pane to the right of the workspace area (see "Report Designer Section Reports Pane" on page 362), drag a design item to the appropriate location on a workspace section of the page.

❖ To add a main table column to a column set that is arranged from left to right

1. Decide where you want to place the additional column.

    - 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.

2. 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.

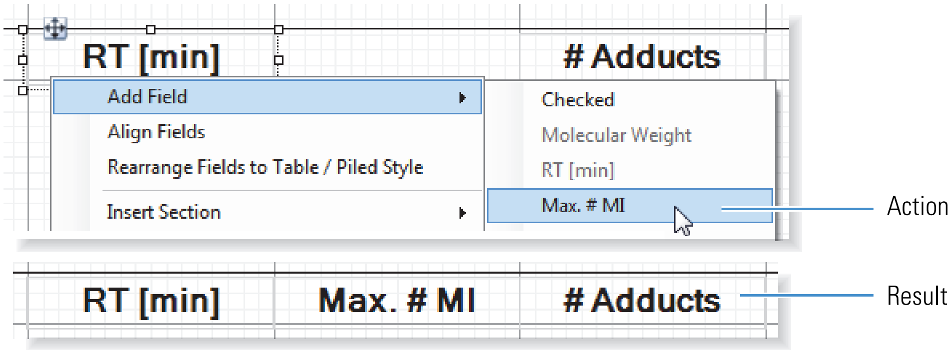
    c. Select an available data column from the list.

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.

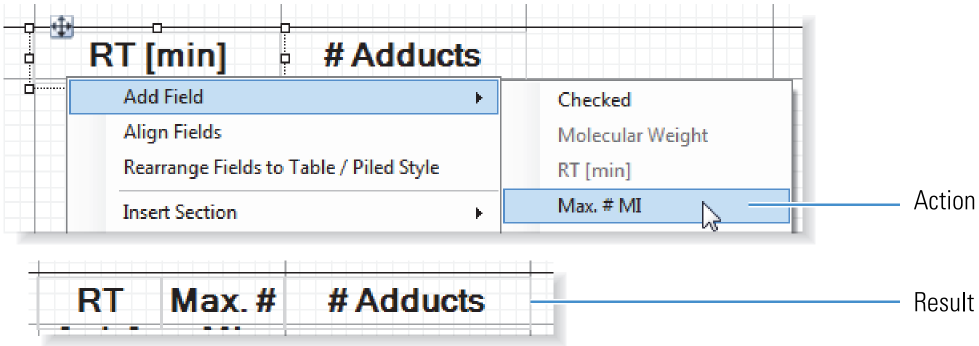
Figure 116 shows that the outcome of adding a column to the right of another column depends on the spacing between the columns.

Figure 116. Adding a data column to the right of another data column

Gap between the RT [min] and #Adducts columns



No gap between the RT [min] and #Adducts columns



❖ To add a main table column to a column set that is vertically arranged

1. Use the sizing bar to display all of the data column rows.
2. 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.

❖ To add a data graph that is associated with the main table to the template

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 selections.

The available items in the list include the data graphs associated with the current main table and the related tables for the current main table.

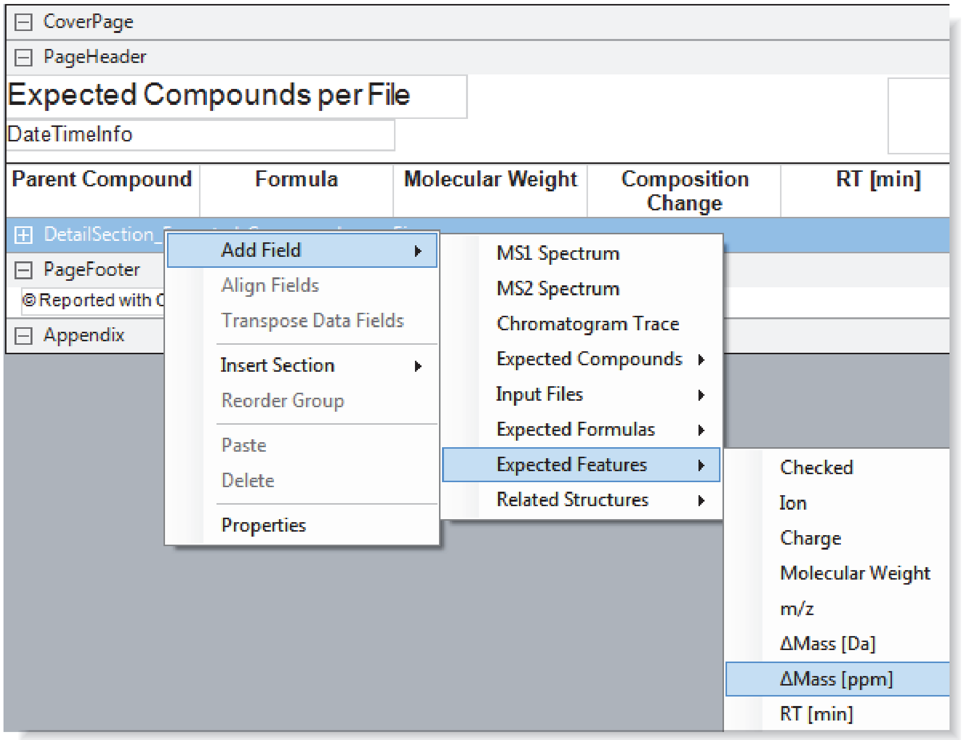
c. Select an available data graph from the list.

When the table columns are positioned from left to right, the data graph appears below the table columns and to the right of any existing data graphs.

❖ To add a column from a related table to the template

1. Do one of the following:

- Right-click the **DetailSection_*Main_Table_Name*** bar and choose **Add Field >** ***Related Table Name*** **>** ***Column of Interest***.



–or–

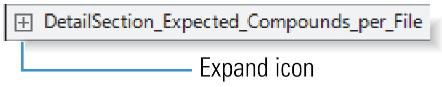
a. Select the **DetailSection_*Main_Table_Name*** bar.

b. In the toolbar, click the **Add Items** icon, , to open a list of data graphs and related table selections.

The available items in the list include the data graphs associated with the current main table and the related tables for the current main table.

c. Select an available related table from the list, and then select a table column.

2. If the DetailSection is collapsed, click the expand icon to open the section.

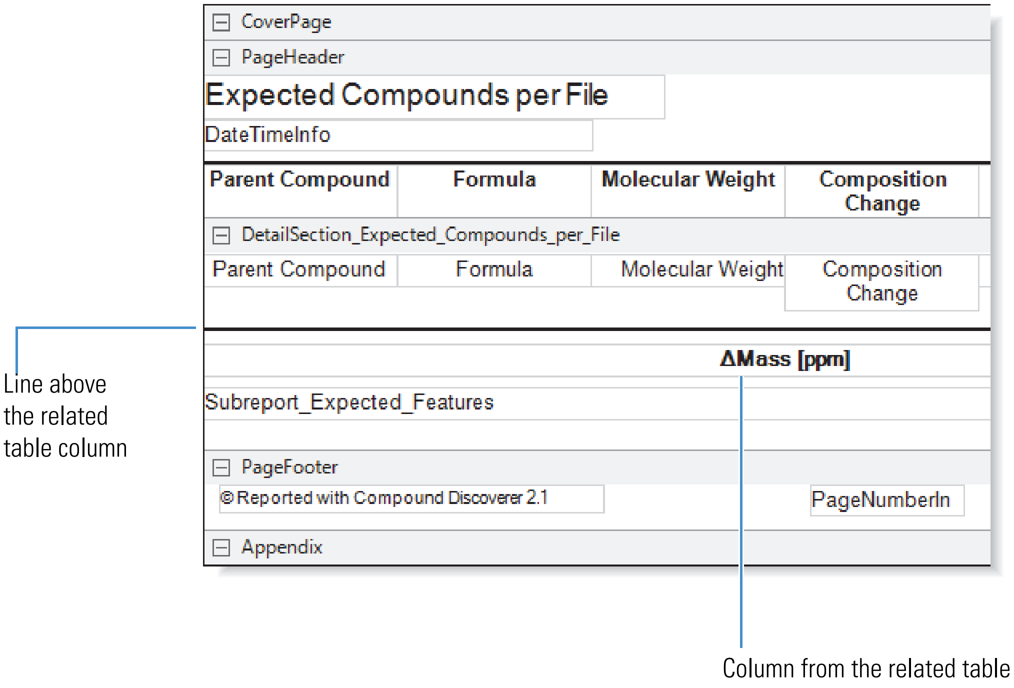


DetailSection_Expected_Compounds_per_File

Expand icon

The added table column appears at the bottom of the DetailSection (data area). The application automatically adds a line above the column heading (Figure 117).

Figure 117. Expected Compounds per File table with the ΔMass [ppm] column from the related Expected Features table



CoverPage
PageHeader
Expected Compounds per File
DateTimeInfo

Parent Compound	Formula	Molecular Weight	Composition Change

DetailSection_Expected_Compounds_per_File

Parent Compound	Formula	Molecular Weight	Composition Change

ΔMass [ppm]
Subreport_Expected_Features
PageFooter
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PageNumberIn
Appendix

Line above the related table column

Column from the related table

❖ To edit the properties of subreport columns

1. To open the subreport editor area, do one of the following:

   - Double-click the **Subreport_*Related_Table_Name*** box.

–or–

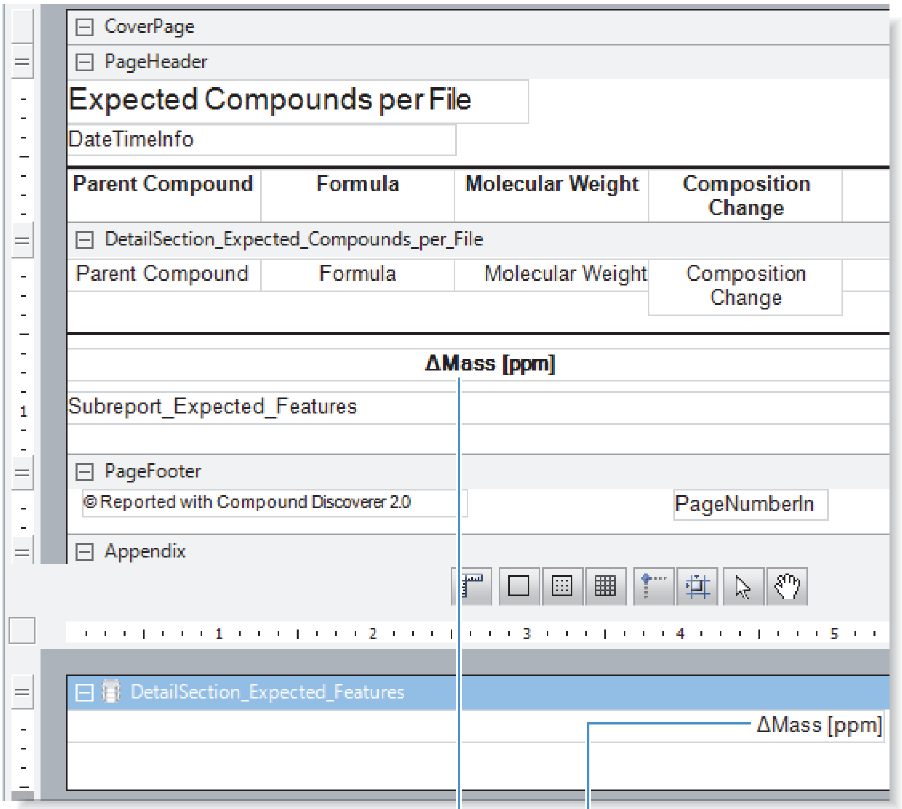
a. Select the **Subreport_*Related_Table_Name*** box.

The Edit Sub-Report icon, , becomes available.

b. Click the **Edit Sub-Report** icon.

The TextBox design item for the related table column appears in a separate section. The item's container is sized to the full page width (Figure 118).

Figure 118. Report designer page with the subreport section open



Column heading for the ΔMass [ppm] column

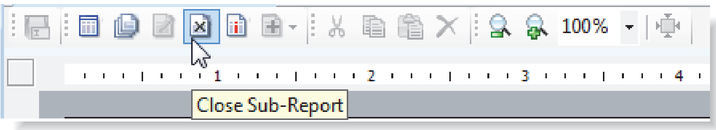
Subreport section with the container for the ΔMass [ppm] data item sized to the full page width

2. To change the properties of the TextBox design item in the subreport section, select it.

   The properties for the selected design item appear in the properties pane to the right of the workspace.

3. 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.

4. To close the subreport section, click the **Close Sub-Report** icon in the report designer toolbar.

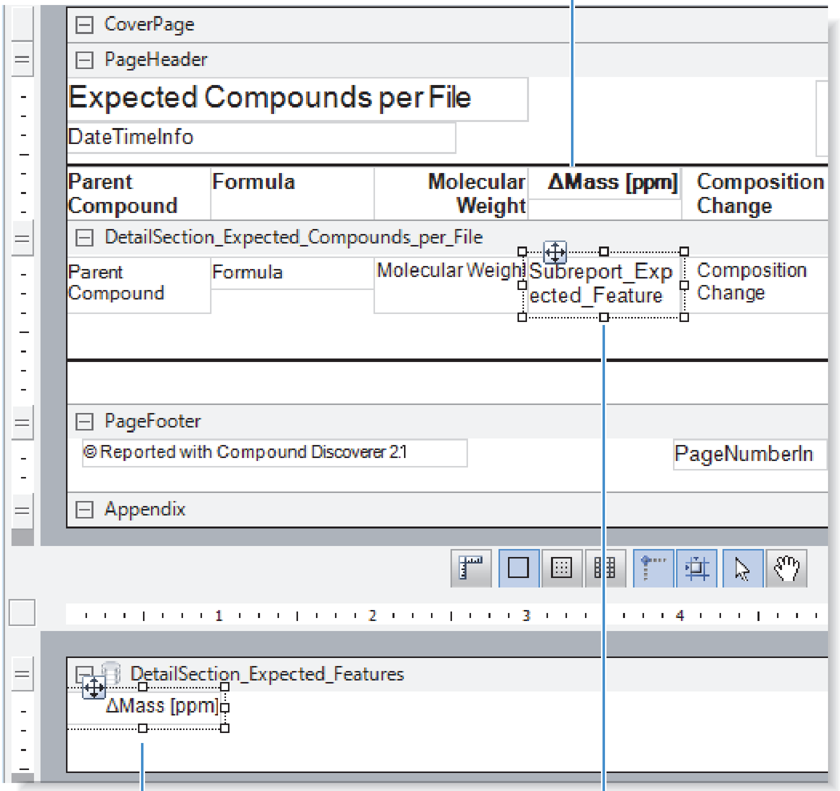


❖ To move a subreport column up to the set of main table columns

1. Resize the column heading container for the subreport column. Then, move it to an appropriate location in the set of main table columns (Figure 119).
2. Resize the Subreport_*Related_Table_Name* container. Then, move it to the appropriate location in the Detail Section.
3. In the related table's Detail Section, resize the data item's container.

Figure 119 shows a report template for the Expected Compounds per File table with an additional column from the related Expected Features table.

Figure 119. Related table column moved up to the main table



Column heading for the related table column

Detail Section for the related table with a resized container for a data item

Subreport container moved to the main table's Detail Section

❖ To edit a design item by using the mouse

1. Select the design item on the report designer page.
2. Modify the item as follows:
    - Move the item by dragging it to a different location (or you can use the arrow keys on the keyboard).
    - Resize the item by dragging the handle points of the container.

❖ To modify the properties of a design item by using the Properties pane

1. Select the design item on the report designer page.

   The properties for the selected design item appear in the Properties pane, at the bottom right of the report designer page. For information about the properties of each design item, see "Report Designer Properties Pane" on page 365.

2. Modify the properties of interest, including the size and location of the selected design item.

❖ To modify the properties of a design item by using its property dialog box

1. Select the design item on the report designer page.
2. Click the **Property Dialog** link at the bottom right of the report designer page (see "Report Designer Property Dialog Links" on page 376).
3. Modify the properties of interest, including the size and location of the selected design item.

Note For the RichTextBox design item, in addition to the Property Dialog link, you can click the Load File link to load text from a file (see "Report Designer Load File Link" on page 379).

❖ To add a page break between reported result table rows

Drag the PageBreak design item from the Section Reports pane to the bottom of the Detail Section of the report template.

❖ To save a modified report template with a different name

1. In the report designer toolbar, click the **Save As** icon, .

   The Save Report Template As dialog box opens.

2. Browse to the folder where you want to store the report template, name the file, and click **Save**.

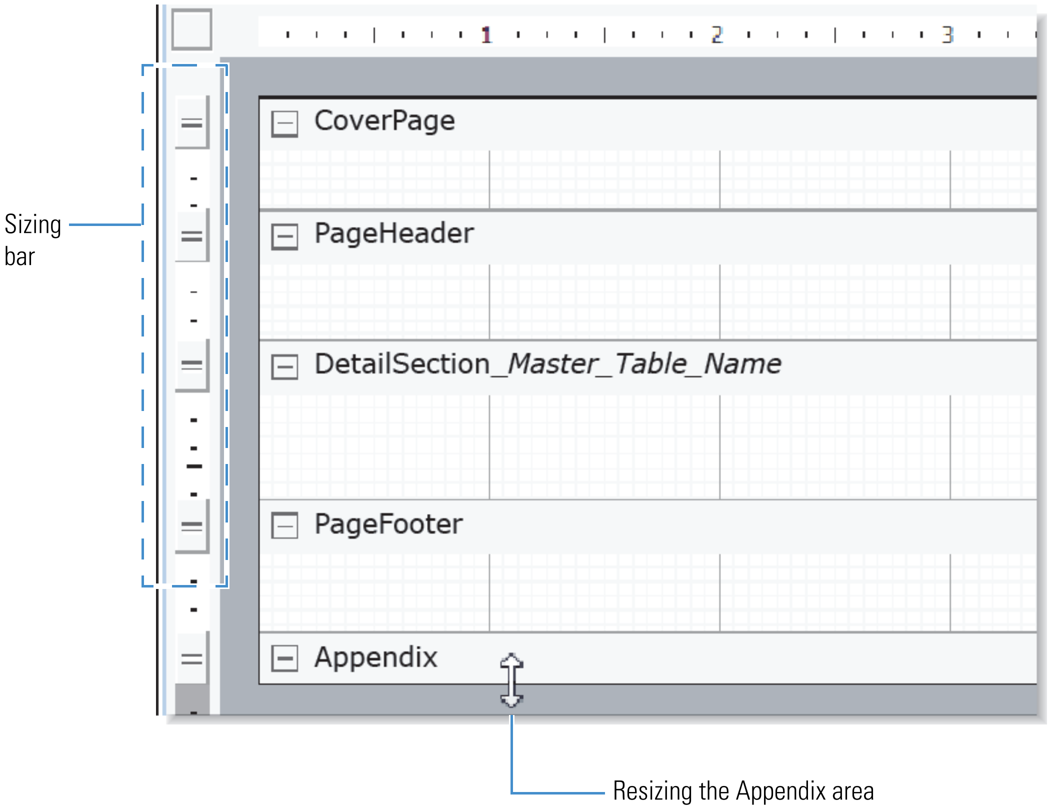
Report Designer Workspace Sections and Sizing Bar

These topics describe the workspace sections and sizing bar on the report designer page:

- Workspace Sections
- Sizing Bar

Figure 120 shows the five workspace sections and the sizing bar:

Figure 120. Workspace sections and sizing bar



For more information about the report designer page, see "Editing an Existing Report Template" on page 344.

Workspace Sections

By default, the template workspace on the report designer page has five sections. Table 90 lists these sections, from top to bottom.

Table 90. 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" on page 373.) 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 design items to the top of each report page. The standard templates include a Label design item with the main table name, a TextBox design item with a time stamp, and a Picture design item with a company logo. The column headings (Label design 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 design 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 design item.

Table 90. 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.

Note The report designer 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. Select one of the workspace sections by clicking the section header or by clicking within the section area.
2. From the shortcut menu, choose **Delete**.

Sizing Bar

Use the sizing bar to the left of the workspace to resize each workspace section vertically, except for the Appendix section.

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 designer page is not necessarily the same as its size in the generated report.

❖ To resize a workspace section (excluding the Appendix section)

In the sizing bar, drag the sizing handle (Figure 120 on page 354).

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 resize the Appendix workspace

To enlarge the Appendix section of the report designer page, drag it down by the bottom edge of the report designer page. To reduce this workspace section, drag the bottom edge up.

Report Designer Toolbars

Table 91 describes the toolbars on the report designer page.

For more information about the report designer page, see "Editing an Existing Report Template" on page 344.

Table 91. Toolbars on the report designer 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 "Creating a Report Template with the Customize Report Dialog Box" on page 334).
💾	Save As—Saves the report template using a different file name.
▦	Preview—Opens the Report Preview dialog box (see "Previewing and Printing a Report" on page 381).
⎙	Print—Opens the Report Print dialog box.

Table 91. Toolbars on the report designer page (Sheet 2 of 4)

Icon	Description
✎	Edit Sub-Report—Enlarges a selected subreport so that you can edit it. Selecting a subreport item activates this icon. 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 designer page. **Note** Related tables that you select in the Customize Report dialog box (see "Creating a Report Template with the Customize Report Dialog Box" on page 334) appear as subreports on the report designer page.
☒	Close Sub-Report—Closes the separate subreport workspace section. Clicking anywhere in the separate subreport workspace activates this icon.
▥	Align Columns—Aligns the Label (column heading) and Textbox (data) containers for the selected column or columns. Selecting a report column activates this icon.
⊞▾	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 activates this icon. 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 design item, and the container for the column data appears in the DetailSection as a TextBox design item.
✂	Cut—Deletes the selected item without confirmation.
⧉	Copy—Copies the selected item.
📋	Paste—Pastes the selected item.

Table 91. Toolbars on the report designer page (Sheet 3 of 4)

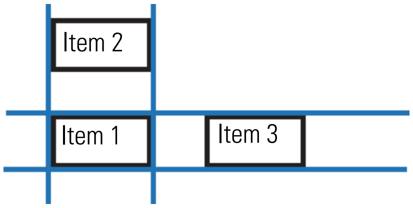
Icon	Description
✕	Delete—Deletes the selected item after you click OK in the confirmation dialog box.
🔍	Zoom Out—Reduces the magnification of the page.
🔍	Zoom In—Increases the magnification of the page.
100% ▾	Magnification box—Displays the magnification percentage.
✥	Actual Size—Displays the page at 100% magnification. Changing the magnification by using the Zoom In and Zoom Out icons or by typing a value in the magnification box activates this icon.
Bottom toolbars	
📏	Dimension Lines—Displays dimension lines (|—1.0 in—|) as you resize a design 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 a design item on the page, blue alignment lines appear. When the selected design item (Item 1 below) is horizontally aligned with another design item, two vertical lines bracket the aligned items. When the selected design item is vertically aligned with another design 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 91. Toolbars on the report designer 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.
100% ⊖ ⊕	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.

Report Designer Shortcut Menu

Table 92 on page 361 describes the shortcut menu commands for the report designer page.

For more information about the report designer page, see "Editing an Existing Report Template" on page 344.

❖ To open the shortcut menu for the report designer page

Right-click the report designer page.

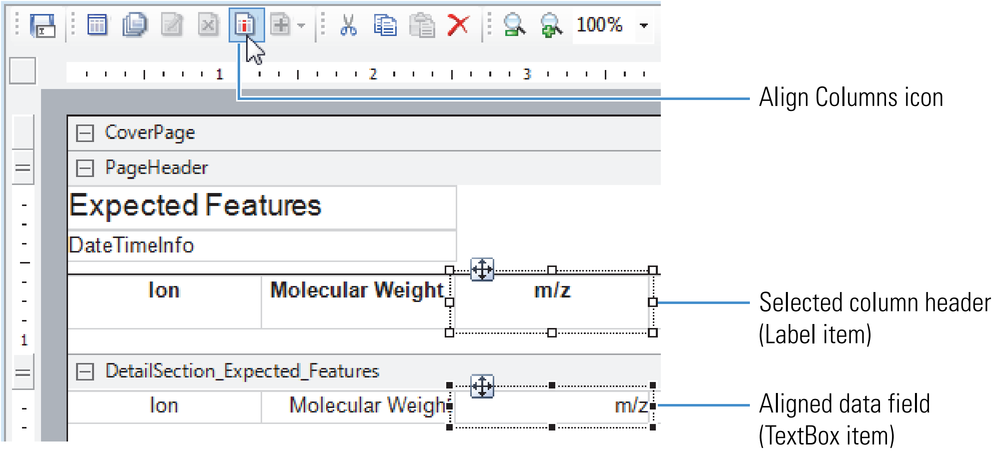
❖ To add a design item to a section of the report

Right-click the section bar within a section area and choose **Add Field** > ***Item of Interest***.

❖ To align a column heading to its associated data field

1. In the PageHeader section, select the column heading (Label design item) that you want to align with its associated data field (TextBox design item).

   The Align Columns icon becomes available.



Align Columns icon

Selected column header (Label item)

Aligned data field (TextBox item)

2. In the report designer page toolbar, click the **Align Columns** icon, .

❖ To transpose the data fields from columns to rows or from rows to columns

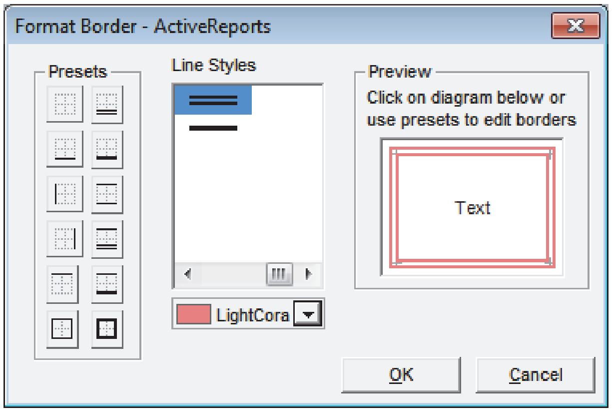
1. Right-click a column heading (Label) or a column data field (TextBox) and choose **Transpose Data Fields**.
2. To undo the change, if necessary, right-click a column heading (Label) or a column data field (TextBox) and choose **Transpose Data Fields**.

❖ To add a border to a design item

1. Right-click the design item in the workspace and choose **Format Border**.

   The Format Border dialog box opens (Figure 121).

   Figure 121. Format Border dialog box with the selection of a coral, double line border



Click on diagram below or use presets to edit borders

LightCora

2. 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 to set up the border.

Table 92 describes the shortcut menu commands for the report designer page.

Table 92. Report designer page shortcut menu (Sheet 1 of 2)

Command	Description
Add Field	Adds more items to the selected workspace section. Choose the item from a submenu.
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.

Table 92. Report designer page shortcut menu (Sheet 2 of 2)

Command	Description
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.
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 designer page.

Report Designer Section Reports Pane

The Section Reports pane to the right of the workspace on the report designer page lists all of the different design items that you can add to the report template.

❖ To add a design item to a report template

1. Drag the item of interest to the appropriate location on the report designer page.

   Some of the items appear as containers (boxes) where you can add text or images.

2. Select the design item to open its properties below the Section Reports pane.
3. Edit the item’s properties as necessary.

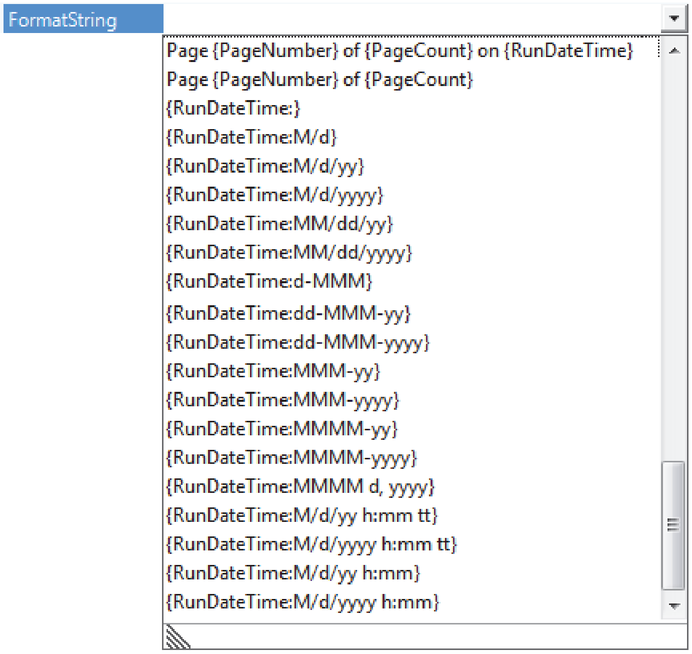
For more information about the report designer page, see “Editing an Existing Report Template” on page 344.

Table 93 describes the design items in the Section Reports pane.

Table 93. Design items in the Section Reports pane (Sheet 1 of 2)

Design item	Description
Label	A text label, usually used as a header or title. The column headers are Label design items.
TextBox	A text box, usually used to group multiple items together. The application uses the TextBox design 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 text to the report's cover page.
CheckBox	A check box that you can select or clear.
RichTextBox	A text box that you can populate by typing text in the box or by loading text from a file. For more information, see "Report Designer Load File Link" on page 379.
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 in the properties pane (see "Report Designer Properties Pane" on page 365).
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 GrapeCity.

Table 93. Design items in the Section Reports pane (Sheet 2 of 2)

Design item	Description
ReportInfo	A variable that the application automatically replaces with real-time data in the generated report. Use the ReportInfo design 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.  FormatString Page {PageNumber} of {PageCount} on {RunDateTime} Page {PageNumber} of {PageCount} {RunDateTime:} {RunDateTime:M/d} {RunDateTime:M/d/yy} {RunDateTime:M/d/yyyy} {RunDateTime:MM/dd/yy} {RunDateTime:MM/dd/yyyy} {RunDateTime:d-MMM} {RunDateTime:dd-MMM-yy} {RunDateTime:dd-MMM-yyyy} {RunDateTime:MMM-yy} {RunDateTime:MMM-yyyy} {RunDateTime:MMMM-yy} {RunDateTime:MMMM-yyyy} {RunDateTime:MMMM d, yyyy} {RunDateTime:M/d/yy h:mm tt} {RunDateTime:M/d/yyyy h:mm tt} {RunDateTime:M/d/yy h:mm} {RunDateTime:M/d/yyyy h:mm}
CrossSectionLine	A line that can span across multiple workspace sections on the report designer 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 designer 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.

Report Designer Properties Pane

The properties pane to the bottom right of the workspace on the report designer page lists all of the property settings used to format an object (a workspace section or a design item) that you select in the report template. The displayed settings vary depending on the selected workspace section or design 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 tables in this topic list all of the possible property settings in alphabetical order. Some of these settings apply only to certain selected objects.

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.

Appearance Properties

Table 94 describes the Appearance properties.

Table 94. Appearance properties in the Properties pane (Sheet 1 of 3)

Property	Description
AnchorBottom	(For the Line design 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 design items) Specifies the horizontal alignment of the text within the container. (For the Barcode design 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 design item only) Specifies the height of the bar code.
CaptionGrouping	(For the Barcode design 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 design 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.

Table 94. Appearance properties in the Properties pane (Sheet 2 of 3)

Property	Description
CharacterSpacing	(For the Label and TextBox design items) Specifies the spacing between the characters in the text, in points. Default: 0
ClassName	Specifies the name of the class for a particular format. Default: Normal
Font	(For the Label, TextBox, and CheckBox design 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 design items) Specifies the font color.
FormatString	(For the ReportInfo design 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 design 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 design 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 94. Appearance properties in the Properties pane (Sheet 3 of 3)

Property	Description
OutputFormat	(For the TextBox design 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 115 on page 347) where you can change the settings. Do not change the OutputFormat settings for data fields from a result table column.
PictureAlignment	(For the Picture design 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 design item only) Specifies the left, right, top, and bottom margins of the quiet zone for the bar code, in inches.
Rotation	(For the Barcode design 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 design item only) Specifies the supplement options (2- or 5-digit add-ons for EAN/UPC bar codes).
TextJustify	(For the Label and TextBox design items) Specifies how to distribute the text when you set the Alignment property to Justify.
VerticalAlignment	(For the Label and TextBox design items) Specifies the vertical alignment of the text within the container. Selections: Top, Middle, and Bottom
VerticalText	Specifies the a 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 95 describes the Behavior properties.

Table 95. 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 design 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 design item only) Specifies whether the barcode design 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 design item only) Specifies the alignment of the check box in the container.
Checked	(For the CheckBox design item only) Specifies whether the CheckBox design 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 design item only) Specifies whether the application computes and includes a checksum in the bar code. Selections: True or False

Table 95. 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 design item only) Specifies whether the PageBreak design 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 design 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 design 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 95. 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 96 describes the Data properties.

Table 96. 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 design 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 design item only) Formats the report data based on the selected culture from a particular country or region. Default: Inherit

Table 96. 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 the design item to another design item, delete the current item. Then, add a new design item as described in "To add a main table column to a column set that is arranged from left to right" on page 347 or "To add a data graph that is associated with the main table to the template" on page 349.
Description	(For the Picture design 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 design 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 RichTextBox design 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 96. 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 design item, you can type text here. For the column headings, this box displays the column heading text. For the TextBox design item, this box displays the name of the data source (table column in the result file).
Title	(For the Picture design item only) Not implemented.

Design Properties

Table 97 describes the Design property.

Table 97. Design properties in the Properties pane

Design property	Description
(Name)	Displays the internal name of an object on the report designer page, used by the application to uniquely identify each individual object.

Layout Properties

Table 98 describes the Layout properties.

Table 98. Layout properties in the Properties pane (Sheet 1 of 2)

Layout property	Description
End	(For the CrossSectionLine and CrossSectionBox design 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 designer 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 design 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 design 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 design 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 98. 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 design item only) Specifies the coordinate of the left end of a line, based on the horizontal ruler at the top of the report designer page.
X2	(For the Line design item only) Specifies the coordinate of the right end of a line, based on the horizontal ruler at the top of the report designer page.
Y1	(For the Line design 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 design 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 99 describes the Miscellaneous properties.

Table 99. Miscellaneous properties in the Properties pane (Sheet 1 of 2)

Miscellaneous property	Description
Code128	(For the Barcode design 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 design 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 design 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 design item only) When you select Pdf417 for the Style property in the Appearance area, use this property to define the code.

Table 99. Miscellaneous properties in the Properties pane (Sheet 2 of 2)

Miscellaneous property	Description
QRCode	(For the Barcode design 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 design item only) When you select RssExpandedStacked for the Style property in the Appearance area, use this property to define the code.

Report Designer Property Dialog Links

The reporting feature for the application includes a property dialog box for each design item in the Section Reports pane. Using this dialog box, you can modify the formatting parameters for a selected design item on the report designer page. The available properties vary depending on the selected workspace section or design item. Most of these parameters are similar to the properties listed in the Properties pane (see "Report Designer Properties Pane" on page 365), although some might have slightly different names.

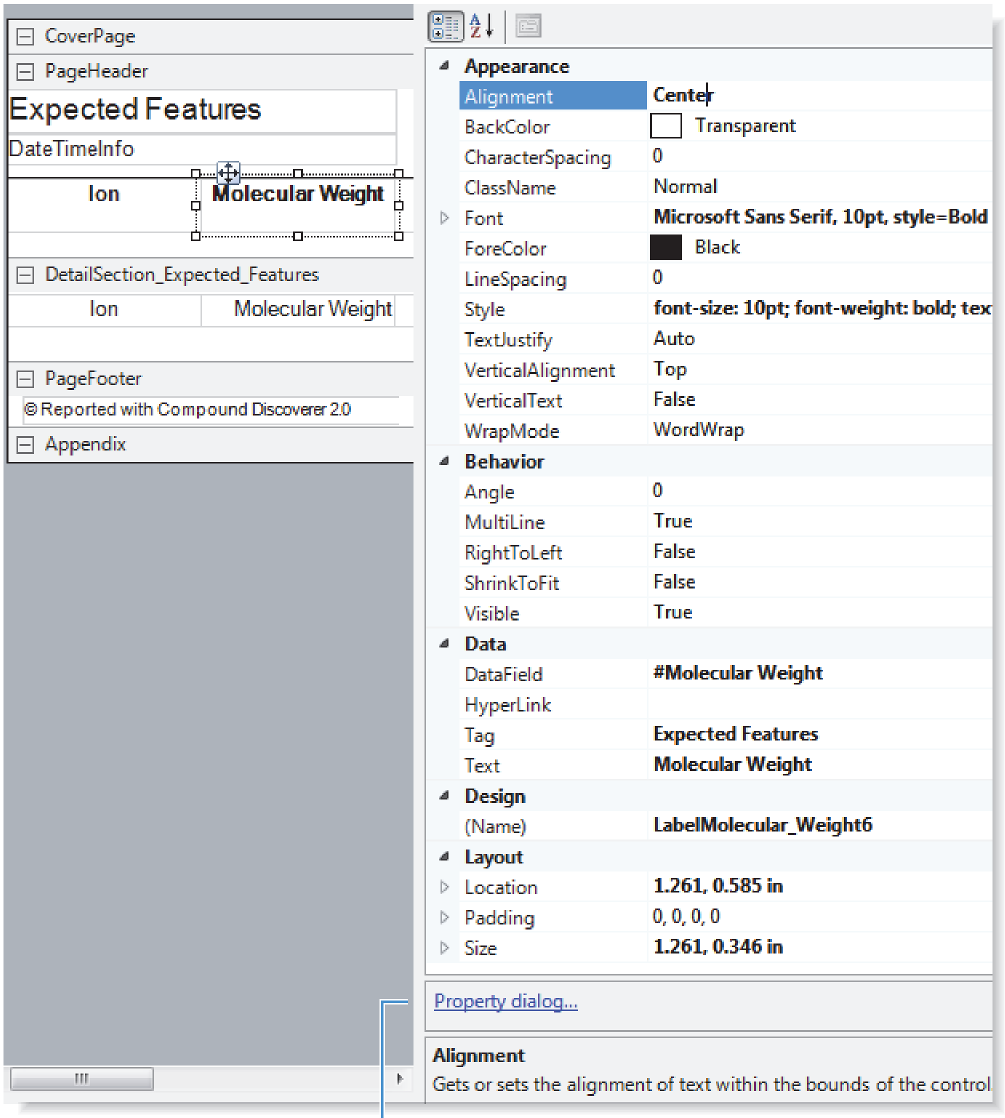
For more information about the report designer page, see "Editing an Existing Report Template" on page 344.

❖ To open the property dialog box for a report design item

1. Select the design item of interest in the workspace.

   The properties pane for the selected item appears (Figure 122).

Figure 122. Properties pane for a label design item



Appearance	
Alignment	Center
BackColor	Transparent
CharacterSpacing	0
ClassName	Normal
Font	Microsoft Sans Serif, 10pt, style=Bold
ForeColor	Black
LineSpacing	0
Style	font-size: 10pt; font-weight: bold; tex
TextJustify	Auto
VerticalAlignment	Top
VerticalText	False
WrapMode	WordWrap
Behavior	
Angle	0
MultiLine	True
RightToLeft	False
ShrinkToFit	False
Visible	True
Data	
DataField	#Molecular Weight
HyperLink	
Tag	Expected Features
Text	Molecular Weight
Design	
(Name)	LabelMolecular_Weight6
Layout	
Location	1.261, 0.585 in
Padding	0, 0, 0, 0
Size	1.261, 0.346 in

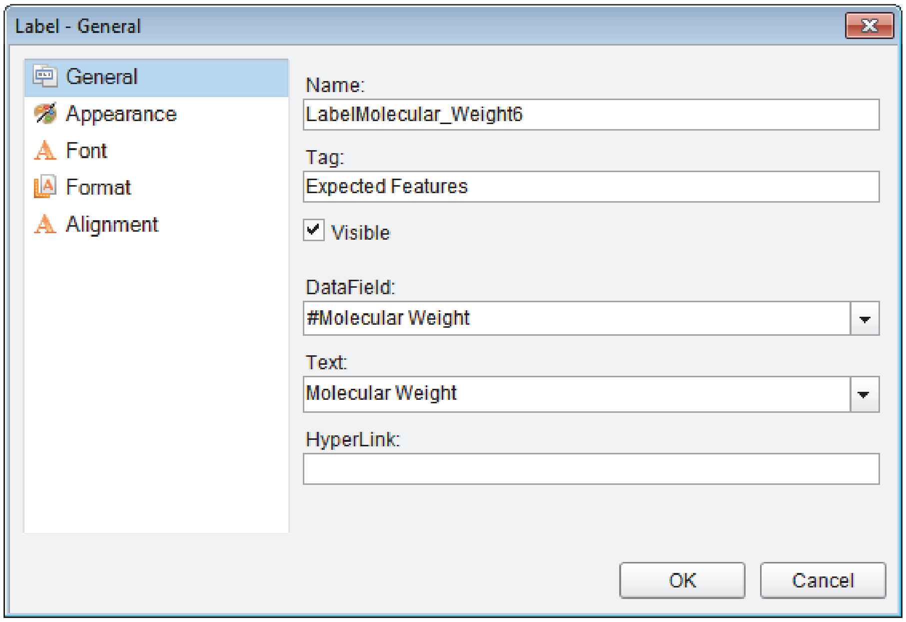
Alignment
Gets or sets the alignment of text within the bounds of the control

Property Dialog link

2. At the bottom right corner of the report designer page, click the **Property Dialog** link.

   The property dialog box for the selected object opens (Figure 123).

Figure 123. Property dialog box for the Label design item



Name: LabelMolecular_Weight6

Tag: Expected Features

☑ Visible

DataField: #Molecular Weight

Text: Molecular Weight

HyperLink:

Note For the RichTextBox design 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 "Report Designer Load File Link" on page 379).

The parameters in the property dialog boxes have equivalent parameters in the properties pane.

Report Designer Load File Link

Use the Load File link at the bottom right corner of the report designer page, (see "Report Designer Properties Pane" on page 365), to populate a RichTextBox design item with data from a file.

❖ To use the Load File link

1. Click the **Load File** link.
2. In the Open dialog box, select the data file and then click **Open**.

   You can load text from one of these file types: RTF, TXT, or HTML or HTM.

Report Designer Report Template Settings

On the report designer 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.

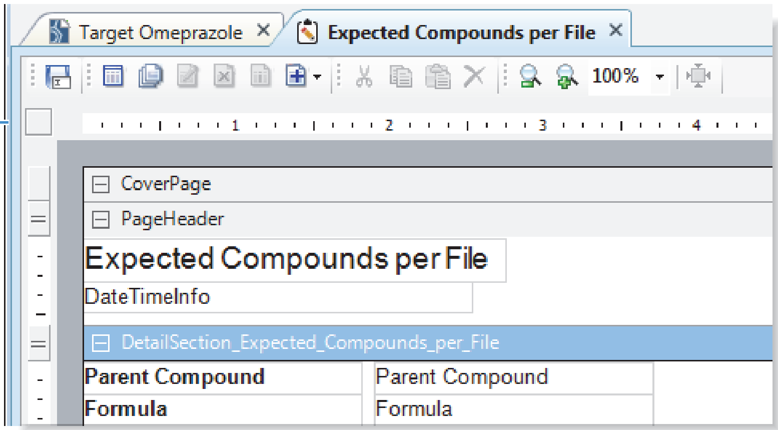
Follow these procedures as needed:

- To open the property settings for the report template
- To add a watermark to the report template
- To change the print width of the template
- To change the page orientation of the report template
- To change the paper size used by the printer

❖ To open the property settings for the report template

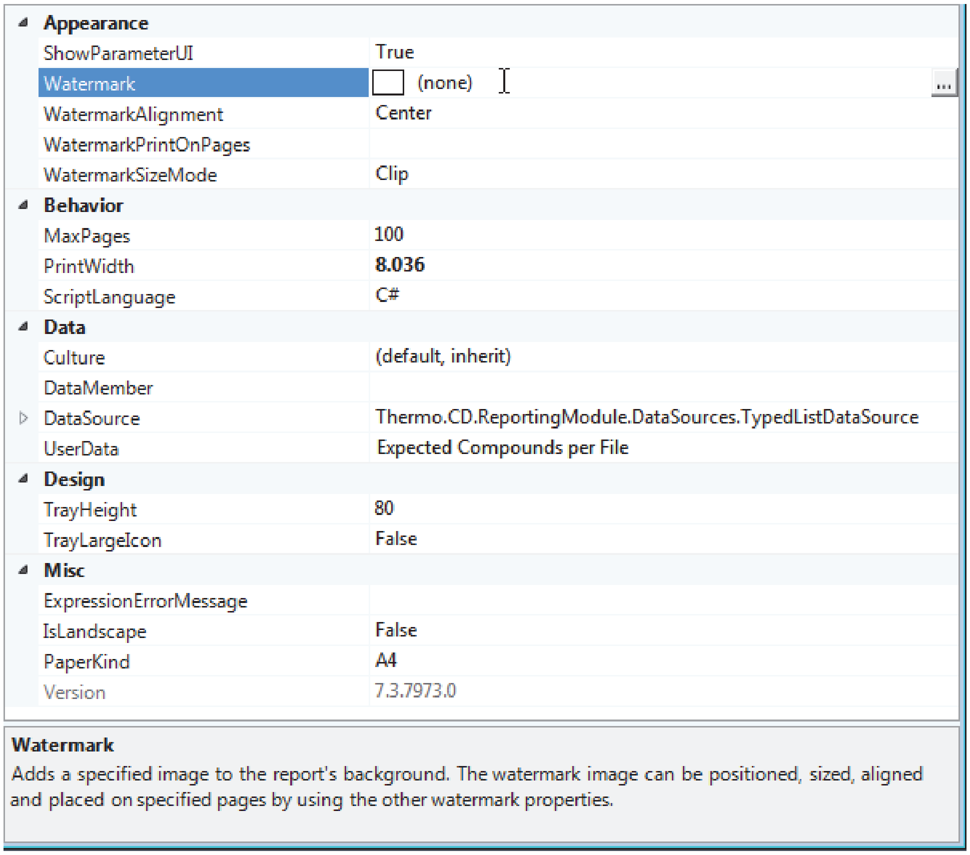
Click the square in the upper left corner (below the toolbar) of the report designer page.

Click this square.



The watermark properties appear in the Appearance group, and the orientation and paper size properties appear in the Miscellaneous group (Figure 124).

Figure 124. Report template properties (in the Properties pane)



Appearance	
ShowParameterUI	True
Watermark	☐ (none)
WatermarkAlignment	Center
WatermarkPrintOnPages	
WatermarkSizeMode	Clip
Behavior	
MaxPages	100
PrintWidth	**8.036**
ScriptLanguage	C#
Data	
Culture	(default, inherit)
DataMember	
DataSource	Thermo.CD.ReportingModule.DataSources.TypedListDataSource
UserData	Expected Compounds per File
Design	
TrayHeight	80
TrayLargeIcon	False
Misc	
ExpressionErrorMessage	
IsLandscape	False
PaperKind	A4
Version	7.3.7973.0

Watermark
Adds a specified image to the report's background. The watermark image can be positioned, sized, aligned and placed on specified pages by using the other watermark properties.

❖ To add a watermark to the report template

1. 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.

2. Find and select the image file of interest and click **Open**.
3. In the WatermarkAlignment list, select the appropriate alignment.
4. In the WatermarkPrintOnPages box, type the page number of the page where you want the watermark to appear.
5. 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.

❖ To change the print width of the template

Under Behavior, type a numeric value in the PrintWidth box.

❖ To change the page orientation of the report template

Under Misc, in the IsLandscape list, select **True** for Landscape or **False** for Portrait.

❖ To change the paper size used by the printer

Under Misc, in the PaperKind list, select the appropriate paper size.

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.

Previewing and Printing a Report

This topic describes how to work with the Report Preview and Report Print dialog boxes and the report resolution page.

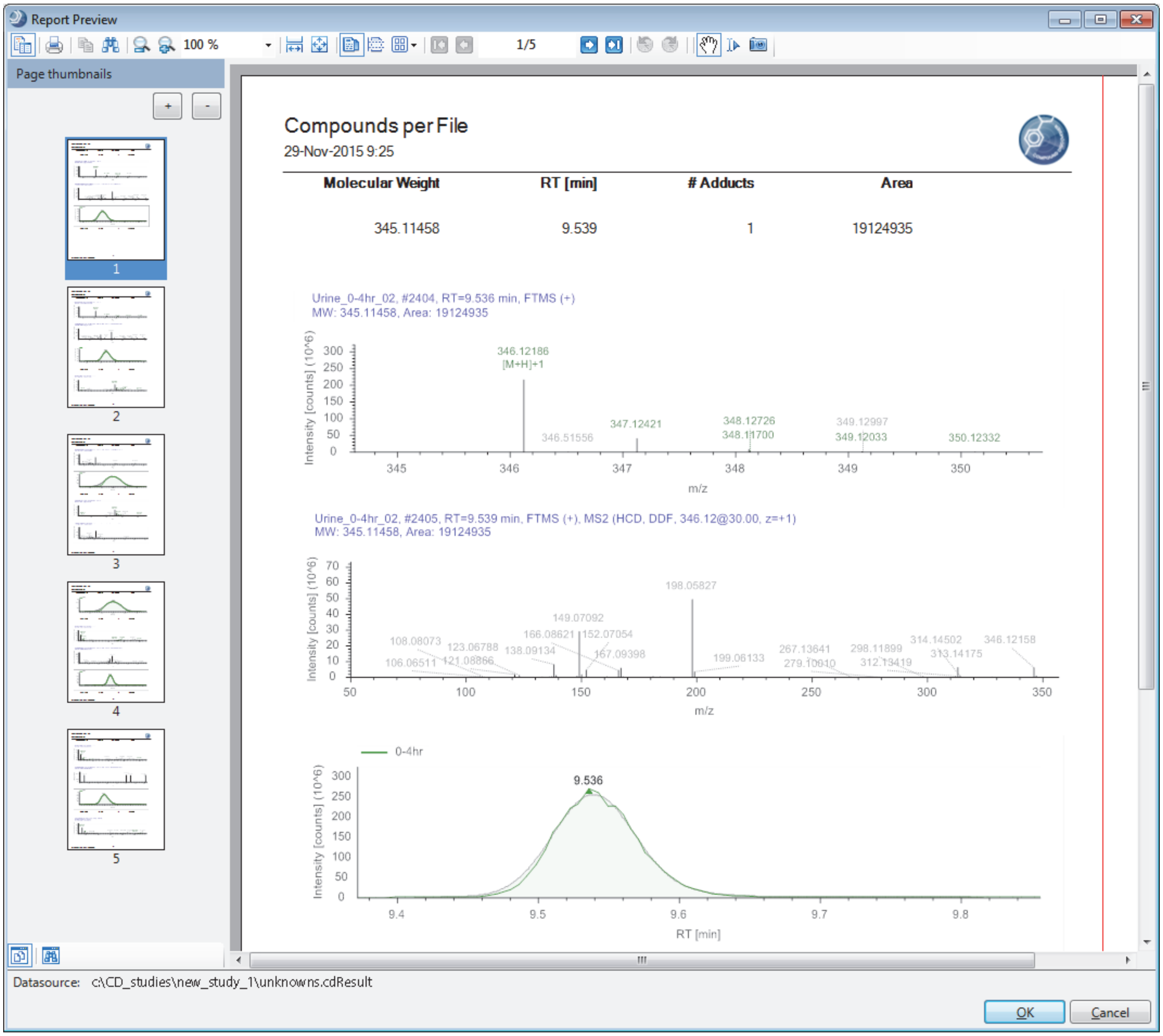
You can print all of the report pages from the report resolution page or the Report Print dialog box. You can print up to five pages from the Report Preview dialog box.

❖ To open the Report Preview dialog box

In the toolbar on the report designer 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 designer 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 To change the print width of the template).

Figure 125. Report Preview dialog box with a red line indicating an insufficient right margin



Compounds per File
29-Nov-2015 9:25

Molecular Weight	RT [min]	# Adducts	Area
345.11458	9.539	1	19124935

Datasource: c:\CD_studies\new_study_1\unknowns.cdResult

❖ To open the Report Print dialog box

In the toolbar on the report designer 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 designer page.The Page Thumbnails pane displays all of the report pages.

❖ 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.

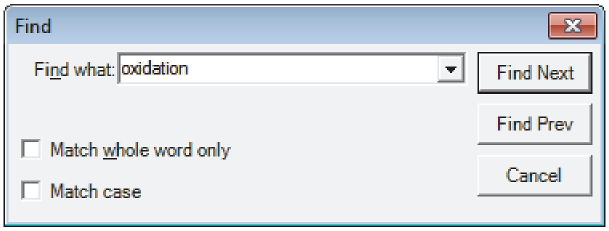
❖ To find a text item in a resolved report

1. In the toolbar, click the **Find** icon, .

   The Find dialog box opens.

2. In the Find What box, type the text that you want to find (see Figure 126).

Figure 126. Find dialog box with a text entry



Find what: oxidation

☐ Match whole word only

☐ Match case

3. 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.
4. Click **Find Next** or **Find Prev**.

❖ To copy a portion of the report to the Clipboard

Do one of the following:

a. To copy a specific item to the Clipboard, in the Report Preview toolbar, click the **Selection Mode** icon, .

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.

❖ To export the contents of the report to an external document

1. Open the Report Print dialog box or the report resolution page.
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

❖ To print the report

1. 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 designer page, open the Report Print dialog box by clicking the **Print Report** icon, .

2. In the toolbar, click the **Print** icon, .

   The Print dialog box opens.

3. Select the appropriate printer and the page range that you want to print.
4. Click **OK** to print the report.

For more information about the toolbar and Page Thumbnails pane, see these topics:

- Report Preview Toolbar
- Page Thumbnails Pane

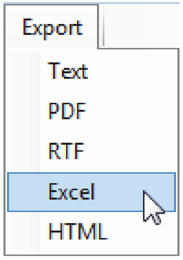
Report Preview Toolbar

The Report Preview and Report Print dialog boxes and the report resolution page share a common toolbar. Table 100 describes the icons in the toolbar, from left to right.

Table 100. Report preview icons (Sheet 1 of 2)

Icon	Description
▤	Toggle Sidebar—Opens and closes the Page Thumbnails pane (see "Page Thumbnails Pane" on page 387).
🖶	Print—Opens the Print dialog box where you select the appropriate print options and send the report to the selected printer.
⎘	Copy—Copies the selected item to the Clipboard. Clicking the Selection Mode icon activates the Copy icon.
	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.
100 % ▾	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.
1/5	Current Page—Indicates the current page and the estimated number of pages in the report.

Table 100. Report preview icons (Sheet 2 of 2)

Icon	Description
➡	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 activates the Backward icon.
↻	Forward—Displays the next selected page in the report. Clicking the Backward icon activates the Forward icon.
✋	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 101 describes the icons in the Page Thumbnails pane, from top left to bottom right.

Table 101. 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.

10

Using the Lists and Libraries Manager

To modify the lists and libraries that are used to process data in the Compound Discoverer application, see the following topics.

Contents

Library Manager Page

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.

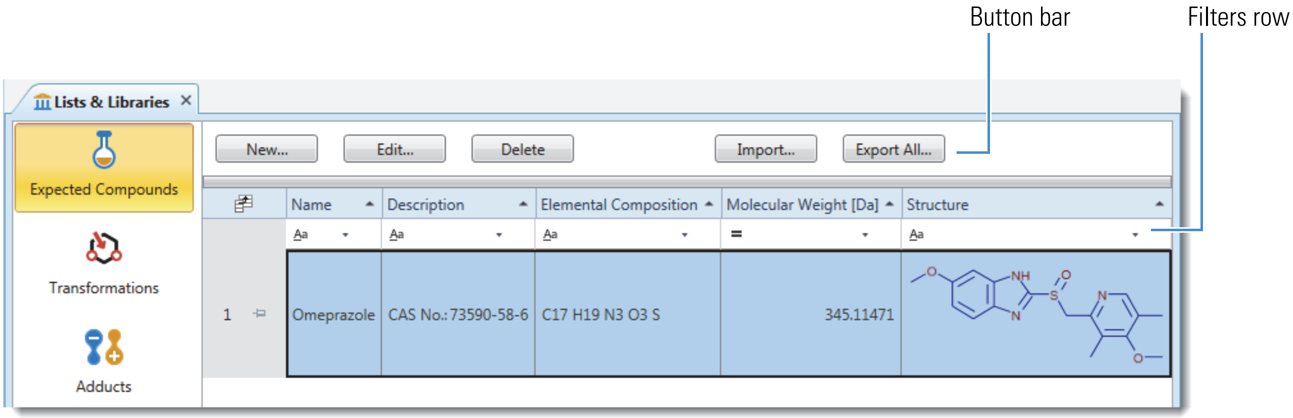
Each view in the Lists & Libraries Manager page includes a table. For information about freezing panes, hiding and showing columns, freezing rows, sorting, and filtering the application tables, see "Working with the Application Tables" on page 531.

Modifying the Expected Compounds List

The initial expected compounds list contains omeprazole (Figure 127), the targeted compound used in the *Compound Discoverer Metabolism Tutorial*.

> **Note** To use 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 127. Expected Compounds view



	Name	Description	Elemental Composition	Molecular Weight [Da]	Structure
1	Omeprazole	CAS No.: 73590-58-6	C17 H19 N3 O3 S	345.11471	

To modify the expected compounds list, see these topics:

- Importing, Exporting, and Deleting Compounds
- Adding and Editing Compounds with the Compound Editor

Importing, Exporting, and Deleting Compounds

Follow these procedures as needed:

- To open the Expected Compounds view
- To delete a compound
- To import a list of compounds from an XML file
- To export the contents of the Expected Compounds view to an XML file

❖ To open the Expected Compounds view

From the application menu bar, choose **Lists & Libraries > Expected Compounds**.

The Expected Compounds view contains your list of expected compounds for targeted analyses.

❖ To delete a compound

1. Select the compound and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import a list of compounds from an XML file

1. In the Expected Compounds view, click **Import**.
2. Select the XML file of interest, click **Open**, and then click **OK** at the prompt.

   The application only imports new entries; it does not import entries that are already in the 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.

❖ To export the contents of the Expected Compounds view to an XML file

1. In the Expected Compounds view, 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**.

Table 102 describes the parameters in the Expected Compounds view.

Table 102. Expected Compounds view parameters (Sheet 1 of 2)

Feature	Description
Buttons	
New	Opens the Compound Editor for adding new compounds to the list.
Edit	Opens the Compound Editor for editing the selected compound. Selecting a compound activates this button.
Delete	Deletes the selected compound. Selecting a compound activates this button.
Import	Opens the Open dialog box for selecting an XML file.
Export All	Opens the Save As dialog box for exporting the entire list as an XML file.

Table 102. Expected Compounds view parameters (Sheet 2 of 2)

Feature	Description
Table 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.

Adding and Editing 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 "Using the Structure Drawing Tools or Commands" on page 434.

Follow these procedures as needed:

- To open the Compound Editor dialog box
- To add a compound to the Expected Compounds list
- To open a structure file
- To edit an existing entry

❖ To open the Compound Editor dialog box

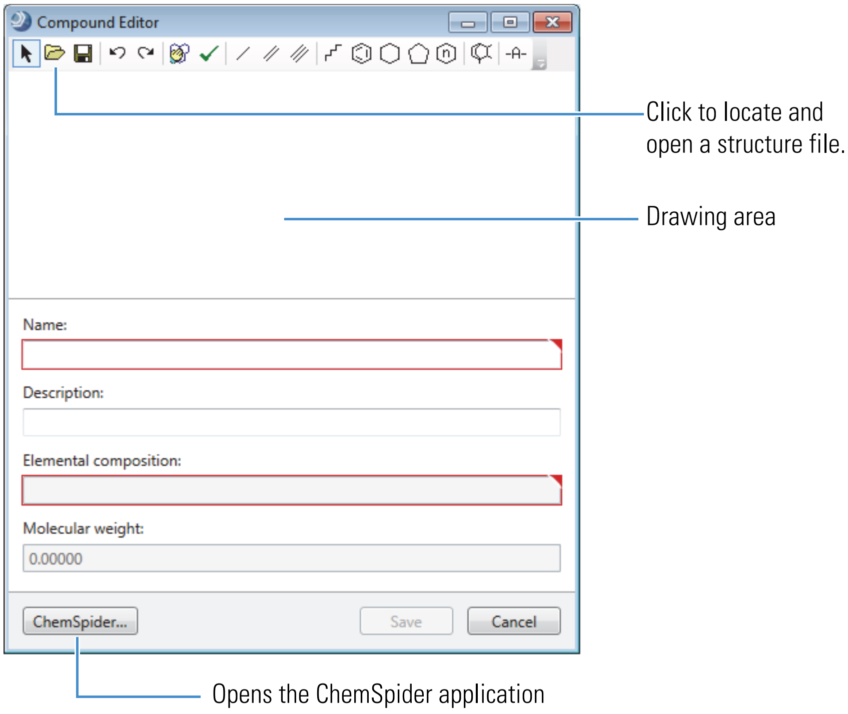
1. Open the Expected Compounds view (see "To open the Expected Compounds view" on page 391).
2. Do one of the following:
   - To add a new compound, click **New**.
   - To edit an existing entry, select the entry and click **Edit**.

❖ To add a compound to the Expected Compounds list

1. In the Expected Compounds view, 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 128. Compound Editor dialog box for a new compound

   Molecular weight: 0.00000

   Click to locate and open a structure file.

   Drawing area

   Opens the ChemSpider application

2. To enter the elemental composition, draw the structure in the drawing area, open a structure file, or click **ChemSpider** to find the structure.

   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.

3. (Optional) In the Description box, type a description of the compound.

4. Click **Save**.

   The dialog box closes and the compound appears in the list.

❖ To open a structure file

See “Loading a Structure from a Structure File” on page 433.

❖ To edit an existing entry

1. In the Expected Compounds view, either double-click the entry or select it and click **Edit**.

   The Compound Editor dialog box opens with information for the selected entry.

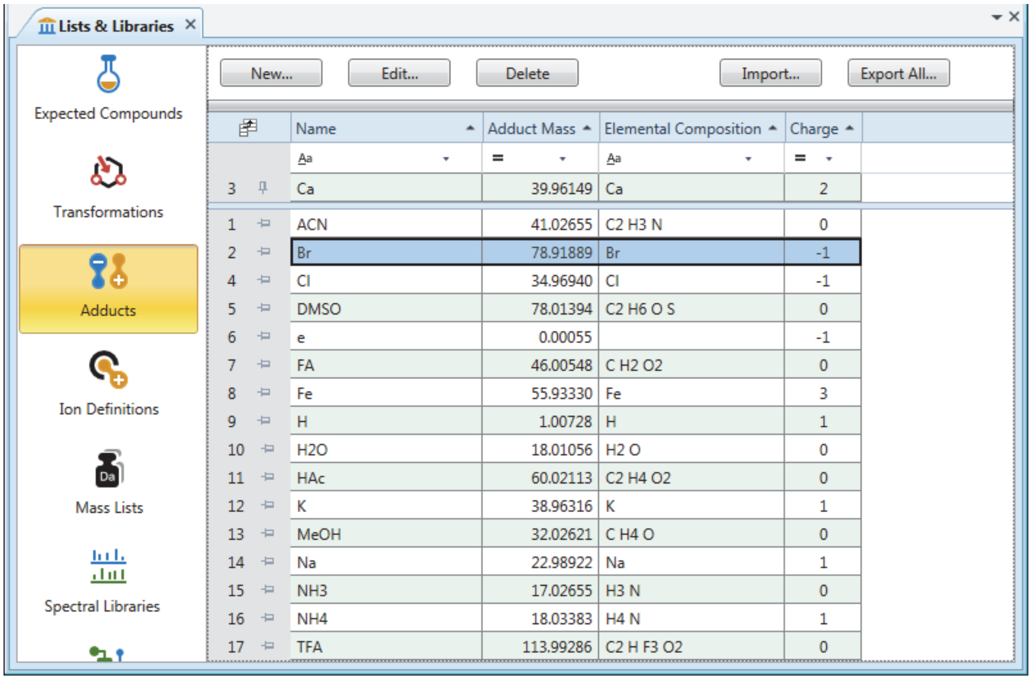
2. Edit the information as applicable.
   - To modify the chemical structure, edit the structure in the drawing area (see “Using the Structure Drawing Tools or Commands” on page 434) or open a different structure file.

     The application automatically populates the Elemental Composition and Molecular Weight boxes.
   - To change the compound name, type alphanumeric text in the Name box.
3. To save the changes, click **Save**, and then click **Yes** at the prompt.

Modifying the Adducts List

Use the Adducts view to define the adducts in your sample solutions (Figure 129).

Figure 129. Adducts view



	Name	Adduct Mass	Elemental Composition	Charge
	Aa	=	Aa	=
3	Ca	39.96149	Ca	2
1	ACN	41.02655	C2 H3 N	0
2	Br	78.91889	Br	-1
4	Cl	34.96940	Cl	-1
5	DMSO	78.01394	C2 H6 O S	0
6	e	0.00055		-1
7	FA	46.00548	C H2 O2	0
8	Fe	55.93330	Fe	3
9	H	1.00728	H	1
10	H2O	18.01056	H2 O	0
11	HAc	60.02113	C2 H4 O2	0
12	K	38.96316	K	1
13	MeOH	32.02621	C H4 O	0
14	Na	22.98922	Na	1
15	NH3	17.02655	H3 N	0
16	NH4	18.03383	H4 N	1
17	TFA	113.99286	C2 H F3 O2	0

To modify the adducts list, see these topics:

- Working with the Adducts List
- Adding and Editing Adducts with the Adduct Editor

Working with the Adducts List

Follow these procedures as needed:

- To open the Adducts view
- To delete an adduct from the list
- To import a list of adducts from an XML file
- To export the entire list of adducts to an XML file

❖ To open the Adducts view

From the application menu bar, choose **Lists & Libraries** > **Adducts**.

❖ To delete an adduct from the list

1. Select the adduct and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import a list of 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**.

❖ To export the entire list of adducts to an XML file

1. Click **Export All**.
2. Select a folder, name the file, and click **Save**.
3. At the prompt, click **OK**.

Adding and Editing Adducts with the Adduct Editor

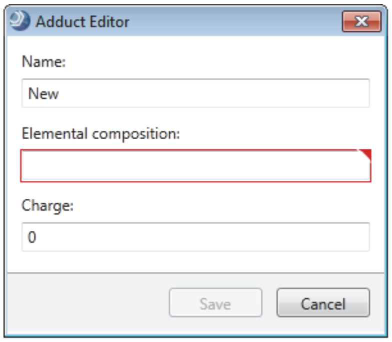
Use the Adduct Editor dialog box to define additional adducts, which are part of the ion definition.

❖ To add adducts to the Adducts library

1. Open the Adducts view (see "Modifying the Adducts List" on page 394).
2. In the button bar, click **New**.

   The Adduct Editor dialog box opens (Figure 130).

Figure 130. Adduct Editor dialog box



Name: New

Elemental composition:

Charge: 0

3. Define the new adduct as follows:
   - In the Name box, select **New** and type a name for the adduct.
   - In the Elemental Composition box, type the elemental composition of the adduct.

     The editor validates the composition entry.
   - In the Charge box, type the charge that the adduct adds to the ion definition.

     Range: –10 to +10
4. Click **Save**.

   The new adduct appears in the library.

❖ To edit an adduct entry

1. Select the entry.
2. Click **Edit**.

   The Adduct Editor opens with the selected entry.
3. Modify the adduct definition as follows:
   - In the Name box, select the current name and type a new name for the adduct.
   - In the Elemental Composition box, select the current elemental composition and type a new elemental composition for the adduct.

     The editor validates the composition.
   - In the Charge box, type the charge that the adduct adds to the ion definition.

     Range: –10 to +10
4. Click **Save**.

Modifying the Ion Definitions List

To modify the Ion Definitions list, see these topics:

- Working with the Ion Definitions List
- Adding or Editing Ion Definitions with the Ion Definition Editor

Working with the Ion Definitions List

The application uses the entries in the Ion Definitions list in the following workflow nodes: Detect Compounds and Generate Expected Compounds.

The default Ion Definitions list contains the most common adducts and dimers formed when using the electrospray-mass spectrometry (ESI-MS) technique in either the positive or negative polarity mode.

Table 103 lists the common adducts and dimers for the positive polarity mode. Table 104 lists the common adducts and dimers for the negative polarity mode.

Table 103. Common adducts and dimers in the positive ion 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 104. Common adducts and dimers in the negative ion mode (Sheet 1 of 2)

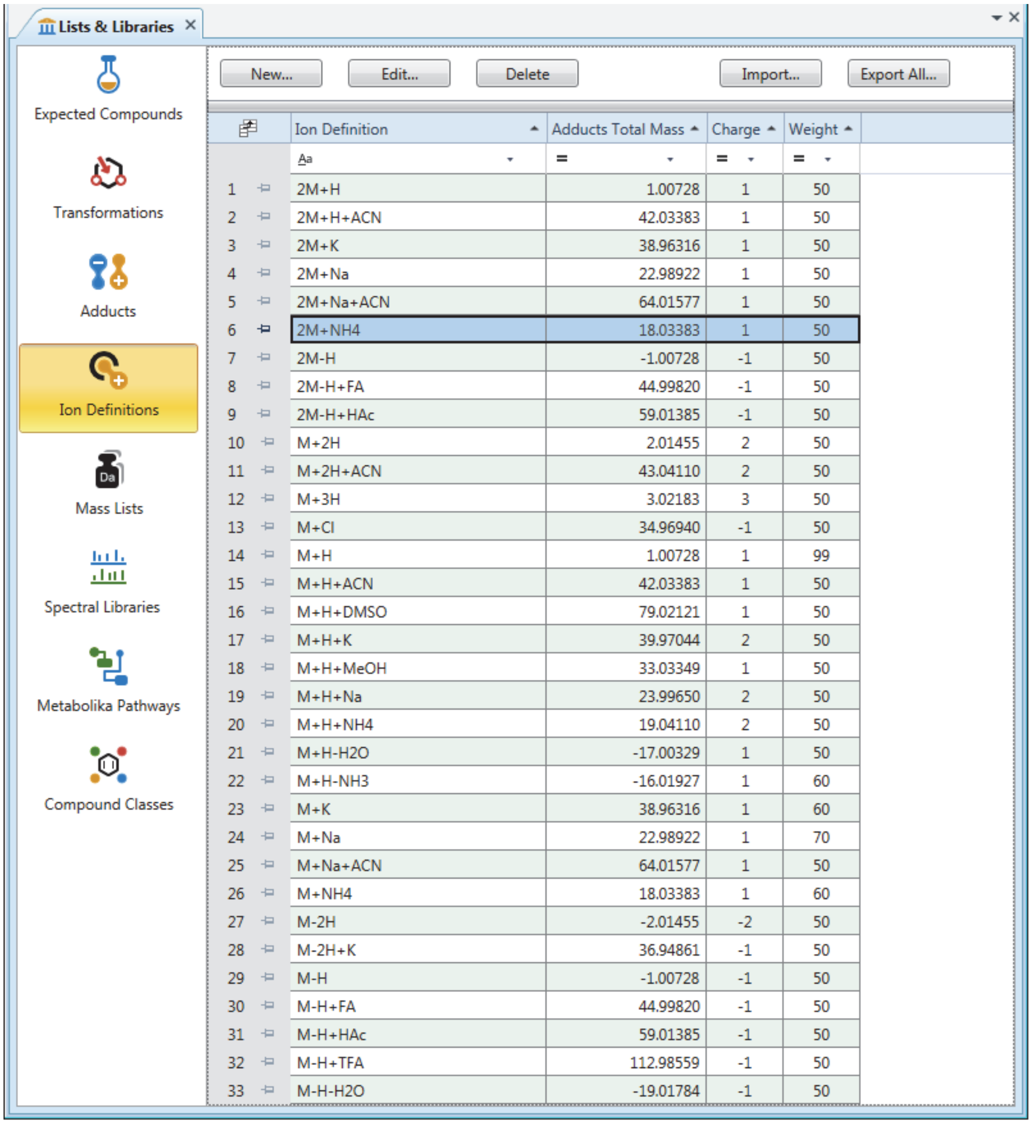
Ion definition	Adducts total mass	Charge	Ion definition	Adducts total mass	Charge
M–H	–1.00728	–1	M–H+FA	44.9982	–1
2M–H	–1.00728	–1	2M–H+FA	44.9982	–1
M–2H	–2.01455	–2	2M–H+HAc	59.01385	–1

Table 104. Common adducts and dimers in the negative ion mode (Sheet 2 of 2)

Ion definition	Adducts total mass	Charge	Ion definition	Adducts total mass	Charge
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 131 shows the default ion definitions.

Figure 131. Ion Definitions view



	Ion Definition	Adducts Total Mass	Charge	Weight
1	2M+H	1.00728	1	50
2	2M+H+ACN	42.03383	1	50
3	2M+K	38.96316	1	50
4	2M+Na	22.98922	1	50
5	2M+Na+ACN	64.01577	1	50
6	2M+NH4	18.03383	1	50
7	2M-H	-1.00728	-1	50
8	2M-H+FA	44.99820	-1	50
9	2M-H+HAc	59.01385	-1	50
10	M+2H	2.01455	2	50
11	M+2H+ACN	43.04110	2	50
12	M+3H	3.02183	3	50
13	M+Cl	34.96940	-1	50
14	M+H	1.00728	1	99
15	M+H+ACN	42.03383	1	50
16	M+H+DMSO	79.02121	1	50
17	M+H+K	39.97044	2	50
18	M+H+MeOH	33.03349	1	50
19	M+H+Na	23.99650	2	50
20	M+H+NH4	19.04110	2	50
21	M+H-H2O	-17.00329	1	50
22	M+H-NH3	-16.01927	1	60
23	M+K	38.96316	1	60
24	M+Na	22.98922	1	70
25	M+Na+ACN	64.01577	1	50
26	M+NH4	18.03383	1	60
27	M-2H	-2.01455	-2	50
28	M-2H+K	36.94861	-1	50
29	M-H	-1.00728	-1	50
30	M-H+FA	44.99820	-1	50
31	M-H+HAc	59.01385	-1	50
32	M-H+TFA	112.98559	-1	50
33	M-H-H2O	-19.01784	-1	50

Follow these procedures as needed:

- To open the Ion Definitions view
- To delete an ion definition
- To import a list of ion definitions from an XML file
- To export the contents of the Expected Compounds view to an XML file

❖ To open the Ion Definitions view

In the application menu bar, choose **Lists & Libraries > Ion Definitions**.

❖ To delete an ion definition

1. In the Ion Definitions view, select the ion definition and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import a list of ion definitions from an XML file

1. In the Ion Definitions view, click **Import**.
2. 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.

3. At the prompt, click **OK**.

❖ To export the entire list of ion definitions to an XML file

1. In the Ion Definitions view, click **Export All**.
2. Select a folder, name the file, and click **Save**.

   The application automatically adds the file name extension (.xml).

3. At the prompt, click **OK**.

Table 105 describes the columns in the Ion Definitions view.

Table 105. Ion Definitions table columns (Sheet 1 of 2)

Column	Description
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.

Table 105. Ion Definitions table columns (Sheet 2 of 2)

Column	Description
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.

Adding or Editing Ion Definitions with the Ion Definition Editor

Use the Ion Definition Editor dialog box to create new ion definitions.

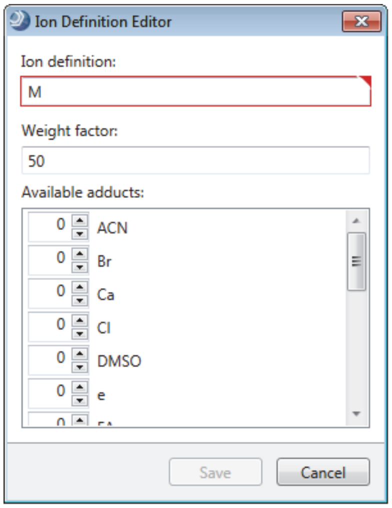
❖ To add ion definitions to the Ion Definitions list

1. Open the Ion Definitions view (see "Working with the Ion Definitions List" on page 397).

2. In the button bar, click **New**.

   The Ion Definition Editor dialog box opens (Figure 132). 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 132. Ion Definition Editor dialog box

   Ion definition: M

   Weight factor: 50

   0 ACN
   0 Br
   0 Ca
   0 Cl
   0 DMSO
   0 e

3. In the Weight Factor box, type the weighting factor for the ion definition.

   Range: 0 to 99

4. To enter an 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–

- Select the current value to the left of the component and type a new integer value.

5. To save the changes, click **Save**.

   The application calculates the ion's charge and difference in mass between the uncharged molecule and the new ion definition. The new ion definition appears in the list.

❖ To edit an ion definition

1. In the Ion Definitions view, select the ion definition.
2. Click **Edit**.

   The Ion Definition Editor opens with the selected definition in the Ion Definition box.

3. To modify an 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–

   - Select the current value to the left of the component and type a new integer value.
4. In the Weight Factor box, type a weighting factor from **0** to **99** for the ion.

   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**, and then click **Yes** at the prompt.

Table 106 describes the parameters in the Ion Definition Editor dialog box.

Table 106. 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. For information about using this list to create ion definitions, see "To add ion definitions to the Ion Definitions list" on page 400.

Modifying the Transformations List

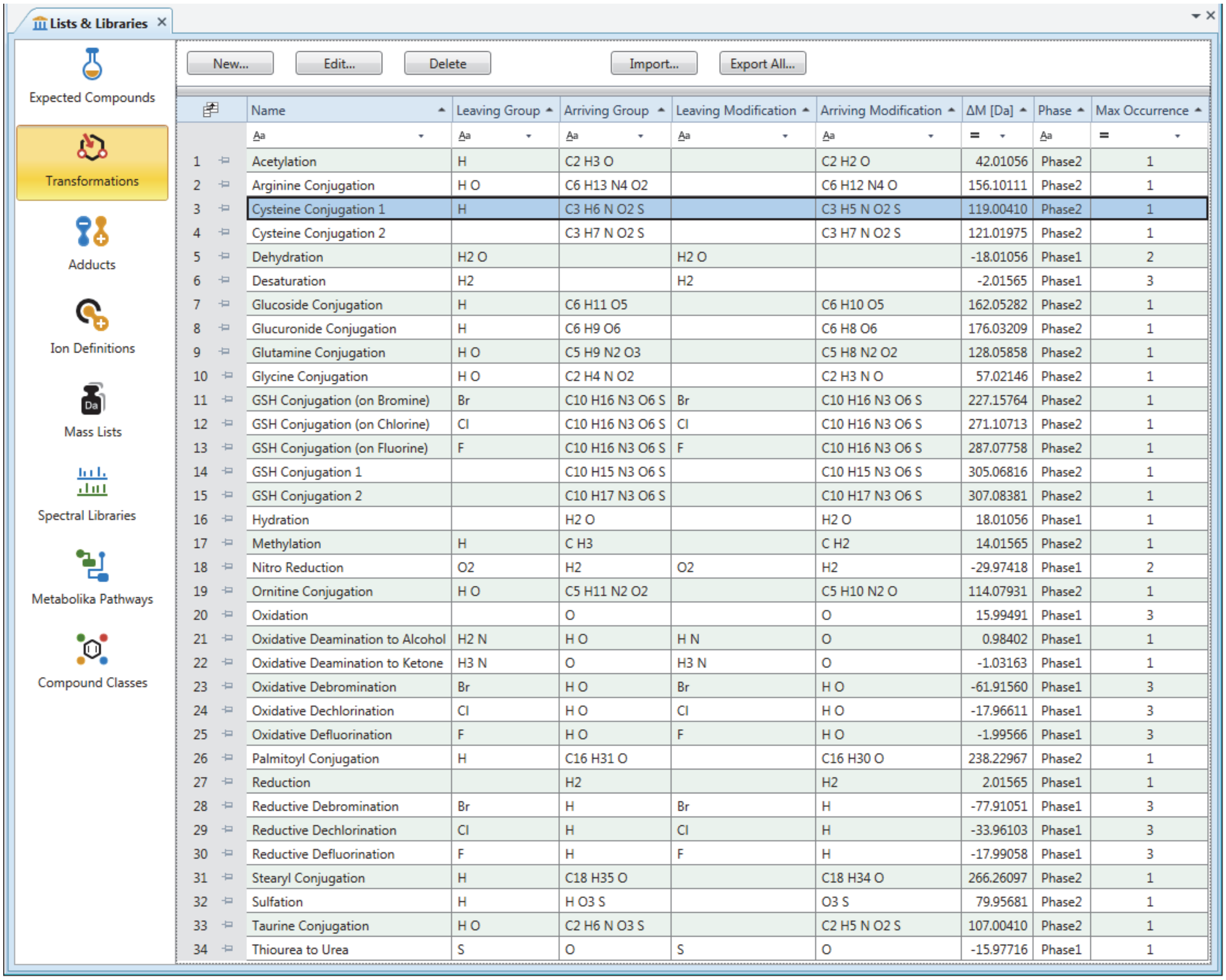
Follow these topics to modify the Transformations list:

- Deleting, Importing, or Exporting Transformations
- Adding or Editing Transformations with the Transformation Editor

Deleting, Importing, or Exporting Transformations

The Transformations view contains a table of possible transformations (Figure 133). 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 compound.

Figure 133. 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	Reduction		H2		H2	2.01565	Phase1	1
28	Reductive Debromination	Br	H	Br	H	-77.91051	Phase1	3
29	Reductive Dechlorination	Cl	H	Cl	H	-33.96103	Phase1	3
30	Reductive Defluorination	F	H	F	H	-17.99058	Phase1	3
31	Stearyl Conjugation	H	C18 H35 O		C18 H34 O	266.26097	Phase2	1
32	Sulfation	H	H O3 S		O3 S	79.95681	Phase2	1
33	Taurine Conjugation	H O	C2 H6 N O3 S		C2 H5 N O2 S	107.00410	Phase2	1
34	Thiourea to Urea	S	O	S	O	-15.97716	Phase1	1

Follow these procedures:

- To open the Transformations view
- To delete an entry from the transformations list
- To import a list of transformations from an XML file
- To export the entire transformations list to an XML file

❖ To open the Transformations view

From the application menu bar, choose **Lists & Libraries > Transformations**.

❖ To delete an entry from the transformations list

1. In the Transformations view, select the entry and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import a list of transformations from an XML file

1. In the Transformations view, click **Import**.
2. 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.

3. At the prompt, click **OK**.

❖ To export the entire transformations list to an XML file

1. In the Transformations view, click **Export All**.
2. Select a folder, name the file, and click **Save**.
3. At the prompt, click **OK**.

Table 107 describes the parameters in the Transformations view.

Table 107. Transformations view features (Sheet 1 of 2)

Feature	Description
Buttons	
New	Opens the Transformation Editor dialog box for creating new transformations.
Edit	Selecting an entry activates this button. Opens the Transformation Editor dialog box for editing the selected transformation.

Table 107. Transformations view features (Sheet 2 of 2)

Feature	Description
Delete	Selecting an entry activates this button. 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.
Table 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.

Adding or Editing Transformations with the Transformation Editor

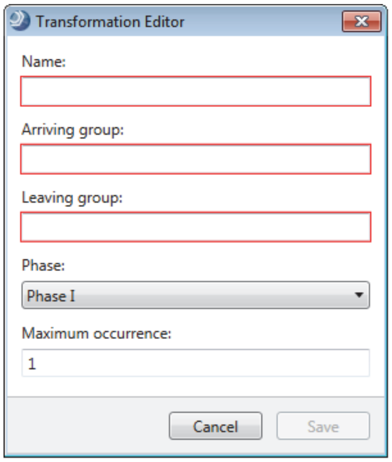
Use the Transformation Editor to add entries to or to edit entries in the transformations list.

❖ To add a transformation to the transformations list

1. In the Transformations view, click **New**.

   The Transformation Editor dialog box opens (Figure 134). 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 134. Transformation Editor dialog box



2. In the Name box, type alphanumeric text to identify the transformation.

   The red outline disappears.

3. Define the transformation as follows:

   a. 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.

   b. 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.

   c. In the Phase list, select **Phase 1** or **Phase 2** for a biotransformation, or select **Other** for other transformation types.

   d. 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.

4. Click **Save**.

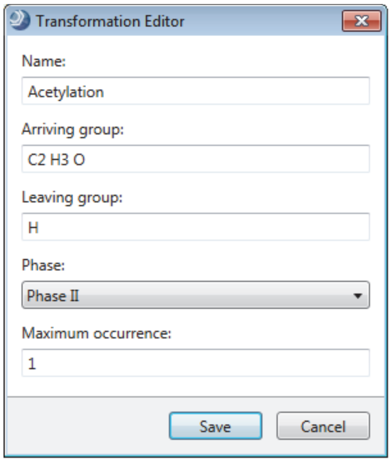
   The Transformation Editor dialog box closes and the new entry appears in the transformations library.

❖ To edit an entry in the transformations list

1. In the Transformations view, 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 135).

   Figure 135. Transformation Editor with information for an acetylation chemical reaction

   Name: Acetylation
   Arriving group: C2 H3 O
   Leaving group: H
   Phase: Phase II
   Maximum occurrence: 1

2. 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.

3. Click **Save** and, at the prompt, click **Yes**.

Table 108 describes the parameters in the Transformation Editor dialog box.

Table 108. 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

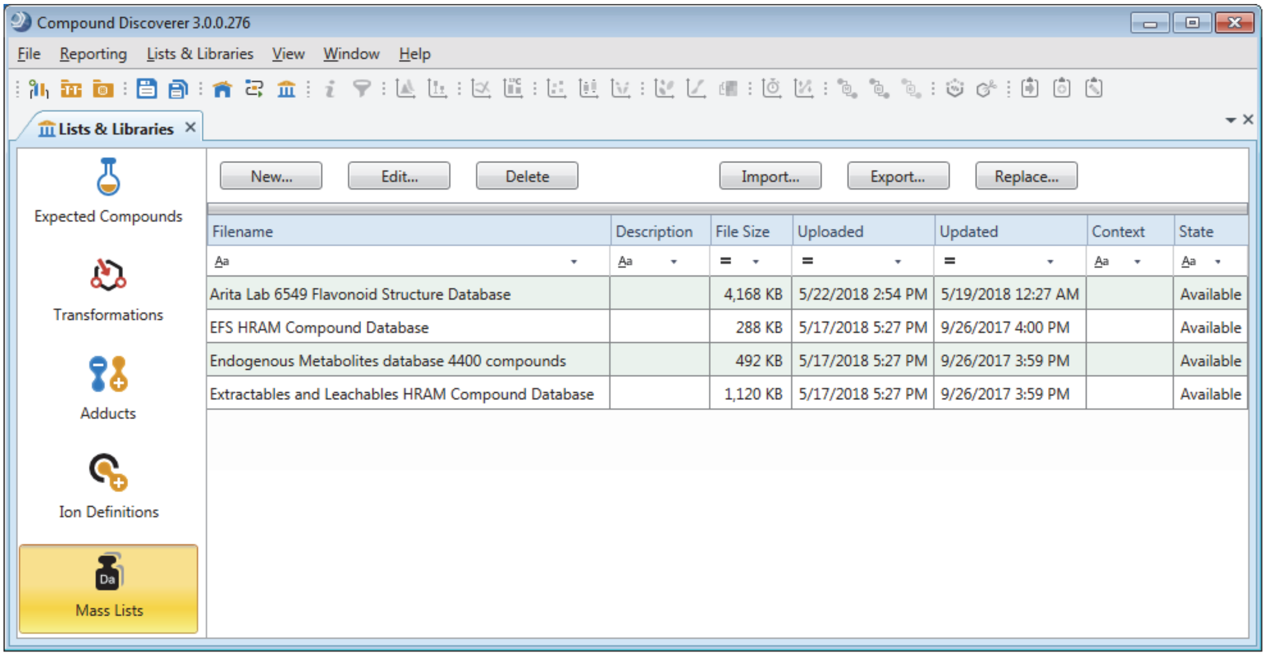
Modifying the Mass Lists Library

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. Figure 136 shows the mass lists that come with the application.

To edit the mass lists library or a mass list, follow these topics:

- Adding, Deleting, Importing, Exporting, and Replacing Mass Lists
- Editing a Mass List
- Adding and Editing Mass List Compounds with the Compound Editor

Figure 136. Mass Lists view



Filename	Description	File Size	Uploaded	Updated	Context	State
Arita Lab 6549 Flavonoid Structure Database		4,168 KB	5/22/2018 2:54 PM	5/19/2018 12:27 AM		Available
EFS HRAM Compound Database		288 KB	5/17/2018 5:27 PM	9/26/2017 4:00 PM		Available
Endogenous Metabolites database 4400 compounds		492 KB	5/17/2018 5:27 PM	9/26/2017 3:59 PM		Available
Extractables and Leachables HRAM Compound Database		1,120 KB	5/17/2018 5:27 PM	9/26/2017 3:59 PM		Available

The application comes with four mass lists:

- Anita Lab Flavenoid Structure Database.massList (with structures)
- Endogenous Metabolites database 4400 compounds.massList
- EFS HRAM Compound Database.massList
- Extractables and Leachables HRAM Compound Database.massList (with structures)

The application can read the following file types:

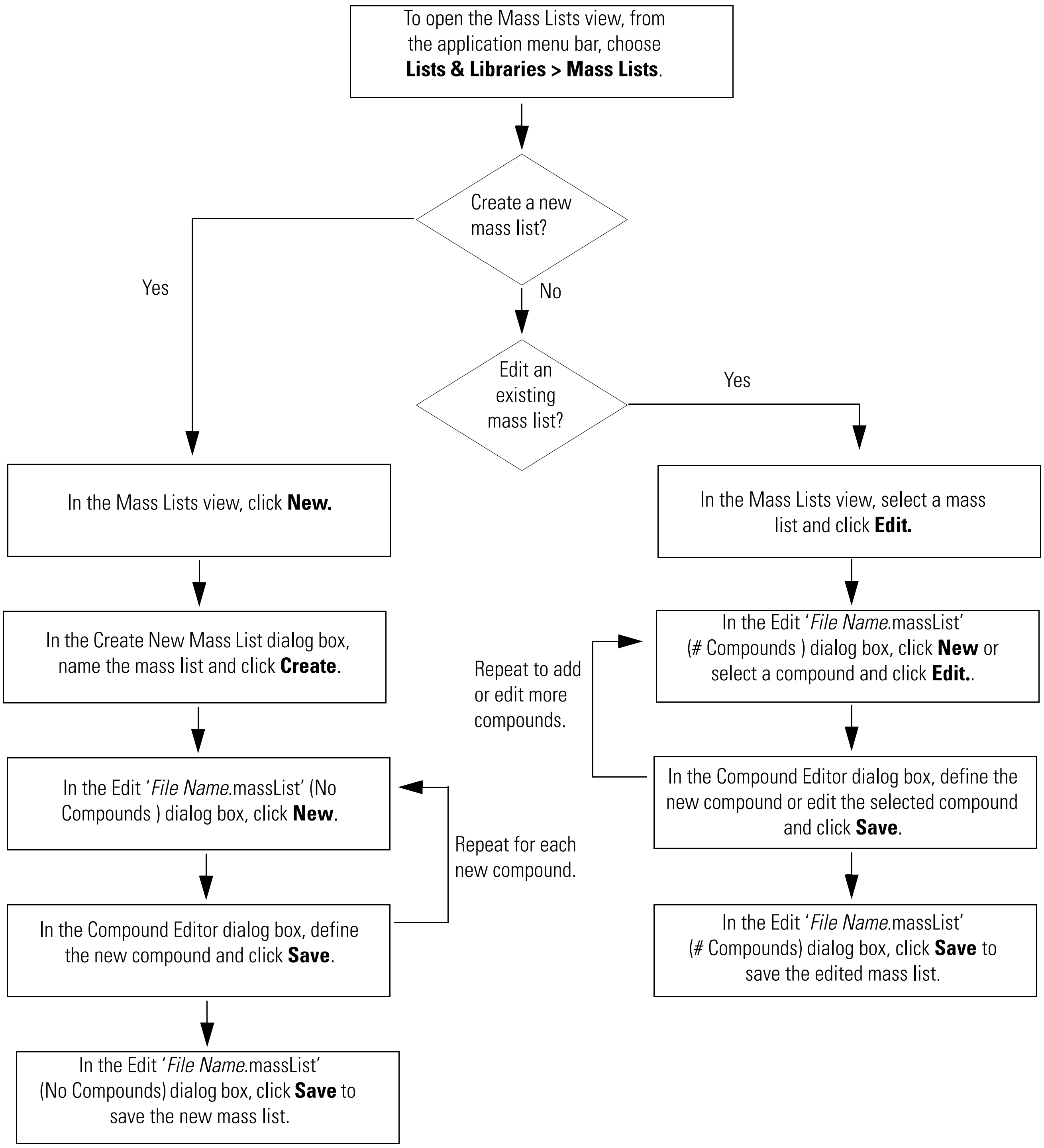
- CSV files with a molecular weight column, an elemental composition column, or both of these columns (For best results, verify that the molecular weight is calculated to five decimal places.)
- CSV files created by exporting a ChemSpider Results table or a Compounds table as plain text.

> **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 (Export All command) in the Expected Compounds library.

Figure 137 shows a flowchart for adding compounds to or editing the compounds in a mass list.

Figure 137. Flowchart for creating and editing mass lists within the application



Adding, Deleting, Importing, Exporting, and Replacing Mass Lists

From the Mass Lists view, you can add, delete, export, and replace mass lists.

Follow these procedures as needed:

- To open the Mass Lists view
- To create a new mass list
- To delete mass list files
- To import a mass list from a CSV file
- To replace a mass list file
- To export a mass list file to a specified file directory

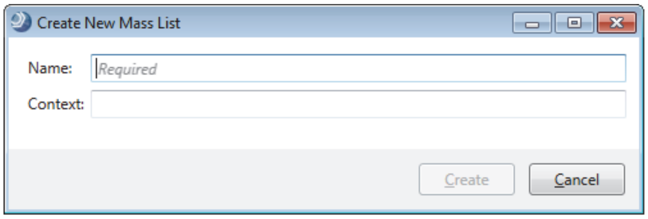
❖ To open the Mass Lists view

From the application menu bar, choose **Lists & Libraries > Mass Lists**.

❖ To create a new mass list

1. In the Mass Lists view, click **New**.

   The Create New Mass List dialog box opens.



2. Name the file and click **Create**.

   The Edit *File Name* (No Compounds) dialog box opens.

3. Go to the next topic, "Editing a Mass List" on page 413.

❖ To delete mass list files

1. In the Mass Lists view, select the entries to delete and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import a mass list from a CSV file

1. In the Mass Lists view, click **Import**.
2. Locate the CSV file and click **Open**.

The Define CSV File Format dialog box opens.

> **Note** Typically, 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. In the Essential Columns area, do the following as needed:
    - 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 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 "Editing a Mass List" on page 413.

❖ To replace a mass list file

1. In the Mass Lists view, select the entry and click **Replace**.
2. Browse to the appropriate folder, select a file, and click **Open**.
    - When you select a result file to replace the existing file, the application automatically reads the mass list.
    - When you select a CSV file, the Define CSV File Format for *file name*.csv dialog box opens if the application does not recognize the file format. Otherwise, the application automatically reads the mass list.

❖ To export a mass list file to a specified file directory

1. In the Mass Lists view, select the file.
2. Click **Export**.
3. Select a folder for the file, rename the file if applicable, and click **Save**.

Table 109 describes the parameters in the Mass Lists view.

Table 109. 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 activates this command.
Delete	Deletes the selected file from the library. Selecting a table row activates this command.
Import	Opens a dialog box for locating and opening a CSV, a massList, 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 activates this command.
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 109. 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.

Editing a Mass List

Use the Edit '*File Name*.massList (# Compounds)' dialog box to modify the compounds list in a mass list. You can add entries to or edit the existing entries in the list.

To edit a mass list, follow these procedures as needed:

- To open a mass list for editing
- To add a compound to or edit a compound in a mass list
- To delete a compound from a mass list
- To import compounds from an XML file into a mass list
- To import compounds from a CSV file into a mass list
- To add a new column to a mass list

❖ To open a mass list for editing

1. From the application menu bar, choose **Lists & Libraries > Mass Lists**.
2. Do one of the following:
   - Create a new mass list (see "To create a new mass list" on page 410).
   - Select a mass list file and click **Edit**.

   –or–

   - Double-click a mass list file.

   The Edit '*File Name* (# Compounds)' dialog box opens with editable entries for the selected mass list.

❖ To add a compound to or edit a compound in a mass list

See "Adding and Editing Mass List Compounds with the Compound Editor" on page 416.

❖ To delete a compound from a mass list

1. Open the mass list for editing.
2. In the Edit '*File Name* (# Compounds)' dialog box, select the compound, and then click **Delete**.
3. Click **Save**.

❖ To import compounds from an XML file into a mass list

1. Open the mass list (see "To open a mass list for editing" on page 413).
2. In the Edit '*File Name* (# Compounds)' dialog box, click **Import**.
3. Locate the XML file and click **Open**.

   Note The XML file must have the same format as an XML file created by exporting all the compounds in the Expected Compounds library to an XML file.

4. Click **Save**.

❖ To import compounds from a CSV file into a mass list

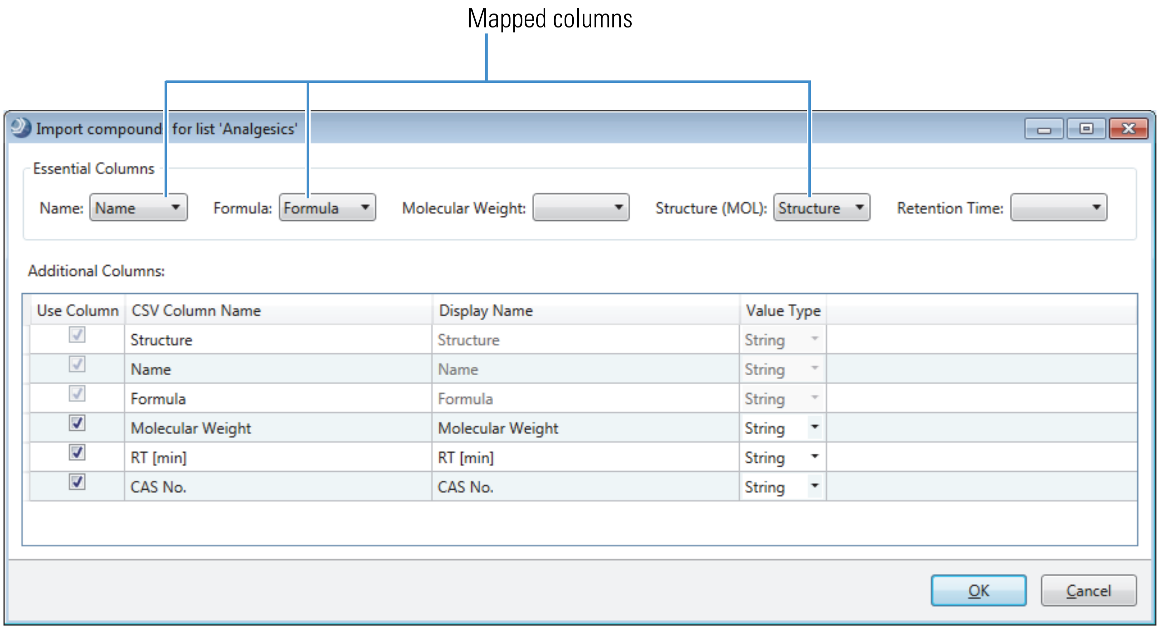
1. Open the mass list (see "To open a mass list for editing" on page 413).
2. In the Edit '*File Name* (# Compounds)' dialog box, click **Import**.
3. Locate the CSV file of interest and click **Open**.

   The Import Compounds for list 'File Name' dialog box opens. When the application maps a CSV column to an essential mass list column, it automatically displays the column name in the appropriate list. In addition, it makes the check box for a recognized essential column unavailable in the Additional Columns area and selects the data type for the column entries.

4. Check the following:
   - In the Essential Columns area, check which CSV columns the application was able to map to the essential columns for a mass list.
   - In the Additional Columns area, check which CSV columns the application was unable to map.

   Figure 138 shows the mapped columns from an imported CSV file.

Figure 138. Import Compounds for list ‘File Name’ dialog box



Essential Columns

Name: Name

Formula: Formula

Molecular Weight:

Structure (MOL): Structure

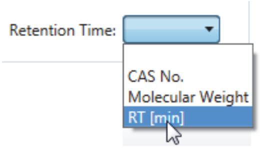
Retention Time:

Additional Columns:

Use Column	CSV Column Name	Display Name	Value Type
☑	Structure	Structure	String
☑	Name	Name	String
☑	Formula	Formula	String
☑	Molecular Weight	Molecular Weight	String
☑	RT [min]	RT [min]	String
☑	CAS No.	CAS No.	String

5. Define any of the remaining columns as appropriate.

   For example, to map the RT [min] column in the CSV file as retention time information that the application can search against, in the Essential Columns area, select RT [min] in the Retention Time list.

6. (Optional) To avoid importing a non-essential CSV column, clear its check box in the Additional Columns area under Use Columns.

7. Click **OK**.

8. In the Edit ‘*File Name* (# Compounds)’ dialog box, click **Save**.

❖ To add a new column to a mass list

1. Open the mass list (see “To open a mass list for editing” on page 413).

2. In the Edit ‘*File Name* (# Compounds)’ dialog box, click **Add Column**.

3. 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**.

4. Click **Save**.

Table 110 describes the buttons at the top of the Edit '*File Name*.massList' (#Compounds) dialog box.

Table 110. 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 activates this command.
Delete	Deletes the selected compound from the mass list. Selecting a compound activates this command.
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.

Adding and Editing 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

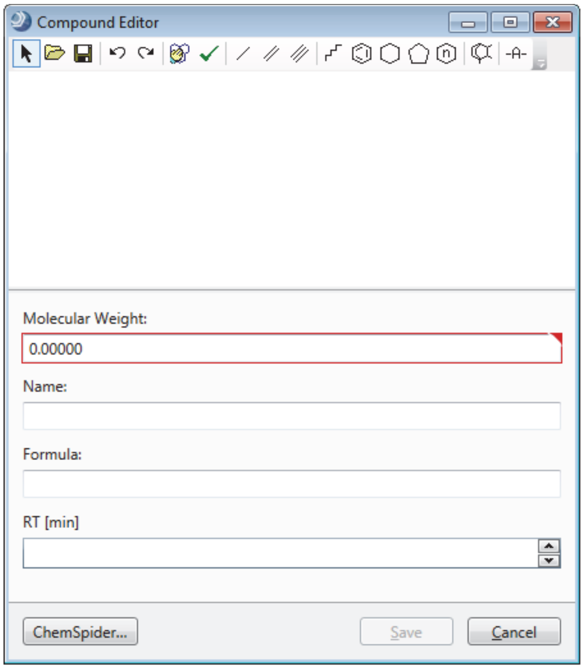
1. From the Mass Lists view, open the mass list for editing (see "Editing a Mass List" on page 413).

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 139). The dialog box is unpopulated for a new compound. The minimum required information is the compound's molecular weight.

   Figure 139. Compound Editor dialog box for editing mass list compounds



0.00000

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: "Using the Structure Drawing Tools or Commands" on page 434, "Loading a Structure from a Structure File" on page 433, and "Finding a Structure in the ChemSpider Database" on page 433.

   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 compound's name.

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 "Filtering Tables" on page 539).

8. To save the changes to the mass list you are editing, click **Save**.

> **Note** If you attempt to close the dialog box without saving the changes, an Unsaved Changes prompt appears.

Modifying the Spectral Libraries List

The mzVault library that comes with the application is a snapshot of the mzCloud database taken in May 2018.

You can create your own custom mzVault libraries by using the mzVault 2.1 application or by exporting the spectral information from a Compound Discoverer result file (see "Exporting Spectral Data to a New or Existing mzVault Library" on page 183).

> **Tip** The Search mzVault node does not require the mzVault application, so installing the mzVault 2.1 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 spectral libraries (created with the Library Manager or mzVault 2.0 or earlier applications) for use in the Compound Discoverer 3.0 application.
>
> You can create new mzVault libraries with the Compound Discoverer 3.0 application, but you are limited to exporting spectra from these result tables: Compounds and Expected Compounds.

> **IMPORTANT** The TraceFinder 5.0 application is compatible with the mzVault 2.1 application. Before converting Library Manager or mzVault libraries to the mzVault 2.1 format, keep copies of the original format so that you can still use them in earlier versions of the TraceFinder application. To use your own mzVault spectral libraries in the Compound Discoverer application, add them to the Spectral Libraries list.

Follow these procedures as needed.

> **Note** You cannot edit spectral libraries in the Compound Discoverer application. The Edit button in the command bar is unavailable.

❖ To open the Spectral Libraries list

From the application menu bar, choose **Lists & Libraries > Spectral Libraries**.

❖ To add an mzVault library to the list

Click **Import**, locate the library, and click **Open**.

❖ To replace an mzVault library

1. In the Spectral Libraries view, select the library.
2. Click **Replace**, locate the library, and click **Open**.

❖ To export an mzVault library

1. In the Spectral Libraries view, select the library.
2. Click **Export**, select a folder, and click **Save**.

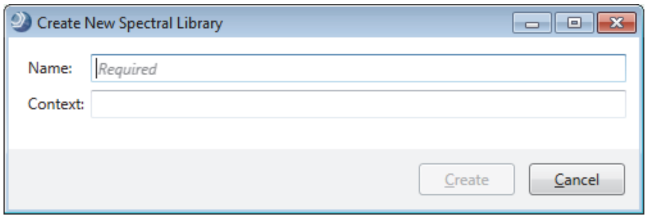
❖ To delete an mzVault library

In the Spectral Libraries view, select the library and click **Delete**.

❖ To create a new empty mzVault library

1. In the Spectral Libraries view, click **New**.

   The Create New Spectral Library dialog box opens.

   Create New Spectral Library

   Name: Required

   Context:

2. Name the file and click **Create**.

Modifying the Metabolika Pathways List

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.

Follow these topics as needed:

- Deleting, Importing, Exporting, and Replacing Metabolika Pathways
- Editing Metabolika Pathways
- Adding and Editing Pathway Structures with the Compound Editor

Deleting, Importing, Exporting, and Replacing Metabolika Pathways

Follow these procedures as needed.

❖ To delete pathways

1. In the Metabolika Pathways view, select the pathways and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import pathway files

1. In the Metabolika Pathways view, click **Import**.
2. Locate the files (.metabolika) and click **Open**.

❖ To export 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.

❖ To replace a pathway

1. In the Metabolika Pathways view, select the pathway, and then click **Replace**.
2. Locate the replacement file and click **Open**.

Editing Metabolika Pathways

Use the Edit '*File Name*.metabolika' dialog box to create a new or edit an existing Metabolika pathway.

To create or edit a pathway, follow these topics:

- Creating a New Pathway
- Editing an Existing Pathway
- Modifying Pathway Arrows
- Shortcut Menu for the Metabolika Pathway Editor

Creating a New Pathway

❖ To edit a new (empty) pathway

1. From the application menu bar, choose **Lists & Libraries** > **Metabolika Pathways**.
1. In the Metabolika Pathways view, click **New**.

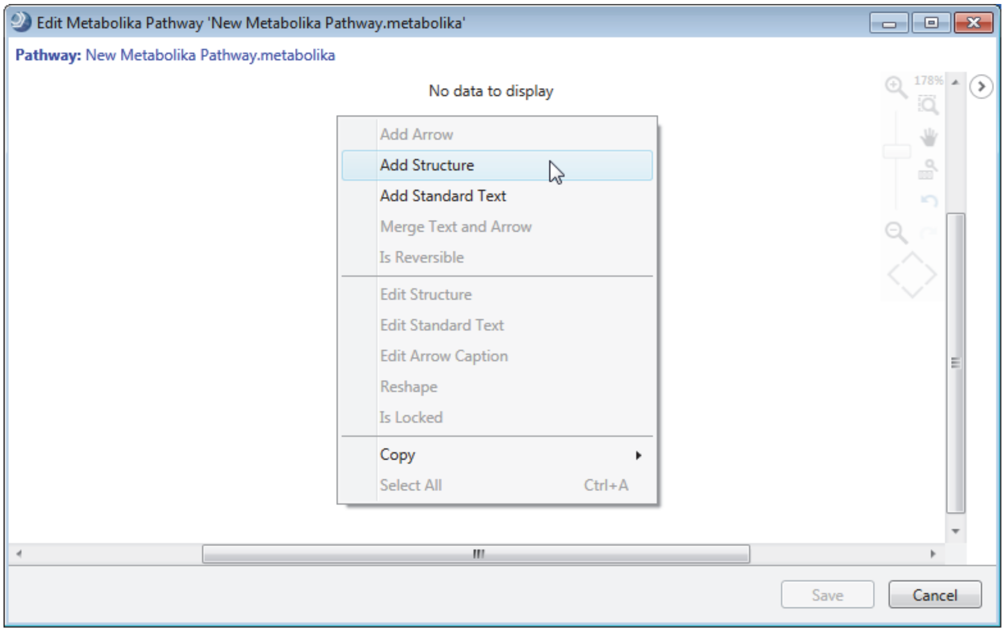
   The Create New Metabolika Pathway dialog box opens.

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 140. Metabolika pathway editor with shortcut menu

   Edit Metabolika Pathway 'New Metabolika Pathway.metabolika'

   Pathway: New Metabolika Pathway.metabolika

   No data to display

   The Compound Editor opens.

4. Use the Compound Editor to add new structures (see "Adding and Editing Pathway Structures with the Compound Editor" on page 425).
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 arrow head and four anchor points (Figure 141). To change the arrow's properties, see "Modifying Pathway Arrows" on page 423.

   Figure 141. 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.

Editing an Existing Pathway

❖ To edit an existing 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 "Modifying Pathway Arrows."
3. To undo a change, use the CTRL+Z keys.

   You can undo up to six changes.

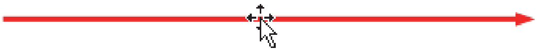
Modifying Pathway Arrows

To modify the arrows in a Metabolika pathway, follow these procedures as needed:

- To move an arrow
- To change an arrow's angle
- To change an arrow's curvature
- To make an arrow bidirectional to represent a reversible reaction
- To merge arrows
- To add an arrow caption

❖ To move an arrow

1. Select the arrow and hold down the left mouse button to display the move pointer (✥).



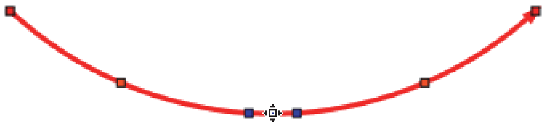
2. Drag the arrow to another location.

❖ To change an arrow's angle

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 needed.

❖ To change an arrow's curvature

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 needed.



❖ To straighten a curved arrow

Right-click it and choose **Reshape**.

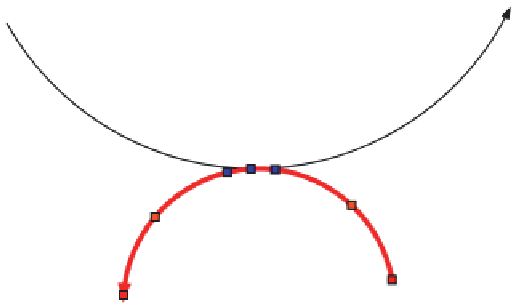
❖ To make an arrow bidirectional to represent a reversible reaction

Right-click it and choose **Is Reversible**.

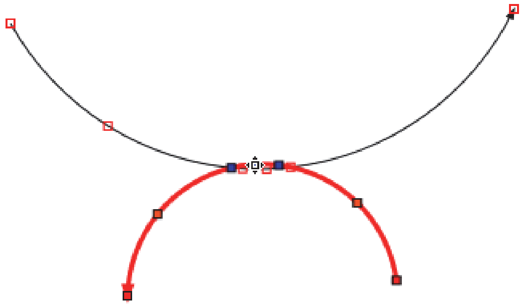
❖ To merge arrows

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. Then, release the mouse button.



5. To straighten one of the merged arrows, right-click it and choose **Reshape**.

❖ To 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**.

Character style	Tag
Bold	
Superscript	
Subscript	

3. To lock the caption to the arrow, right-click the arrow and choose **Is Locked**.

Shortcut Menu for the Metabolika Pathway Editor

Table 111 describes the shortcut menu for the Metabolika pathway editor.

Table 111. 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.

Adding and Editing Pathway Structures with the Compound Editor

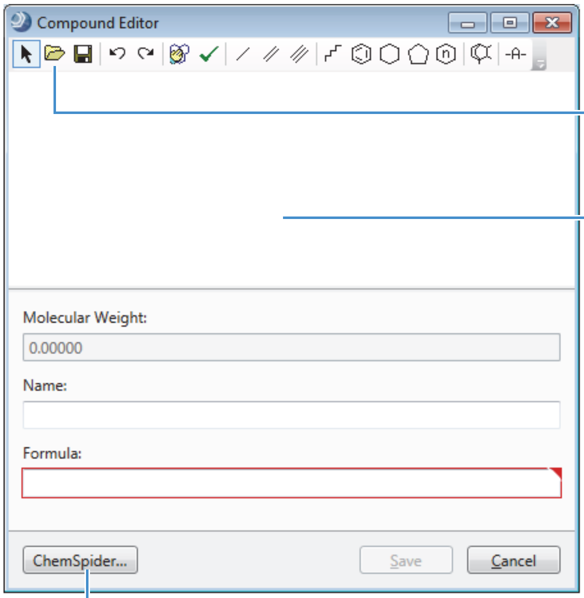
Use the Compound Editor to add structures to and edit the structures in a Metabolika pathway.

❖ To edit or add a pathway structure

1. Open the Compound Editor for editing and adding Metabolika pathway structures (see "Adding and Editing Mass List Compounds with the Compound Editor" on page 416).

   Figure 142 shows the Compound Editor dialog box for a new structure.

Figure 142. Compound Editor dialog box for editing Metabolika pathway structures



Molecular Weight: 0.00000

Click to locate and open a structure file.

Drawing area

Opens the ChemSpider application

2. Do one of the following:

   - When adding a new structure, use the drawing tools, load a structure file, or use the ChemSpider application (see “Using the Structure Drawing Tools or Commands” on page 434, “Loading a Structure from a Structure File” on page 433, or “Finding a Structure in the ChemSpider Database” on page 433).

     The application automatically populates the Molecular Weight and Formula boxes.

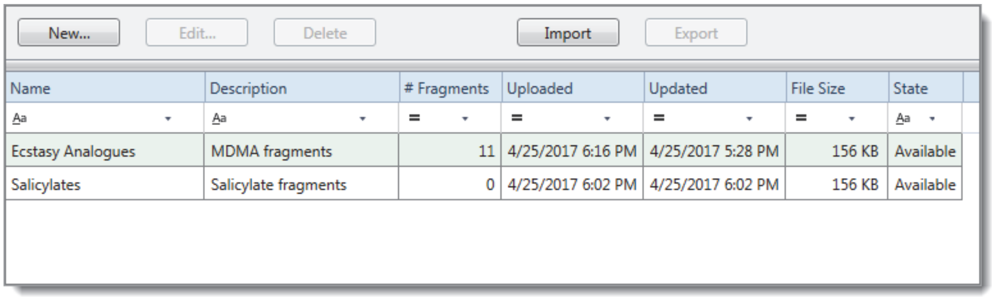
   - When editing an existing structure, you are limited to structures that match the current molecular weight and formula.

Modifying the Compound Classes List

When the processing workflow includes the Compound Class Scoring Node, the application can determine the probability that an unknown compound belongs to the user-defined compound classes by comparing the ions detected in the fragmentation scans to user-defined compound classes.

Use the Compound Classes view, the Edit '*Named Compound Class*' dialog box, and the Fragmentation Editor to create a list of compound class libraries. Figure 143 shows the Compound Classes view.

Figure 143. Compound Classes view



Name	Description	# Fragments	Uploaded	Updated	File Size	State
Ecstasy Analogues	MDMA fragments	11	4/25/2017 6:16 PM	4/25/2017 5:28 PM	156 KB	Available
Salicylates	Salicylate fragments	0	4/25/2017 6:02 PM	4/25/2017 6:02 PM	156 KB	Available

Follow these procedures as needed:

- To open the Compound Classes library
- To add new compound classes to the Compound Classes library
- To edit a compound class
- To delete a compound class
- To import a compound class library file (.clib)
- To export a compound class

❖ To open the Compound Classes library

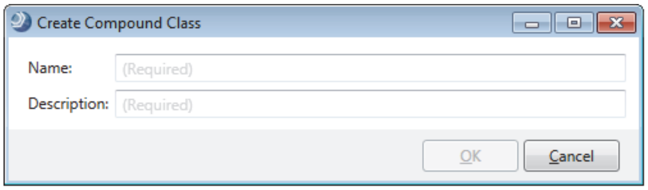
From the menu bar, choose **Lists & Libraries > Compound Classes**.

❖ To add new compound classes to the Compound Classes library

1. In the Compound Classes view, click **New**.

   The Create Compound Class dialog box opens (Figure 144).

Figure 144. Create Compound Class dialog box

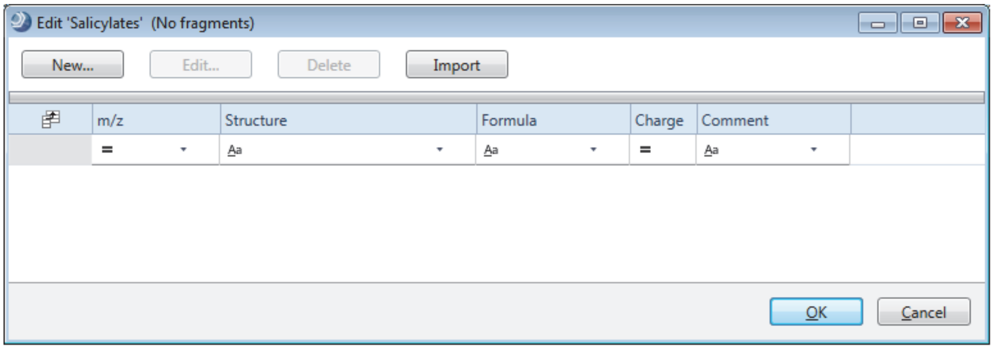


Name: (Required)
Description: (Required)

2. Name the class, provide a brief description, and click **OK**.

   The named compound class appears as a new row in the Compound Classes view and the Edit '*Named Compound Class*' dialog box opens (Figure 145). For information about this dialog box, see "Compound Class Editor" on page 430.

   Figure 145. Edit '*Named Compound Class*' dialog box



3. In the Edit '*Named Compound Class*' dialog box, click **New**.
4. In the Fragment Editor, define the fragments for the compound class as described in "Using the Fragment Editor" on page 431.
5. Click **OK** to close the Edit '*Named Compound Class*' dialog box.

❖ To edit a compound class

1. In the Compound Classes view, select the compound class of interest and click **Edit**.

   The Edit '*Named Compound Class*' dialog box opens with a list of fragments.

2. Do the following as needed:
   - To add a new fragment by using the Fragment Editor, click **New**. Then, use the Fragment Editor to define the fragment (see "Using the Fragment Editor" on page 431).
   - To add new fragments by importing their structures from a CSV or SDF file, click **Import**.
   - To edit a fragment, select it and click **Edit**.
   - To delete a fragment, select it and click **Delete**.
3. Close the dialog box to return to the library.

❖ To delete a compound class

1. In the Compound Classes view, select the compound class of interest and click **Delete**.
2. At the prompt, click **Yes**.

❖ To import a compound class library file (.clib)

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 > Server Files 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.

❖ To export a compound class

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 as needed, and click **Save**.

Table 112 describes the features of the Compound Classes view.

Table 112. Compound Classes view parameters (Sheet 1 of 2)

Feature	Description
Commands	
New	Opens the Create Compound Class dialog box for naming and describing the new compound class.
Edit	Opens the Edit '*Named Compound Class*' dialog box for editing the selected compound class file.
Delete	Deletes the selected compound class file.
Import	Opens the Open dialog box for selecting a .clib file.
Export	Opens the Save As dialog box for selecting a file name and location for the exported .clib file.
Table columns	
Name	Displays the name of the .clib file.
Description	Displays a description of the file.
# Fragments	Displays the number of fragments in the file.

Table 112. Compound Classes view parameters (Sheet 2 of 2)

Feature	Description
Uploaded	Displays the date (month/day/year) and time (hour/minute) when you added the class to the library in the following format: MM/DD/yyyy HH:mm
Updated	Displays the data and time when the file was updated.
File Size	Displays the size of the file.
State	Displays Available when an uncorrupted file with the specified name exists in the following folder: *Drive X* > ProgramData > Thermo > Compound Discoverer *X.X* > ServerFiles

Compound Class Editor

Table 113 describes the buttons and columns in the compound class editor. For information about using the compound class editor, see "Modifying the Compound Classes List" on page 427.

Table 113. Edit 'Named Compound Class dialog box parameters

Parameters	Description
Buttons	
New	Opens the Fragment Editor for defining a fragment (see "Using the Fragment Editor" on page 431).
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 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.

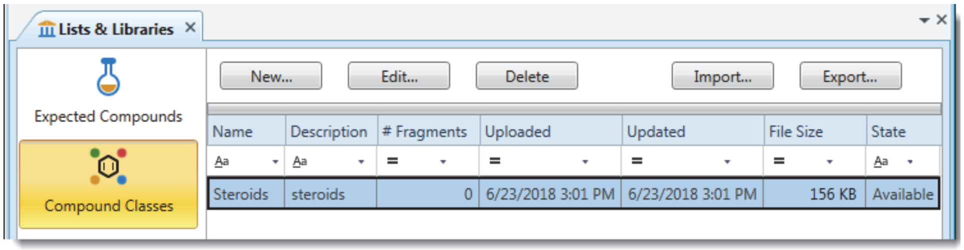
Using the Fragment Editor

Use the Fragment Editor to define fragments for a compound class.

> **Note** For information about using the Fragment Editor's drawing tools, see "Using the Structure Drawing Tools or Commands" on page 434.

❖ 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:
   a. Select a library and click **Edit**.

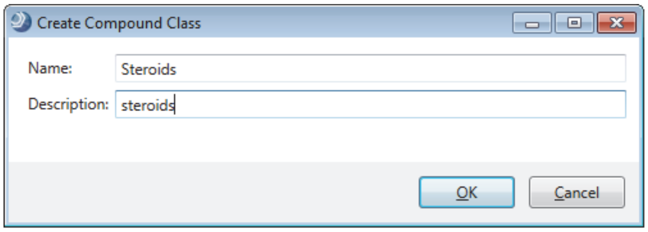


Name	Description	# Fragments	Uploaded	Updated	File Size	State
Steroids	steroids	0	6/23/2018 3:01 PM	6/23/2018 3:01 PM	156 KB	Available

   b. In the Edit '*Named Compound Class*' dialog box, select a fragment and click **Edit**.

–or–

   a. Click **New**.
   b. In the Create Compound Class dialog box, name the library, type a description, and click **OK**.



Name: Steroids

Description: steroids

   c. In the Edit '*Named Compound Class*' (No Fragments) dialog box, click **New**.

mk:@MSITStore:C:\Users\alison.cook\Desktop\CompoundDiscoverer.chm::/Compound_Discoverer_User_Libraries.11.30.htm

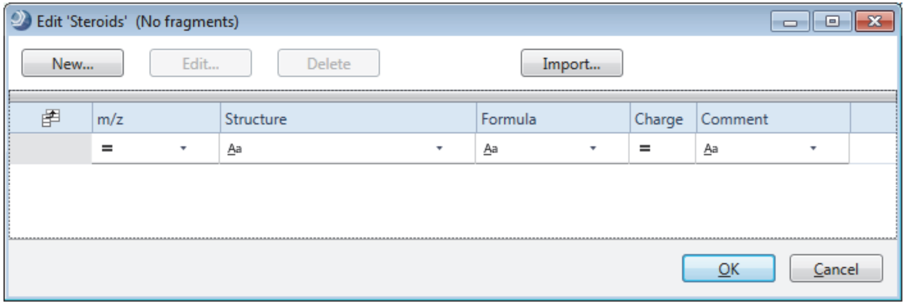
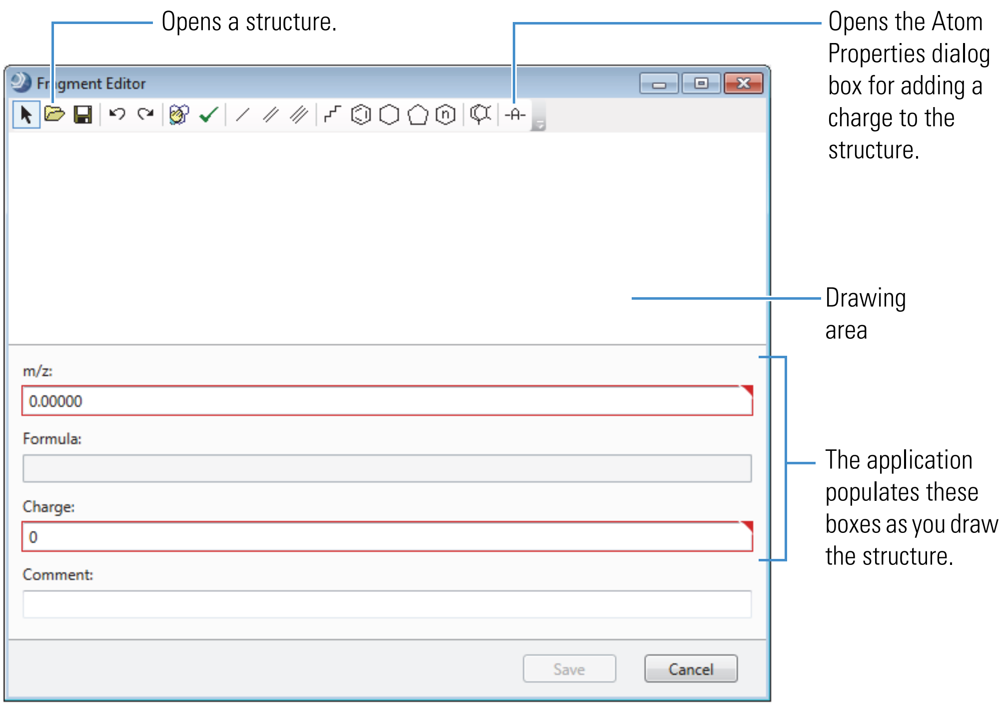


Figure 146 shows the Fragment Editor dialog box.

Figure 146. Fragment Editor dialog box



m/z: 0.00000

Formula:

Charge: 0

Comment:

Opens a structure.

Opens the Atom Properties dialog box for adding a charge to the structure.

Drawing area

The application populates these boxes as you draw the structure.

❖ To use the drawing tools to add a structure to the drawing area

See “Using the Structure Drawing Tools or Commands” on page 434.

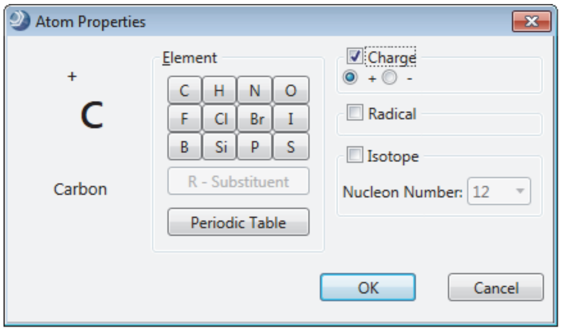
❖ To open a structure file

See “Loading a Structure from a Structure File” on page 433.

❖ To add a charge to a structure

1. In the drawing area of the Fragment Editor, select the atom where you want to add a charge.
2. Click the **Atom Properties** icon, -A-.
3. In the Atom Properties dialog box, select the **Charge** check box (Figure 147).

Figure 147. Atom Properties dialog box with an available Charge check box



4. Select the positive or negative option.
5. Click **OK**.

Loading a Structure from a Structure File

From the Compound Editor or the Fragment Editor, you can load a structure from a structure file.

❖ 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.

Finding a Structure in the ChemSpider Database

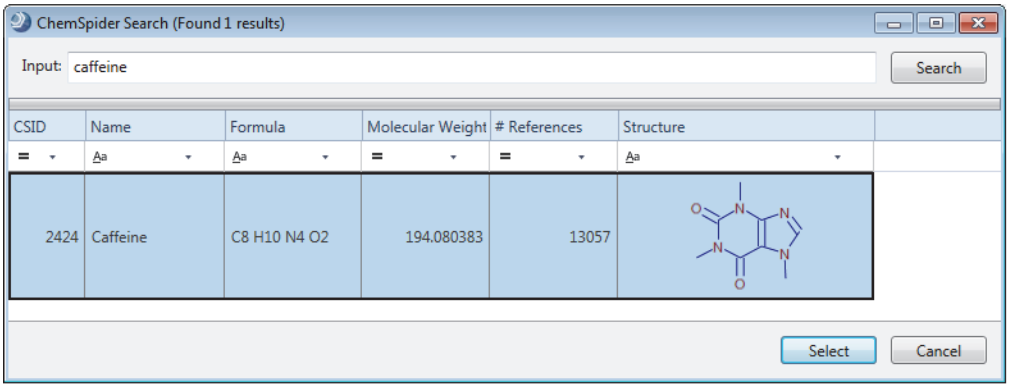
You can access the ChemSpider database from the Compound Editor dialog box, the Compound Annotation Editor dialog box, or the mzLogic Analysis view and search for a compound entry with a structure file.

❖ To load a structure into the drawing area

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.



Input: caffeine

CSID	Name	Formula	Molecular Weight	# References	Structure
2424	Caffeine	C8 H10 N4 O2	194.080383	13057	

5. Click **Select**.

   The chemical structure appears in the drawing pane and the compound's molecular weight, name, and formula appear in their respective fields.

Using the Structure Drawing Tools or Commands

The Compound Editors and the Fragment Editor include a set of drawing tools.

Use the editor toolbar and the shortcut menu for the drawing area to draw, manipulate, and save structures as described in the following topics:

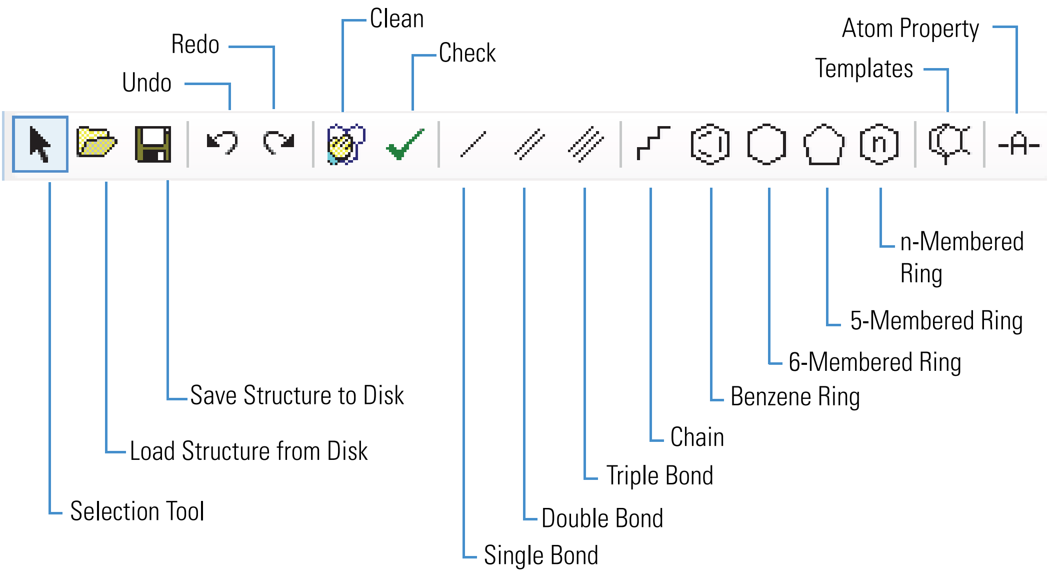
- Compound Editor Toolbar and Fragment Editor Toolbar
- Shortcut Menu Commands for the Drawing Area
- Using the Structure Icons
- Using the Template Tool
- Checking the Validity of a Structure
- Manipulating Structures
- Modifying Atoms and Bonds
- Saving a Structure
- Editing Atom Properties

> **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.

Compound Editor Toolbar and Fragment Editor Toolbar

The Compound Editor and Fragment Editor dialog boxes have the same set of toolbar icons (Figure 148).

Figure 148. Editor toolbar



Shortcut Menu Commands for the Drawing Area

The Compound Editor dialog boxes and the Fragment Editor dialog box include a drawing area for adding a two-dimensional structure.

Table 114 describes the drawing area's shortcut menu commands.

Table 114. Shortcut menu commands for the drawing area (Sheet 1 of 2)

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 (see "To resize a structure" on page 439).

Table 114. Shortcut menu commands for the drawing area (Sheet 2 of 2)

Menu command	Description
Rotate	Rotates the structure around the selected axis of rotation (see "To rotate a structure" on page 439).
Mirror	Reflects the structure along its vertical or horizontal axis (see "To mirror a structure" on page 439).

Using the 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 as described in "Using the Template Tool."

   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 as described in "Modifying Atoms and Bonds" on page 440.

Using the Template Tool

Use the template tool to draw closely related chemical structures as described in these procedures:

- To open a template structure
- To create a template structure

❖ To open a template structure

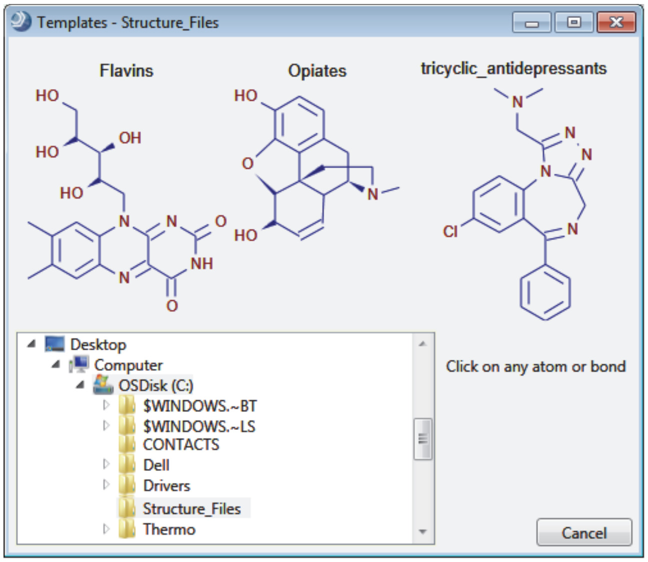
1. Click the **Templates** icon, .

   The Templates dialog box opens.

2. 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 (Figure 149). The application displays all of the structures in the folder. It does not differentiate between MOL files and Template files.

   Figure 149. Templates dialog box with a view of the stored structures



3. 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.

4. To place the selected structure in the drawing area, click the drawing area.

❖ To create a template structure

1. Open a structure file or draw a structure in the drawing area.
2. In the Compound Editor 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**.

Checking the Validity of a Structure

The application does 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.

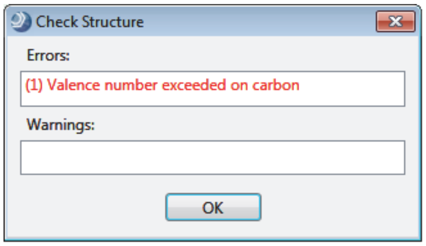
Note The check structure tool does not perform quantum mechanical or thermodynamical calculations that address possible structural stability.

❖ 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 150).

   Figure 150. Check Structure message

   Check Structure

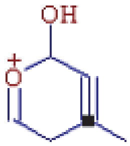
   Errors:

   (1) Valence number exceeded on carbon

   Warnings:

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.

Manipulating Structures

To manipulate a structure, follow these procedures:

- To resize a structure
- To rotate a structure
- To mirror a structure
- To clean a structure

❖ To resize a structure

1. Select the structure or part of the structure you want to resize.
2. Right-click and choose **Resize**.
3. Drag one of the small rectangles on the structure's edge and release the mouse button.

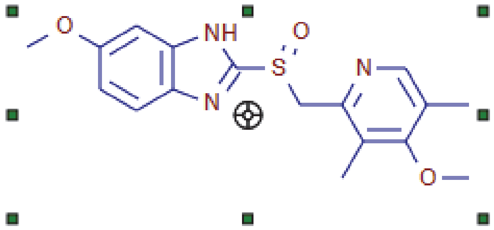
   Dragging one of the diagonal rectangles keeps the aspect ratio constant during structure resizing.

❖ To rotate a structure

1. Select the structure or part of the structure 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 structure's edge.

❖ To mirror a structure

1. Select the structure or part of the structure you want to mirror.
2. Right-click and choose **Mirror**.
3. Click one of the small rectangles on the structure's edge.
   - 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.

❖ To clean a structure

1. Do one of the following:

   - Select an entire structure.

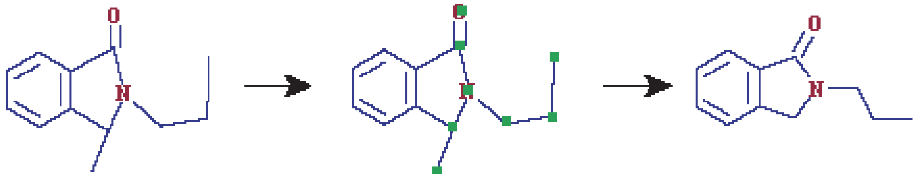
   –or–

   - Select only the atoms 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.



Note In some complicated cases, the Clean function can lead to structures that you might not find satisfactory. If this occurs, click the **Undo** icon, ↶.

After finishing a structure drawing, always check for errors before proceeding.

Modifying Atoms and Bonds

To modify or add elements to a structure or to modify or add bonds to a structure, follow these procedures:

- Selecting Atoms and Bonds
- Editing Bond Properties

For information about editing the atom properties, see "Editing Atom Properties" on page 442.

Selecting Atoms and Bonds

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.

Follow these procedures:

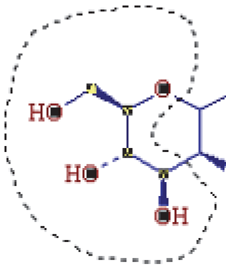
- To select an individual atom or bond
- To choose a selection mode
- To select a group of atoms that are adjacent to each other
- To select all of the atoms and bonds in the structure
- To move a structure

❖ To select an individual atom or bond

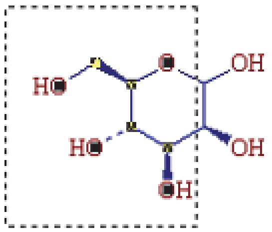
Click the **Selection Tool** icon, and then click the individual atom or bond.

❖ To 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

❖ To select a group of atoms that are adjacent to each other

Do one of the following:

- Right-click and choose **Rectangle Selection**. Then drag the cursor to form a rectangle around the atoms.

–or–

- Right-click and choose **Lasso Selection**. Then draw a free-form shape around the atoms.

❖ To select all of the atoms and bonds in the structure

Do one of the following:

- Right-click the drawing area and choose **Select All**.

–or–

- Click the **Selection Tool** icon, and then double-click anywhere in the drawing area, except on atoms or bonds.

❖ **To move a structure**

1. Select the atoms or bonds that you want to move.
2. Drag the selected structures to a new location.

❖ **To move all of 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.

Editing Bond Properties

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.

Saving a Structure

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**.

Editing 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 "Using the Structure Drawing Tools or Commands" on page 434.

IMPORTANT The application does not support compounds with a charge or radical nor does it support the R-Substituent feature.

❖ To edit the element or nucleon number of a single atom

1. Open the Compound Editor dialog box as described in “To open the Compound Editor dialog box” on page 392.

2. Click the **Selection Tool** icon, .

3. Do one of the following:

   - Double-click the atom that you want to change.

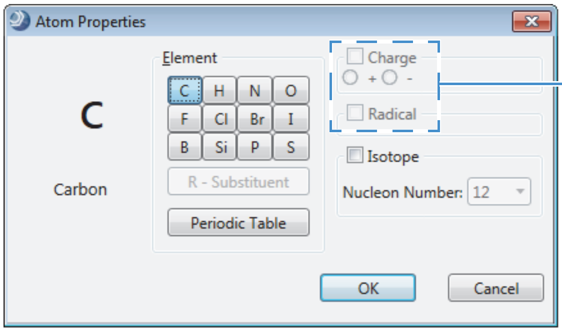
   –or–

   - Select the atom that you want to change and click the **Atom Properties** icon, -A-.

   The Atom Properties dialog box opens with the properties of the selected atom displayed. The Charge and Radical check boxes are not available for compounds.

   > **Tip** To add charges to fragment structures for a Compound Class library, see “Using the Fragment Editor” on page 431.

   Figure 151. Atom Properties dialog box, showing the properties for carbon



Nucleon Number: 12

The Charge and Radical check boxes are not available for compounds.

4. To change the element, do the following:

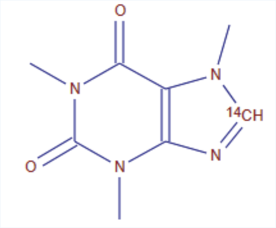
   - To change the atom to an element that is in the Element area, click the appropriate Element button.

   - 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 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.



6. When you finish editing the selected atom, click **OK**.

   Changes you make in the Atom Properties dialog box affect only the selected atom.

11

Using the License Manager

Use the License Manager to install new processing workflow nodes as they become available and to activate the software license.

Contents

Opening the License Manager

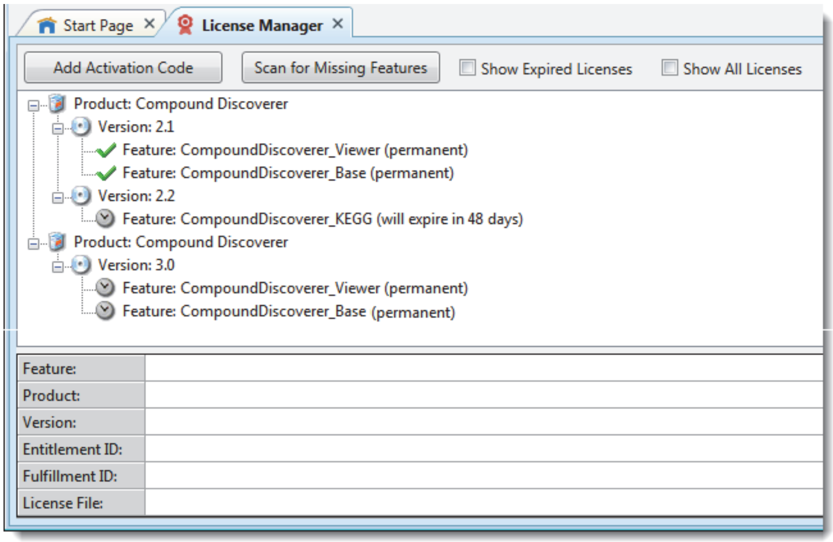
Access the License Manager page from the Help menu.

❖ 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 152). For information about the shortcut menu commands for the License Manager page, see "Working with Tabbed Pages and Dockable Views" on page 44.

Figure 152. License Manager page



```
Product: Compound Discoverer
    Version: 2.1
        Feature: CompoundDiscoverer_Viewer (permanent)
        Feature: CompoundDiscoverer_Base (permanent)
    Version: 2.2
        Feature: CompoundDiscoverer_KEGG (will expire in 48 days)
Product: Compound Discoverer
    Version: 3.0
        Feature: CompoundDiscoverer_Viewer (permanent)
        Feature: CompoundDiscoverer_Base (permanent)
```

Table 115 describes the License Manager command bar.

Table 115. License Manager command bar

Command or feature	Description
Add Activation Code	Opens the License Activation dialog box where you can apply a new license and activate the application on the current computer.
Scan for Missing Features	Activates a scan for newly installed processing workflow nodes.
Show Expired Licenses	Selecting this check box displays any expired licenses.
Show All Licenses	Selecting this check box displays the status of your licensed Thermo Scientific software applications.

Installing or Updating 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.

12

Setting Up the Configuration Options

To set up the application's configuration options, follow these topics.

Contents

Opening the Configuration Page

Use the Configuration page to set up the application's global configuration options.

❖ **To open the Configuration page**

From the menu bar, choose **Help > Configuration**.

Selecting the Maximum Number of Parallel Processing Jobs

Use the Parallel Options 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 left pane of the Configuration page, under Server Settings, select **Parallel Options**.

2. In the Parallel Options view, 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.

3. Click **Save Current Settings**.

Selecting Where to Store Temporary Data

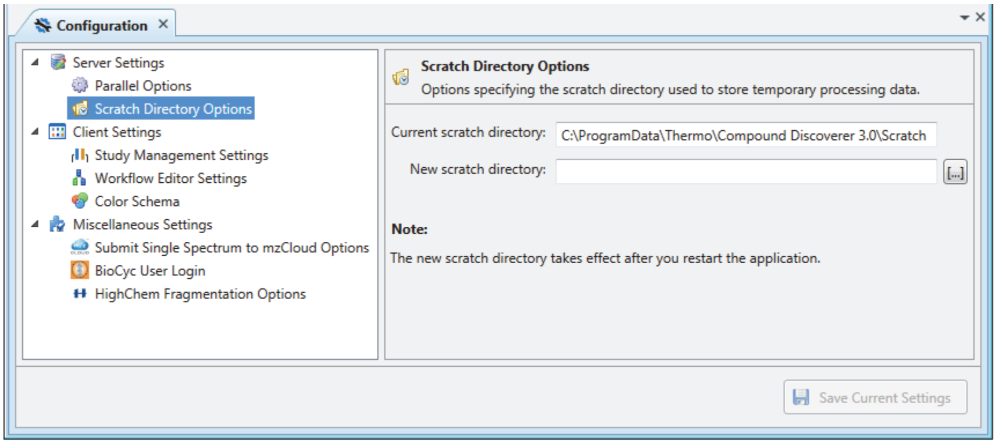
Use the Scratch Directory Options view of the Configuration page to change the folder where the application stores temporary data during data processing.

❖ To change the scratch directory

1. In the left pane of the Configuration page, under Server Settings, select **Scratch Directory Options**.

   The Current Scratch Directory box lists the current location of the scratch folder.

   Figure 153. Scratch Directory Options view



Scratch Directory Options

Options specifying the scratch directory used to store temporary processing data.

Current scratch directory: C:\ProgramData\Thermo\Compound Discoverer 3.0\Scratch

New scratch directory:

Note:

The new scratch directory takes effect after you restart the application.

2. Click the browse button next to New Scratch Directory and locate the new directory.

3. Click **Save Current Settings**.

4. Restart the application.

5. Reopen the Scratch Directory Options view and make sure that the Current Scratch Directory box lists the new scratch directory.

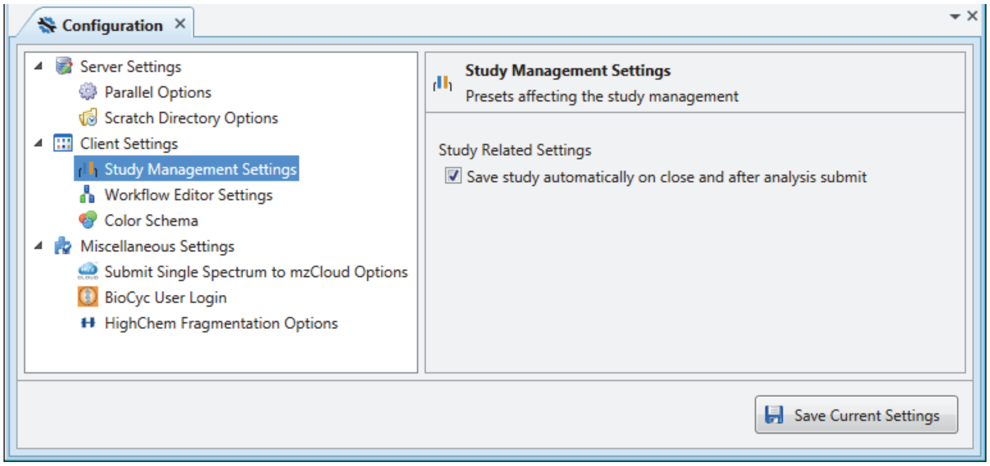
Turning Off the Auto-Save Feature for Studies

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 left pane of the Configuration page, under Client Settings, select **Study Management Settings** (Figure 154).

   Figure 154. Study Management Settings view with the default setting



Study Management Settings
Presets affecting the study management

Study Related Settings
☑ Save study automatically on close and after analysis submit

2. Clear the **Save Study Automatically On Close and After Analysis Submit** check box.
3. Click **Save Current Settings**.
4. Restart the application.

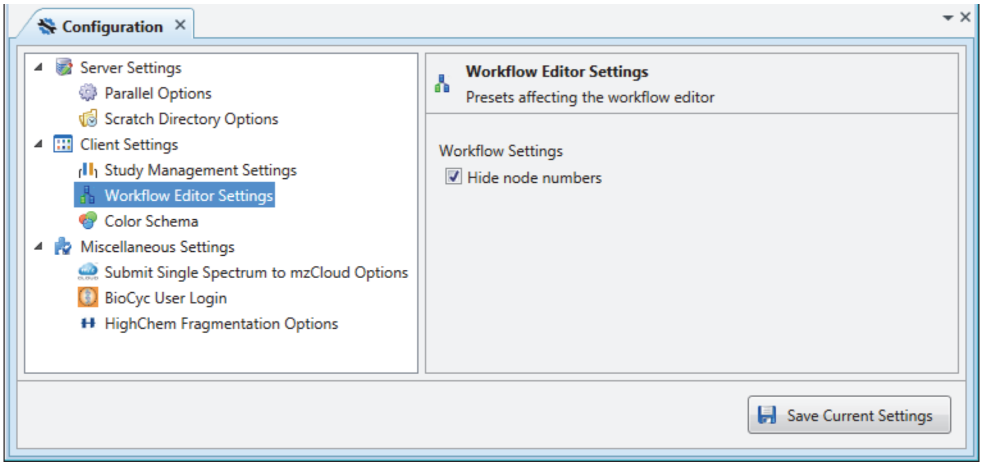
Hiding the Workflow Node Numbers

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 left pane of the Configuration page, under Client Settings, select **Workflow Editor Settings**.
2. Under Workflow Settings, select the **Hide Node Numbers** check box (Figure 155).

Figure 155. Workflow Editor Settings view



Workflow Editor Settings
Presets affecting the workflow editor

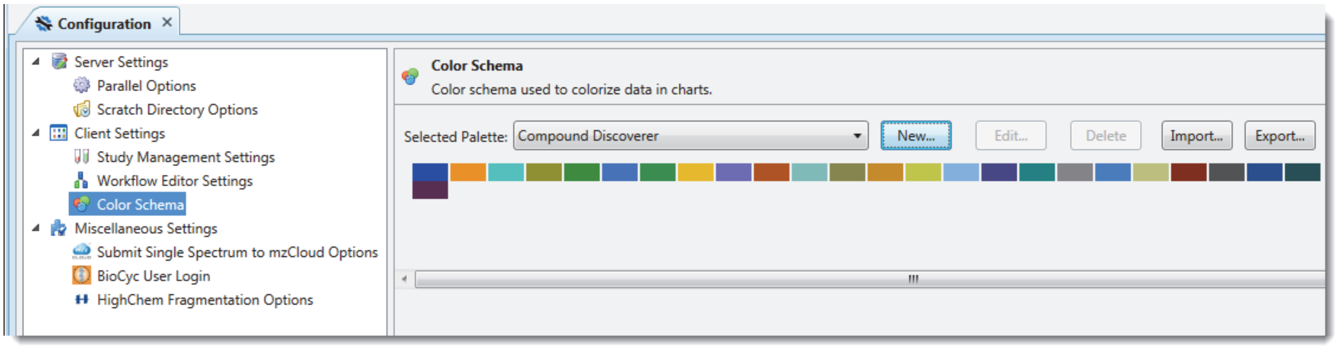
Workflow Settings
☑ Hide node numbers

3. Click **Save Current Settings**.

Selecting the Global Color Palettes

Use the Color Schema view of the Configuration page (Figure 156) 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 156. Color Schema view



Color Schema
Color schema used to colorize data in charts.

Selected Palette: Compound Discoverer

To set up the global color palette, follow these topics as needed:

- Selecting a Standard Color Palette
- Creating, Deleting, Importing, or Exporting a Custom Color Palette
- Editing a Custom Color Palette

Selecting a Standard Color Palette

For visualizing chart data, you can select from four standard color palettes.

❖ To select a standard color palette

1. In the left pane of the Configuration page, under Client Settings, select **Color Schema**.
2. In the Selected Palette list, select from four palettes.
   - Compound Discoverer

   - Proteome Discoverer

   - 60 Distinct Colors

   - Deuternopia, Protanopia, and Tritanopia

3. Click **Save Current Settings**.

Creating, Deleting, Importing, or Exporting a Custom Color Palette

To set up custom color palettes, follow these topics as needed.

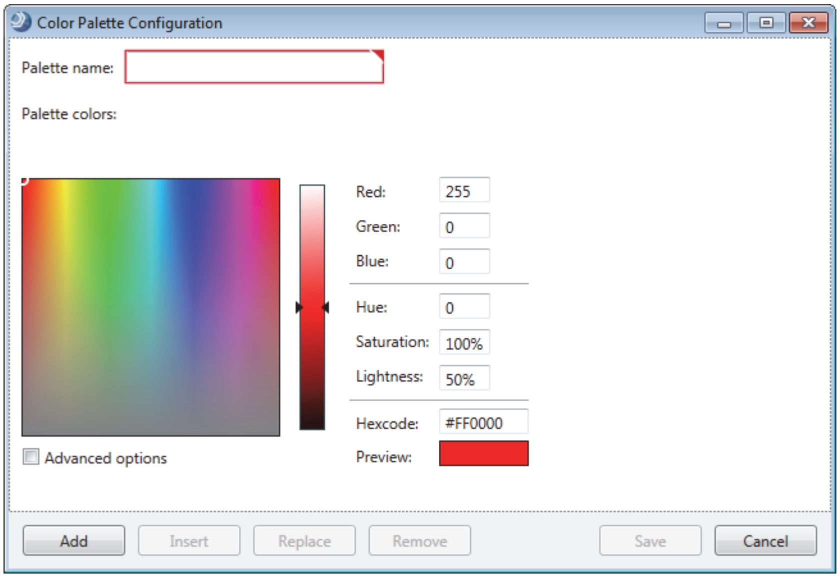
- To create a custom color palette
- To delete a custom color palette
- To import a custom color palette
- To export a custom color palette

❖ To create a custom color palette

1. In the left pane of the Configuration page, under Client Settings, select **Color Schema**.
2. Click **New**.

   The Color Palette Configuration dialog box opens (Figure 157).

Figure 157. Color Palette Configuration dialog box



Red: 255
Green: 0
Blue: 0
Hue: 0
Saturation: 100%
Lightness: 50%
Hexcode: #FF0000
☐ Advanced options

3. Name the custom color palette.

4. Add selected colors to the custom color palette (see "Editing a Custom Color Palette" on page 453).

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**.

❖ To delete a custom color palette

1. In the Color Schema view, select the custom color palette in the Selected Palette list.
2. Click **Delete**.

❖ To import a custom color palette

1. In the Color Schema view, click **Import**.
2. Locate the color palette file (XML) and click **Open**.

   The import color palette appears in the Selected Palette list.

❖ To export a custom color palette

1. In the Color Schema view, select the custom color palette in the Selected Palette list.
2. Click **Export**.
3. Name the palette and click **Save**.

Editing a Custom Color Palette

To edit a custom color palette, follow these procedures as needed.

- To open a custom color palette for editing
- To edit a custom color palette
- To select a color in the gradient color chart

❖ To open a custom color palette for editing

1. In the left pane of the Configuration page, under Client Settings, select **Color Schema**.
2. In the Selected Palette list, select the custom color palette.
3. Click **Edit**.

   The Color Palette Configuration dialog box opens.

❖ To edit a custom color palette

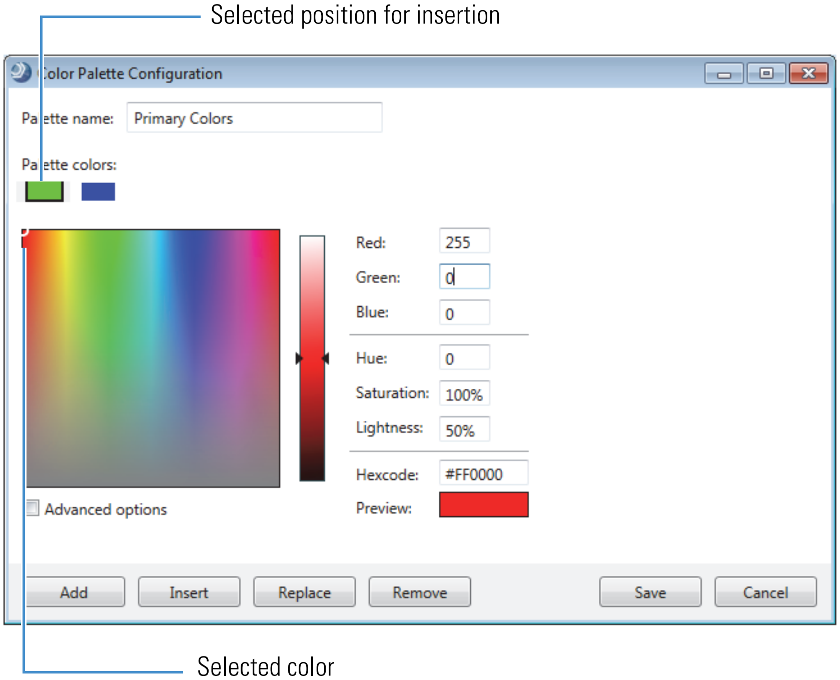
1. Open the palette for editing.
2. Do any of the following:
   a. To add a color to a custom color palette, select the color in the gradient color chart.
   b. Click **Add**.

      In the Palette Colors area, the new color appears to the right of the current colors.

   –or–

   a. 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.
   b. Select the new color in the gradient color chart (Figure 158).

Figure 158. Color Palette Configuration dialog box with the basic options view



Selected position for insertion

Palette name: Primary Colors

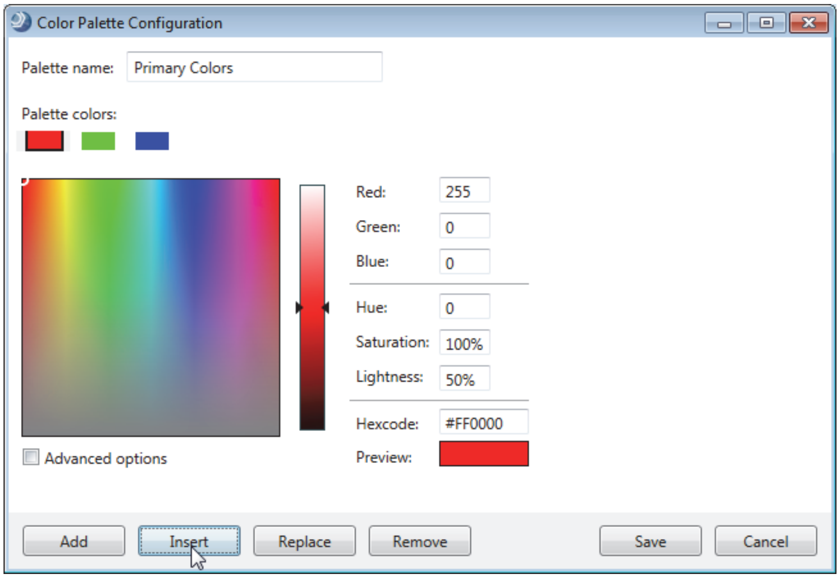
Red: 255
Green: 0
Blue: 0
Hue: 0
Saturation: 100%
Lightness: 50%
Hexcode: #FF0000
Preview: 🟥

☐ Advanced options

Selected color

c. Click **Insert**.

In the Palette Colors area, the new color appears to the left of the currently selected color.



Palette name: Primary Colors

Red: 255
Green: 0
Blue: 0
Hue: 0
Saturation: 100%
Lightness: 50%
Hexcode: #FF0000
Preview: 🟥

☐ Advanced options

–or–

a. To replace a color with another color, select the color to replace in the Palette Colors area.

b. Select a color in the gradient color chart.

c. Click **Replace**.

–or–

a. To remove a color from a custom color palette, select the color in the Palette Colors area.

b. Click **Remove**.

3. Click **Save**.

❖ To select a color in the gradient color chart

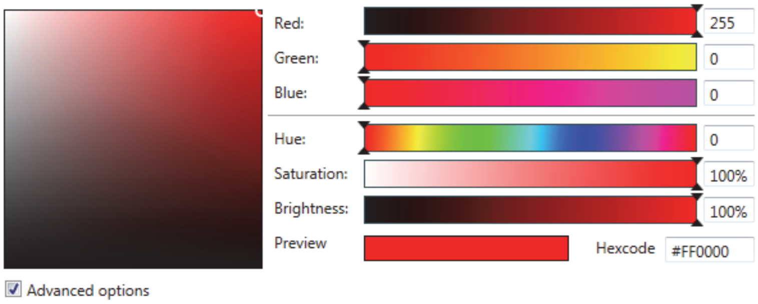
Do any of the following:

- 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 159).

Figure 159. Advanced Options view



Red: 255
Green: 0
Blue: 0
Hue: 0
Saturation: 100%
Brightness: 100%
Preview
Hexcode #FF0000
☑ Advanced options

–or–

- Enter the hexadecimal code.

Specifying 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.

❖ To set up the mass tolerance settings for a manual mzCloud search

1. In the left pane of the Configuration page, under Miscellaneous settings, select **Submit Single Spectrum to mzCloud Options**.

2. Do 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 include the Search mzCloud node, select the **Use mzCloud Node Settings** check box to use the node's settings (see "Search mzCloud Node" on page 517).
3. Click **Save the Current Settings**.

Table 116 describes the options for submitting single scans to the mzCloud database.

Table 116. 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

Setting Up a BioCyc Account or Subscription

Follow the instructions in the BioCyc User Login view on the Configuration page to set up your BioCyc subscription or user account. You must have either an organization subscription and a user account or an individual subscription to access all BioCyc databases. A user account alone allows you to access only the EcoCyc and MetaCyc databases.

To set up a BioCyc account or individual subscription and enter your credentials in the BioCyc User Login view, follow these topics as needed:

- Opening the BioCyc User Login View
- Setting Up a BioCyc Account or Individual Subscription
- Entering, Testing, and Saving Your Account Information

Note To set up a user account or an individual user subscription, you must have Internet access.

Opening the BioCyc User Login View

❖ To open the BioCyc User Login view

1. From the application window, choose **Help > Configuration**.

   The Configuration page opens.

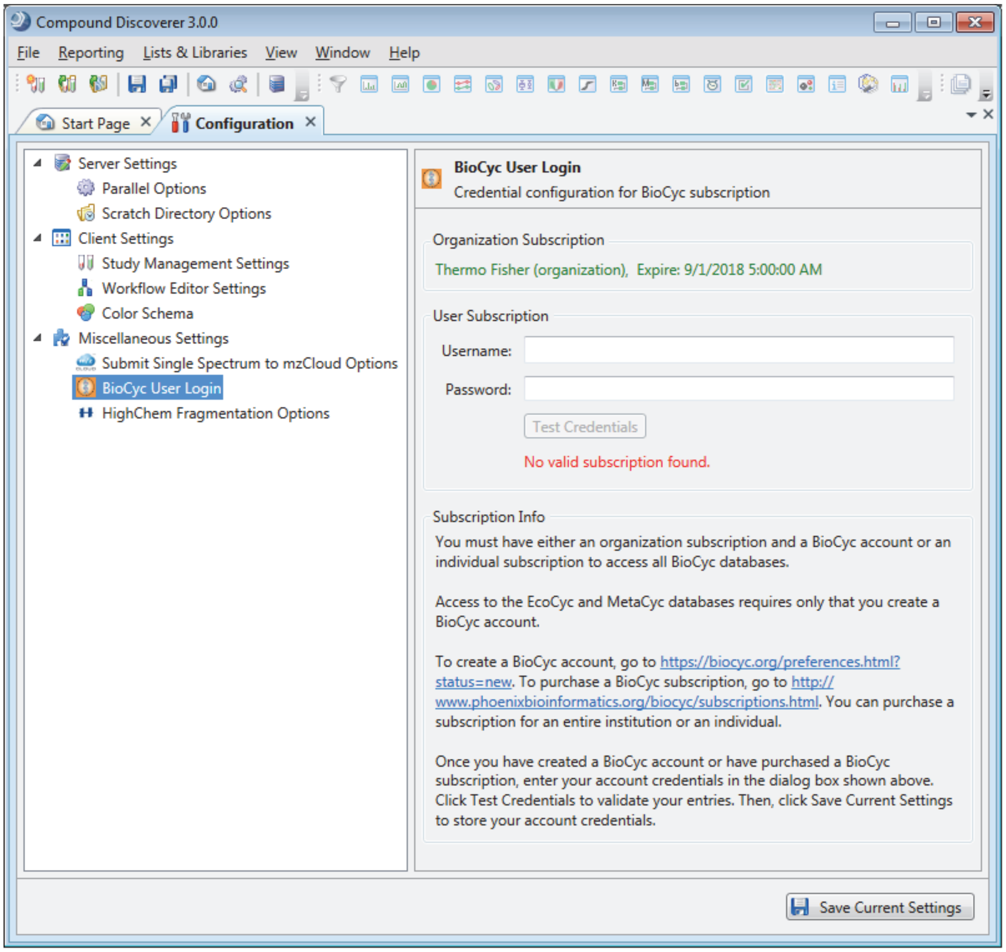
2. In the left pane, under Miscellaneous settings, select **BioCyc User Login**.

   - 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 already have a BioCyc user account, 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 160 shows a BioCyc User Login page for a user without a subscription.

Figure 160. BioCyc User Login page for a user without a subscription



BioCyc User Login
Credential configuration for BioCyc subscription

Organization Subscription
Thermo Fisher (organization), Expire: 9/1/2018 5:00:00 AM

User Subscription
Username:
Password:

No valid subscription found.

Subscription Info

You must have either an organization subscription and a BioCyc account or an individual subscription to access all BioCyc databases.

Access to the EcoCyc and MetaCyc databases requires only that you create a BioCyc account.

To create a BioCyc account, go to https://biocyc.org/preferences.html?status=new. To purchase a BioCyc subscription, go to http://www.phoenixbioinformatics.org/biocyc/subscriptions.html. You can purchase a subscription for an entire institution or an individual.

Once you have created a BioCyc account or have purchased a BioCyc subscription, enter your account credentials in the dialog box shown above. Click Test Credentials to validate your entries. Then, click Save Current Settings to store your account credentials.

Setting Up a BioCyc Account or Individual Subscription

❖ To set up a BioCyc account or individual subscription

Open the BioCyc User Login view on the Configuration page, and follow the instructions in the view.

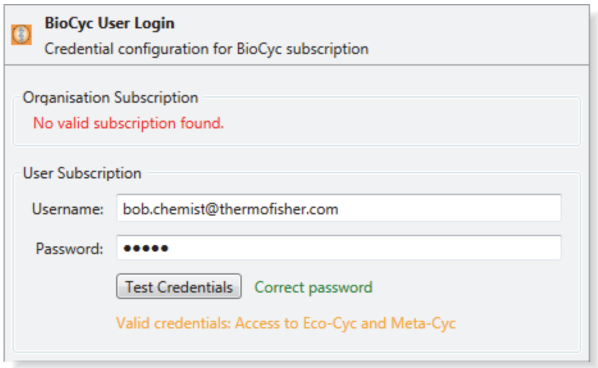
Entering, Testing, and Saving Your Account Information

❖ To enter, test, and save your account information

1. In the User Subscription area of the BioCyc User Login view on the Configuration page, enter your user name (email address) and password.
2. Click **Test Credentials**.
3. Click **Save Current Settings**.

Figure 161 shows the subscription information for a user who has a user account but does not have an organization subscription or an individual subscription. When running analyses that map compounds to the BioCyc pathways, the user can access only the EcoCyc and MetaCyc databases.

Figure 161. Settings for a user with a only a user account



BioCyc User Login

Credential configuration for BioCyc subscription

Organisation Subscription

No valid subscription found.

User Subscription

Username: bob.chemist@thermofisher.com

Password: •••••

Correct password

Valid credentials: Access to Eco-Cyc and Meta-Cyc

Specifying the Fragmentation Libraries

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**.

13

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 5, “Creating and Editing Processing Workflows.”

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.

Contents

Input and Output Nodes

These topics describe the input and output nodes:

- Export Spectra Node
- 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 162 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 162. Minimum processing workflow for the Export Spectra node

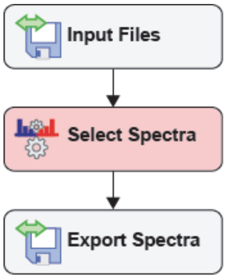


Table 117 describes the parameters for the Export Spectra node.

Table 117. 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.

Table 117. Export Spectra node parameters (Sheet 2 of 2)

Parameter	Description
File Name Suffix	Specifies the suffix that the application appends to the file name of the exported file.
Export Format	Specifies the data format of the exported file. Selections: • DTA archive (*.dta.zip)—Generates a zip file that contains an individual DTA file for each MS scan in the raw data file. The individual file names include the scan number of the scan. The DTA file format is a simple text file that contains a peak table of mass and intensity. This format does not store information about data acquisition, such as the instrument method or mass resolution, and you cannot reprocess DTA files with a mass spectrometry application. • 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 a result file’s input files, open its Input Files Table.

Spectrum Processing Nodes

These nodes extract the mass spectral data from the input file set:

- Align Retention Times Node
- Filter By Mass Defect Node
- Filter By Scan Event Node
- Filter Centroids Node
- Select Spectra Node

Align Retention Times Node

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.

For information about adding the node to a processing workflow, see "Building a Processing Workflow" on page 130.

To check the chromatographic alignment of the input files, see "Viewing the Corrected Retention Times of the Alignment Features" on page 257 and "File Alignments Table" on page 277.

IMPORTANT Do not apply a scan filter that excessively reduces the retention time window (see "Select Spectra Node" on page 471), 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.

Table 118 describes the parameters for the Align Retention Times node.

Table 118. Align Retention Times node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Alignment Model	Specifies the curve fitting algorithm that the workflow uses to chromatographically align the input files. Default: Adaptive Curve Selections: Adaptive Curve or Linear
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

Table 118. Align Retention Times node parameters (Sheet 2 of 2)

Parameter	Description
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

Filter By Mass Defect Node

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.

Table 119 describes the parameters for the Filter By Mass Defect node.

Table 119. 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: $\text{Fractional Mass} = \text{exact mass} - \text{floor (exact mass)}$ $\text{Standard Mass Defect} = \text{exact mass} - \text{nominal mass}$ $\text{Relative Mass Defect} = \frac{1e6 \times (\text{exact mass} - \text{nominal mass})}{(\text{exact mass})}$ $\text{Kendrick Mass Defect} = \text{Kendrick mass} - \text{nominal Kendrick mass}$ Where: $\text{Exact mass} = \text{Monoisotopic mass of the elemental composition}$ $\text{Nominal mass} = \text{Integer mass}$ 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 Kendrick Mass Defect as the 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 119. Filter By Mass Defect node parameters (Sheet 2 of 2)

Parameter	Description
2. Tolerances	
Using the mass defect values calculated above 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. To create new ion definitions, see "Adding or Editing Ion Definitions with the Ion Definition Editor" on page 400.

Filter By Scan Event Node

Use the Filter By Scan Event node to filter the mass spectra by scan events.

Table 120 describes the parameters for the Filter By Scan Event node.

Table 120. 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 120. 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 120. 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 121 describes the parameters for the Filter Centroids node.

Table 121. Filter Centroids node parameters

Parameter	Description
1. General Settings	
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. 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 acquired by your Thermo Scientific mass spectrometer and 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 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 When using settings other than the defaults for the Select Spectra node, follow these guidelines:

- The application uses the full (MS1) scans to measure the accurate mass and isotope patterns of the mass spectral peaks; therefore, do not filter out the full (MS1) scans when the processing workflow includes the Find Expected Compounds and Detect Compounds nodes.
- Both the Align Retention Times and Find Expected Compounds nodes require a representative amount of data to function properly. If you excessively reduce the retention time window (for example, by using an RT or scan number range), the Align Retention Times node's chromatographic alignment algorithm and the Find Expected Compounds node's automatic peak width detection algorithm might fail to produce satisfactory results.

Table 122 describes the parameters in the Select Spectra node.

Table 122. Select Spectra node parameters (Sheet 1 of 8)

Parameter	Description
1. General Settings	
Precursor Selection	Specifies the MS order of the precursor scans for higher-order MS^n scans, like MS^3, MS^4, and so forth. Default: Use MS(n – 1) Precursor Selections: Use MS1 Precursor or Use MS(n – 1) Precursor

Table 122. Select Spectra node parameters (Sheet 2 of 8)

Parameter	Description
Use New Precursor Reevaluation	Specifies the algorithm used to determine the monoisotopic mass of the precursor ion for a higher-order scan when the full (MS1) scan has been acquired with an FT analyzer. Default: True Selections: • True—The node uses a sophisticated algorithm to determine the best precursor mass peak for a given MS/MS spectrum from the corresponding MS1 master scan. Using the monoisotopic mass and charge reported by the instrument in the scan header (or if that is not available, the isolation mass), the algorithm goes into the master scan and tries to find the corresponding peak in the MS1 spectrum both to improve the mass accuracy of the monoisotopic mass reported by the instrument and to correct for inaccurate precursor masses corresponding to one of the ^{13}C isotopes. • False—Instead of reevaluating the monoisotopic mass, the node uses the monoisotopic mass provided by the instrument in the scan header. The instrument uses a simplified algorithm that looks for matching masses only to the left of a reported peak and performs a rough check of the detected isotopic intensities.
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.
Store Chromatograms	Specifies whether the application creates a TIC trace and a BPC trace for each input file and lists these traces in the Specialized Traces table. Default: False

Table 122. Select Spectra node parameters (Sheet 3 of 8)

Parameter	Description
2. Spectrum Properties Filter	
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
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 a mass spectrometry viewer application, such as Qual Browser or 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 122. Select Spectra node parameters (Sheet 4 of 8)

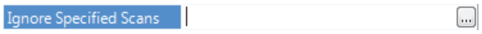
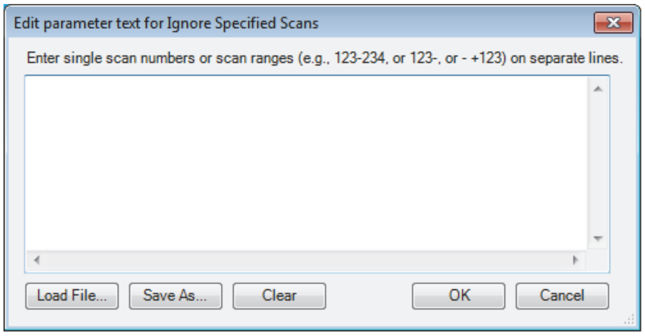
<table>
<tr><th>Parameter</th><th>Description</th></tr>
<tr><td>Ignore Specified Scans</td><td>Specifies the scan numbers that the analysis ignores. Placing the cursor in the Ignore Specified Scans box and clicking the More icon, ..., opens the Edit Parameter Text for Ignore Specified Scans dialog box where you can do the following:
• Manually enter the scan numbers to ignore.
• Load a text file that lists the scans numbers to ignore.
• Create and save a list of scans numbers to ignore.


Enter single scan numbers or scan ranges (e.g., 123-234, or 123-, or - +123) on separate lines.</td></tr>
<tr><td colspan="2">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.</td></tr>
<tr><td>Lowest Charge State</td><td>Excludes higher-order scans of precursor ions with a lower charge state than the specified charge state.
Default: 0 Minimum: 0</td></tr>
<tr><td>Highest Charge State</td><td>Filters out scans from precursor ions with a higher charge state than the specified charge state.
Default: 0 (specifies no upper limit)</td></tr>
<tr><td>Min. Precursor Mass</td><td>Specifies the minimum precursor mass for a higher-order scan.
Default: 0 (no filtering)
Minimum value: 0 Maximum value: Unchecked</td></tr>
<tr><td>Max. Precursor Mass</td><td>Specifies the maximum precursor mass for a higher-order scan.
Default: 0 (no filtering)
Minimum value: 0 Maximum value: Unchecked</td></tr>
</table>

Table 122. Select Spectra node parameters (Sheet 5 of 8)

Parameter	**Description**
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).
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
3. Scan Event Filters	
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 **Note** 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 122. Select Spectra node parameters (Sheet 6 of 8)

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: • 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 122. Select Spectra node parameters (Sheet 7 of 8)

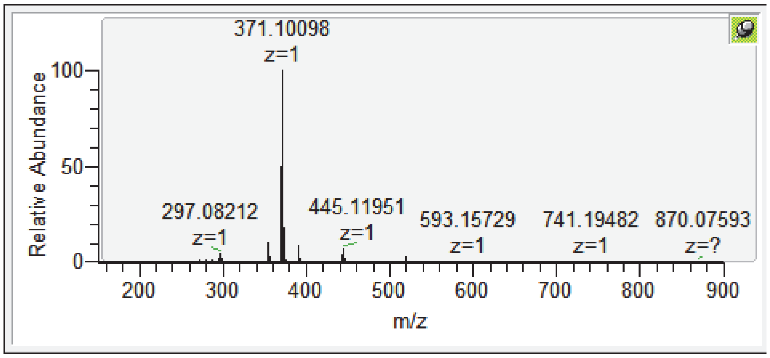
Parameter	Description
Polarity Mode	Specifies the polarity mode for the scan. Filter selection: Any, Is, Is Not Default: (Not Specified)—The node does not filter the scan events by polarity mode. Check box selections: • Positive • Negative
4. Peak Filters	
S/N Threshold (FT-only)	Specifies the signal-to-noise threshold for mass peaks in an FTMS scan. Mass peaks below this threshold are filtered out. Default: 1.5
5. 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, and 8

Table 122. Select Spectra node parameters (Sheet 8 of 8)

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: • 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

Trace Creation Nodes

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

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.

❖ To extract a UV trace or an analog trace from the RAW data file

1. Under General Settings, select **UV** or **Analog** from the Trace Type list.

2. 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 detected the sample simultaneously.

3. In the Custom Label box, type text to identify the trace in the Specialized Traces table of the result file window.

❖ To extract a PDA trace from the raw data

1. In the General Settings area, do the following:
   - 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.
2. In the PDA Settings area, do 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.

Table 123 describes the parameters for the Analog Traces node.

Table 123. 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.

Table 123. Create Analog Trace node parameters (Sheet 2 of 2)

Parameter	Description
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
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: 190 Range: 190–800 nm

Create FISh Trace Node

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 124 describes the parameters for the Create FISh Trace node.

Table 124. 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 Expected Compounds library (see "Modifying the Expected Compounds List" on page 390). **IMPORTANT** To run an analysis that includes the Create FISh Trace node, you must select a compound from this list (see "Troubleshooting Common Analysis Errors" on page 101).
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 124. Create FISh Trace node parameters (Sheet 2 of 3)

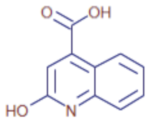
Parameter	**Description**
3. Scan Filter Settings	
Scan Polarity	Specifies the polarity of the scan. Default: + (Positive) Selections: Positive or Negative
Fragment Mode	Specifies the fragmentation mode of the fragmentation scans that you want the node to extract. Default: All-Ion Selections: All-Ion and Data-Dependent
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. $4n + 2$ = 0 or a positive integer for the number of electrons in the delocalized, conjugated p-orbital cloud For example, the following structure is aromatic with an *n* value of 2.  Default: True

Table 124. 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 125 describes the parameters for the Create Mass Trace node.

Table 125. 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 125. 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.

Table 126 describes the parameters for the Create Pattern Trace node.

Table 126. 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 (see "Setting Up Isotope Patterns for Pattern Scoring or Pattern Traces" on page 120). 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 126. 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.

- Find Expected Compounds Node
- FISh Scoring Node
- Generate Expected Compounds Node
- Group Expected Compounds Node
- Mark Background Compounds Node–Expected Compounds
- Merge Features Node

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 Workflows for Expected Compounds" on page 23.

Table 127 describes the parameters for the Find Expected Compounds node.

Table 127. Find Expected Compounds node parameters (Sheet 1 of 2)

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
SN Threshold	Specifies the signal-to-noise threshold for the pattern search. Isotopes that are expected to be below this intensity level are not required. This means that if the intensity for an isotope in the theoretical isotope pattern (based on the expected elemental composition) is below the signal-to-noise threshold, the application ignores the isotope and requires one less matching isotope in the measured isotope pattern. Range: 1 or greater
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
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 127. Find Expected Compounds node parameters (Sheet 2 of 2)

Parameter	Description
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" on page 471. • 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.

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.

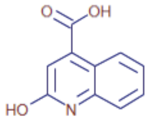
For information about how the node calculates the confirmation score, see "FISh Scoring for Targeted Compounds and Proposed Structures" on page 41.

Table 128 describes the parameters for the FISh Scoring node.

Table 128. 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 "Working with the Mass Spectrum View" on page 198. 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 128. 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. $4n + 2$ = 0 or a positive integer for the number of electrons in the delocalized, conjugated p-orbital cloud For example, the following structure is aromatic with an *n* value of 2.  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

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 "Adding or Editing Transformations with the Transformation Editor" on page 404.

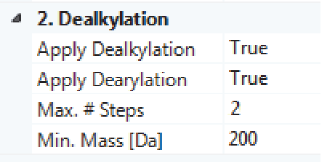
When you add transformations to the library, you can assign them to one of the following groups: Phase I, Phase II, or Others. The Generate Expected Compounds node treats transformations assigned to the Others group as Phase I transformations; that is, it applies Phase I and Others transformations before it applies Phase II transformations.

To predict the transformation products for the selected parent compounds, the Generate Expected Compounds node follow 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.

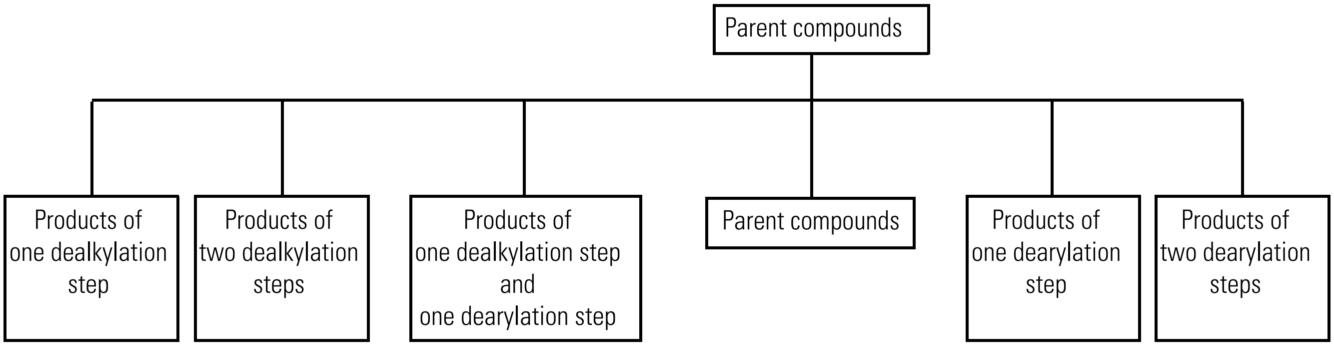
   Consider all steps under Dealkylation together as one step. For example, consider the selections shown in Figure 163 as one step in the total set of reaction pathways and create separate reaction pathways. Apply the transformation steps on the parent compound and the reaction products from the dealkylation pathways.

   Figure 163. Dealkylation step example



2. Dealkylation

Apply Dealkylation	True
Apply Dearylation	True
Max. # Steps	2
Min. Mass [Da]	200



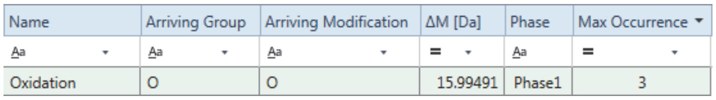
2. When more than one reaction pathway produces the same elemental composition, use the pathway with the lowest number of transformation steps.

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.

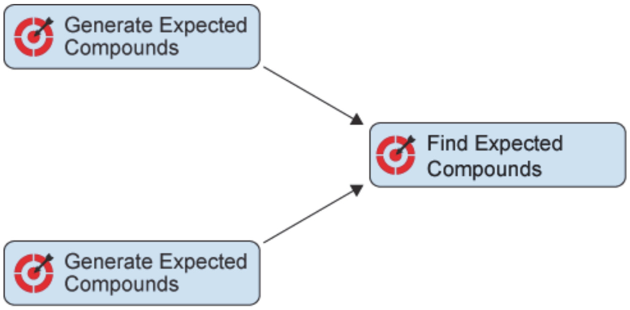
5. For Phase II transformations, limit the maximum number of times to apply the transformation on a single compound to the lowest of these three values:
   - Max Occurrence setting for the transformation in the Transformations library
   - Maximum number of steps for all reactions (setting for node's 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.

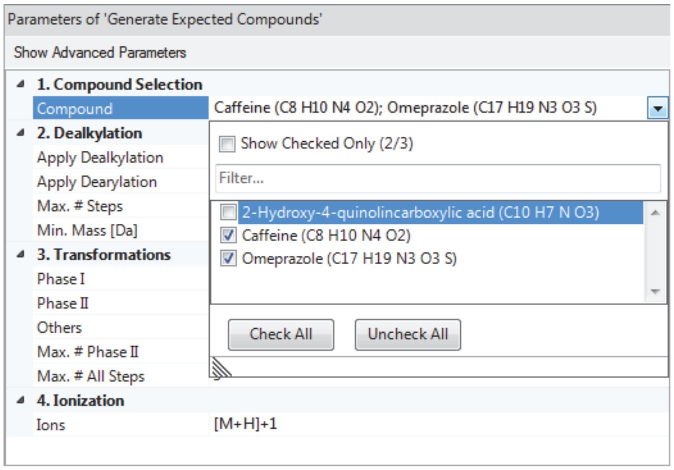
Table 129 describes the parameters for the Generate Expected Compounds node. The application cannot use the processing workflow until you select a compound from the Compound list.

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.



Parameters of 'Generate Expected Compounds'

Show Advanced Parameters

1. Compound Selection

Compound: Caffeine (C8 H10 N4 O2); Omeprazole (C17 H19 N3 O3 S)

☐ Show Checked Only (2/3)

Filter...

☐ 2-Hydroxy-4-quinolincarboxylic acid (C10 H7 N O3)
☑ Caffeine (C8 H10 N4 O2)
☑ Omeprazole (C17 H19 N3 O3 S)

2. Dealkylation

Apply Dealkylation
Apply Dearylation
Max. # Steps
Min. Mass [Da]

3. Transformations

Phase I
Phase II
Others
Max. # Phase II
Max. # All Steps

4. Ionization

Ions: [M+H]+1

Table 129. 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 129. Generate Expected Compounds node parameters (Sheet 2 of 3)

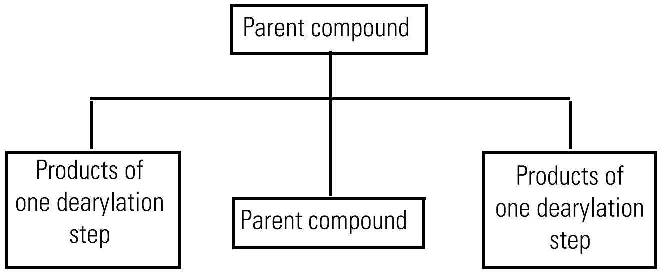
Parameter	Description
Max. # Steps	Specifies the maximum number of Dealkylation steps. For example, if you select True for Dealkylation, True for Dearylation, and 1 for the Max. # Steps, the node applies up to one dealkylation step and up to one dearylation step as the initial Dealkylation step in the set of reaction pathways. For another example, see Figure 163 on page 492.  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 129. 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 "Modifying the Ion Definitions List" on page 397.

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 130 describes the parameters for the Group Expected Compounds node.

Table 130. Group Expected Compounds node parameters (Sheet 1 of 2)

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: 0.05 Range: 1.0

Table 130. Group Expected Compounds node parameters (Sheet 2 of 2)

Parameter	Description
2. Fragment Data Selection	
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.

Mark Background Compounds Node–Expected Compounds

Use the Mark Background Compounds node to flag compounds that are also found in the sample blanks (Sample Type—Set to Blank). The Mark Background Compounds node for a targeted analysis has a blue background.

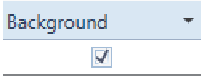
For information about editing the assigned sample types, see "Editing the Sample Type and Study Factor Values" on page 91.

Table 131 describes the parameters for the Mark Background Compounds node.

Table 131. Mark Background Compounds node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Max. Sample/Blank	Below this ratio threshold, the node labels the expected compound as a background compound in the Expected Compounds table. If the input file set includes more that 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.

Table 131. Mark Background Compounds node parameters (Sheet 2 of 2)

Parameter	Description
Max. Blank/Sample	Below this ratio threshold, the node labels the expected compound as a background compound in the Expected Compounds table. If the input file set includes more that 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 Expected Compounds Table includes a filter icon (Expected Compounds ▼), and the expected 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 Expected Compounds table. When a compound is flagged as a background compound, its Background check box is selected.  Background ☑ Default: True

Compound Detection Nodes

Use these nodes to detect unknown compounds:

- Analyze Labeled Compounds 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.

Table 132. 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 132. 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 Node

Use the Detect Compounds node to detect unknown compounds. The processing results for the Detect Compounds node appear in the Compounds per File table and the Features table.

For information about an untargeted processing workflow, see "Untargeted Workflows for Identifying Unknown Compounds" on page 31.

Table 133 describes the parameters for the Detect Compounds node.

Table 133. Detect Compounds node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Mass Tolerance	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%
S/N Threshold	Specifies the signal-to-noise threshold for mass spectral peaks (centroids). The unknown compound detection algorithm ignores centroids below this user-specified threshold. Default: 3 Range: 0 to no upper limit
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 134). 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 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 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.	
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 133. Detect Compounds node parameters (Sheet 2 of 2)

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
2. Peak Detection	
Filter Peaks	Specify whether you want to turn on the chromatographic peak filtering parameters. Default: True
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
Min. #Scans per Peak	Specifies the minimum number of scans (data points) required to define a chromatographic peak. Default: 5 Range: 3 to 20
Min. #Isotopes	Specifies the minimum number of isotopes required in the mass spectral scans that define the chromatographic peak. Default: 1

Table 134 lists the recommended range for the minimum peak intensity parameter. The optimal setting depends on the sensitivity of the mass spectrometer.

Table 134. 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

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 "Marking Background Compounds in an Untargeted Analysis" on page 35.

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 The Fill Gaps node 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 using the Parameterless Peak Detection (PPD) algorithm. 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.

Table 135 describes the parameters for the Fill Gaps node.

Table 135. Fill Gaps 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
S/N Threshold	Specifies the minimum signal-to-noise threshold for centroids. Default: 1.5 Minimum: 1
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 analysis 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 analysis uses only a peak simulation algorithm to fill the gaps with simulated chromatographic peaks.

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 136 describes the parameters for the Group Compounds node.

Table 136. Group Compounds node parameters (Sheet 1 of 2)

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

Table 136. Group Compounds node parameters (Sheet 2 of 2)

Parameter	Description
2. Fragment Data Selection	
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

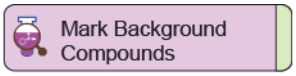
Peak Area Refinement Nodes

Use these nodes to hide background compounds or to normalize the chromatographic peak areas:

- Mark Background Compounds Node–Unknown Compounds
- Normalize Areas Node

Mark Background Compounds Node–Unknown Compounds

Use the Mark Background Compounds node to identify the background compounds (compounds also found in the blank samples) in the Compounds Table.



For information about the parameter settings, see “Mark Background Compounds Node–Expected Compounds” on page 497.

Always place the Mark Background Compounds node at the end of the processing workflow by following these examples:

- Group Compounds > Mark Background Compounds
- Group Compounds > Fill Gaps > Mark Background Compounds
- Group Compounds > Fill Gaps > Normalize Areas > Mark Background Compounds

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 “Marking Background Compounds in an Untargeted Analysis” on page 35.

Normalize Areas Node

Use the Normalize Areas node to normalize the chromatographic peak areas when you need the analysis to compensate for batch effects.

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 Normalized Area column to the Compounds Table. When the analysis includes quality control samples, the node also adds the "QC" columns in the Compounds table. You can view the corrected compound areas in the Compound Area Corrections view (see "Viewing the QC-Based Compound Area Correction Curves" on page 259).

> **IMPORTANT** When the Normalize Areas and Mark Background Compounds nodes are part of a processing workflow, connect the Normalize Areas node to the Mark Background Compounds node.

If the input files include Quality Control samples, the application automatically performs a batch normalization on each compound that meets the user-specified criteria.

Table 137 describes the parameters for the Normalize Areas node.

Table 137. Normalize Areas node parameters (Sheet 1 of 3)

Parameter	Description
1. QC-based Area Correction	
The analysis uses the QC samples to create a regression curve for each detected compound. The analysis does not create a regression curve for a particular compound or does not correct the areas in the non-QC samples unless all three of these conditions are met: • 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).	
Regression Model	Specifies the regression model as Linear or Cubic Spline. Default: Linear

Table 137. Normalize Areas node parameters (Sheet 2 of 3)

Parameter	Description
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 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. Default: 30% Range: 10 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
2. Area Normalization	
Normalization Type	For selections other than None, the analysis normalizes the chromatographic peaks areas after performing a batch normalization based on the QC samples. Selections: • None (Default)—The analysis does not normalize the chromatographic peak areas for injection variability. • 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 137. Normalize Areas node parameters (Sheet 3 of 3)

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. Otherwise, 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.

Compound Identification Nodes

Use these nodes to identify unknown compounds:

- Assign Compound Annotations Node
- Predict Compositions Node
- Search ChemSpider Node
- Search Mass Lists Node
- Search mzCloud Node
- Search mzVault Node

Assign Compound Annotations Node

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. 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.

Table 138 describes the parameters for the Assign Compound Annotations node.

Table 138. Assign Compound Annotation node parameters

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, 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

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 when the processing workflow also includes the Assign Compound Annotations node.

Table 139 describes the parameters for the Predict Compositions node.

Table 139. 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 Na2 O15 P2 S5

Table 139. 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: $D = 1 + \frac{\left[\sum_{i}^{imax} Ni(Vi-2)\right]}{2}$ where: • D is the value for the RDB equivalents • $imax$ 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 The value of 0 means no limit. The application does not accept negative values.

Table 139. 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: 10% Range: 0 to 100%

Table 139. 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. $\frac{\text{Summed intensity of the matching isotope peaks} \times 100}{\text{Summed intensity of the theoretical isotope pattern}}$
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 15, "Testing Communication to the Online Databases."

Table 140 describes the parameters for the Search ChemSpider node.

Table 140. Search ChemSpider node parameters (Sheet 1 of 2)

Parameter	Description
1. Search Settings	
Database(s)	Specifies the databases for the ChemSpider search.
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 140. 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 requires input from the Group Compounds node, adds the #Matched Masses to the Compounds Table, and creates the Mass List Search Results Table.

❖ To select input files for the mass list search

1. 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**.

Table 141 describes the parameters for the Mass List Search node.

Table 141. Search Mass List node parameters

Parameter	Description
1. Search Settings	
Input File(s)	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.
Show Extra Fields as Columns	Specifies whether information from the non-required columns in the mass list table appears in additional columns in the Mass List Search Results table or only in the Annotation column of the Mass List Search Results table. Default: False—Additional information appears in the Annotation column of the Mass List Search Results table.
Consider 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: 0.05 Range: 1.0
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 142 describes the table columns in the Select Input Files dialog box.

Table 142. Select Input File(s) dialog box parameters (Sheet 1 of 2)

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.

Table 142. Select Input File(s) dialog box parameters (Sheet 2 of 2)

Table column	Description
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 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.

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 and mzCloud Best Match columns to the Compounds table.

The Search mzCloud node requires input from the Group Compounds node.

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 test. See Chapter 15, “Testing Communication to the Online Databases.”

Table 143 describes the parameters for the Search mzCloud node.

Table 143. Search mzCloud node parameters (Sheet 1 of 4)

Parameter	Description
1. Search Settings	
Compound Classes	Specifies the compound classes for the search. Select **All** or select specific classes. Default: All

Table 143. Search mzCloud node parameters (Sheet 2 of 4)

Parameter	Description
Match Ion Activation Type	Specifies whether to search for fragmentation spectra generated by the same ion activation type: collision-induced dissociation (CID) or higher energy collision-induced dissociation (HCD). Default: True
Match Ion Activation Energy	Specifies whether to search for fragmentation spectra generated by the same ion activation energy within a tolerance. Default: True
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
Apply Intensity Threshold	Specifies whether to apply an automatic intensity threshold that sets the threshold intensity by calculating the spectrum noise level. Default: True
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

Table 143. Search mzCloud node parameters (Sheet 3 of 4)

Parameter	Description
Identity Search	Specifies the identity search algorithm. Selections: • HighChem DP—Alternative score using a modified dot product • HighChem HighRes—Use for high-resolution data. • NIST • Cosine Default: HighChem HighRes
Similarity Search	Specifies the similarity search algorithm. Selections: • None (Default)—Does not run a similarity search. • 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).
Library	Specifies the mzCloud library for the search. Reference is the only selection.
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 143. Search mzCloud node parameters (Sheet 4 of 4)

Parameter	Description
Match Factor Threshold	Specifies the minimum match factor for reporting a spectrum match. Default: 60 Range: 0 to 100%
Max. # Results per Compound and Spectrum	Specifies the maximum number of hits for each compound to store in the result file. Displays the hits with the highest match score above the cutoff storage number in the result file. Default: 10

Search mzVault Node

Use the Search mzVault node to search a local mass spectra database for compounds of interest. This node requires input from the Group Compounds node and creates the mzVault Results table.

For information about the parameter settings, see "Search mzCloud Node" on page 517.

❖ 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**.

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. This node requires input from the Group Compounds node—that is, it requires a list of molecular weights or chemical formulas.

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 145 describes the parameters for the Map to BioCyc Pathways node.

Table 144. Map to BioCyc Pathways node parameters

Parameter	Description
1. Search Settings	
BioCyc Database/Organism to be Searched	Specifies the databases for the search.
Search Mode	Default: By Formula or Mass Selections: By Formula or Mass, By Formula and Mass, By Formula or Mass, 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 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 input from the Group Compounds node—that is, it requires a list of molecular weights or chemical formulas.

The Map to KEGG Pathways node adds the following items 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. See Chapter 15, "Testing Communication to the Online Databases."

Follow these procedures as needed:

❖ To search the KEGG Pathways database by formula, mass, or both

1. Select the **Map to KEGG Pathways** node to open its parameter set.
2. Select the search mode.
3. Do the following:
    - For a formula search, type the number of formulas that you want to search per compound in the box for the Max. # of Predicted Compositions to be Searched per Compound.
    - For a mass search, type an appropriate mass tolerance in the Mass Tolerance box.
4. Go to this procedure To limit the number of pathways displayed individually in the Pathways column of the Compounds table.

❖ To limit the number of pathways displayed individually in the Pathways column of the Compounds table

1. Select the **Map to KEGG Pathways** node to open its parameter set.
2. In the Maximum # of Pathways in "Pathways" Column box, type the maximum number of pathways that you want the node to display individually in the Pathways column of the Compounds table.

Table 145 describes the parameters for the Map to KEGG Pathways node.

Table 145. 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 and Mass, By Formula or Mass, 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 Compound Discoverer 3.0 application. You can edit these pathways or create your own pathways by using the Metabolika pathway editor (“Modifying the Metabolika Pathways List” on page 420).

Table 146 describes the parameters for the Map to Metabolika Pathways node.

Table 146. 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 and Mass, By Formula Only, By Formula or Mass, 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 these nodes to score the explanations for each detected compound.

- Apply mzLogic Node
- Compound Class Scoring Node
- Pattern Scoring Node

To specify the isotope pattern for the Pattern Scoring node or the Pattern Trace node, see this topic "Setting Up Isotope Patterns for Pattern Scoring or Pattern Traces" on page 120.

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 147. 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

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 "Modifying the Compound Classes List" on page 427.

Table 148 describes the parameters for the Compound Class Scoring node.

Table 148. 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 (see "Modifying the Compound Classes List" on page 427).
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
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

Table 148. Compound Class Scoring node parameters (Sheet 2 of 2)

Parameter	Description
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
Allow AIF Scoring	Specifies whether the node uses AIF scans for scoring when there are no available data-dependent scans. If set to false, the node annotates AIF scans, but it does not use them for scoring. Default: True

Pattern Scoring Node

Use the Pattern Scoring node to provide a spectrum fit score (SFit%) for each detected compound. 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 a 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 149 describes the parameters for the Pattern Scoring node.

Table 149. Pattern Scoring node parameters (Sheet 1 of 2)

Parameter	Description
1. General Settings	
Isotope Patterns	Specifies the isotope patterns to be used for scoring.
Mass Tolerance	Specifies the mass tolerance for calculated elemental compositions and pattern matching. Default: 5 ppm Range: 0.0–no limit
Intensity Tolerance [%]	Specifies the relative intensity tolerance of the mass spectral peaks in the pattern. Default: 30 Range: 0.01–100.0
S/N Threshold	Specifies the signal-to-noise threshold for the search. The application ignores isotopes with a theoretical intensity value below this threshold.

Table 149. Pattern Scoring node parameters (Sheet 2 of 2)

Parameter	Description
Min. Spectral Fit [%]	Specifies the minimum required spectral fit value as a percentage. Range: 0 to 100%

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 150 describes the parameters for the Merge Features node.

Table 150. 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

Post-Processing Nodes

These nodes provide additional information about the detected compounds.

- Descriptive Statistics Node
- Differential Analysis Node
- Export Xcalibur Inclusion or Exclusion List 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 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 the Group Compounds node or the Group Expected Compounds node for a sample set with replicate data points and generated ratios. If the Grouping and Ratios page of an analysis does not contain generated ratios, the following confirmation message appears:

> No quan ratios defined in ‘Grouping & Ratios’ tab

Table 151 describes the parameter for the Differential Analysis node.

Table 151. 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

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 152 describes the parameters for the Export Xcalibur Inclusion or Exclusion List node.

Table 152. 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. 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
Left 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
3. LTQ Orbitrap Settings	
Maximum Concurrent Entries	Specifies the maximum number of entries with overlapping time windows. Default: 500
Mass Precision Decimals	Specifies the required number of decimal places for the mass values. Default: 5

14

Working with the Application Tables

These 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.

Contents

Moving Up and Down Table Rows

Use the following procedures to move through the rows in a data table.

❖ **To move down through the rows of a result or library table**

Press TAB.

❖ **To move up through the rows of a result or library table**

Hold down the SHIFT key and press TAB.

Sorting Tables

Use the following procedures to sort the data tables.

❖ To sort the rows based on the contents of one or more columns

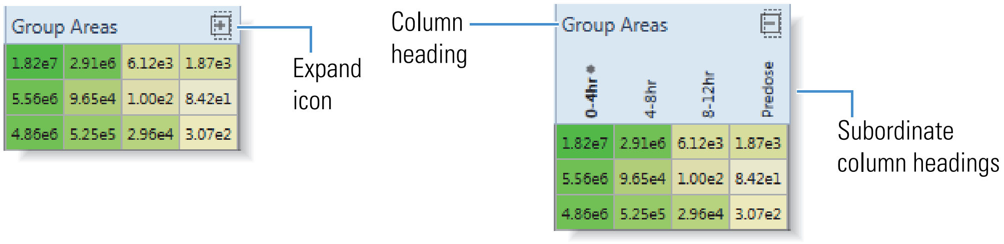
1. Click a column header to sort the rows between ascending order (A, B, C …) and descending order (Z, Y, X …), based on the contents of the column.

   > **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.

❖ 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.



Group Areas			
1.82e7	2.91e6	6.12e3	1.87e3
5.56e6	9.65e4	1.00e2	8.42e1
4.86e6	5.25e5	2.96e4	3.07e2

Group Areas			
0-4hr	4-8hr	8-12hr	Predose
1.82e7	2.91e6	6.12e3	1.87e3
5.56e6	9.65e4	1.00e2	8.42e1
4.86e6	5.25e5	2.96e4	3.07e2

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.

Freezing Table Rows

Use the following procedure to freeze table rows.

❖ To affix rows at the top of the table

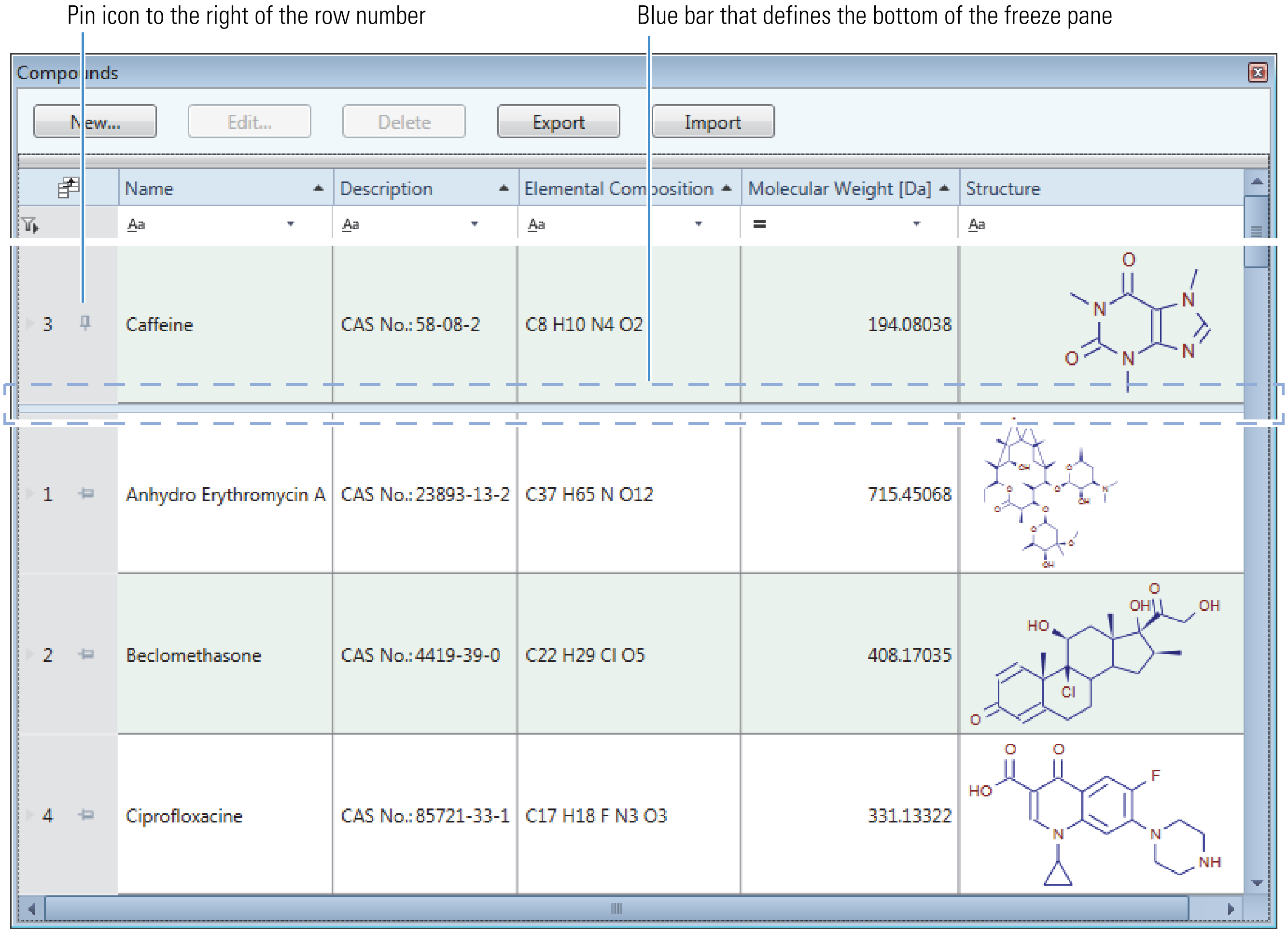
1. Click the pin icon, 📌, next to the row number of the row that you want to freeze.

   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.

2. 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 164 shows a compound library with caffeine in the freeze pane.

Figure 164. Compound library with a freeze pane



Pin icon to the right of the row number

Blue bar that defines the bottom of the freeze pane

	Name	Description	Elemental Composition	Molecular Weight [Da]	Structure
3	Caffeine	CAS No.: 58-08-2	C8 H10 N4 O2	194.08038	
1	Anhydro Erythromycin A	CAS No.: 23893-13-2	C37 H65 N O12	715.45068	
2	Beclomethasone	CAS No.: 4419-39-0	C22 H29 Cl O5	408.17035	
4	Ciprofloxacine	CAS No.: 85721-33-1	C17 H18 F N3 O3	331.13322	

Grouping 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

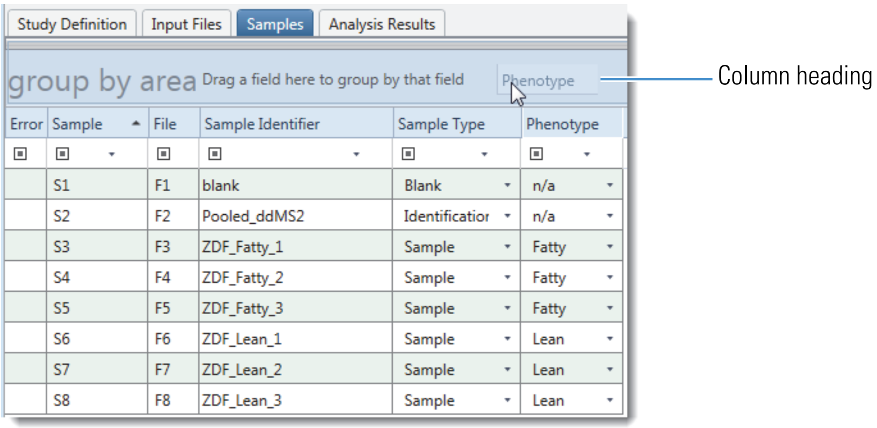
1. Right-click the page and choose **Enable Row Grouping**.

   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 165 shows the column heading for a study factor being dragged to the Group by Area bar.

Figure 165. Group by Area bar above the table heading row

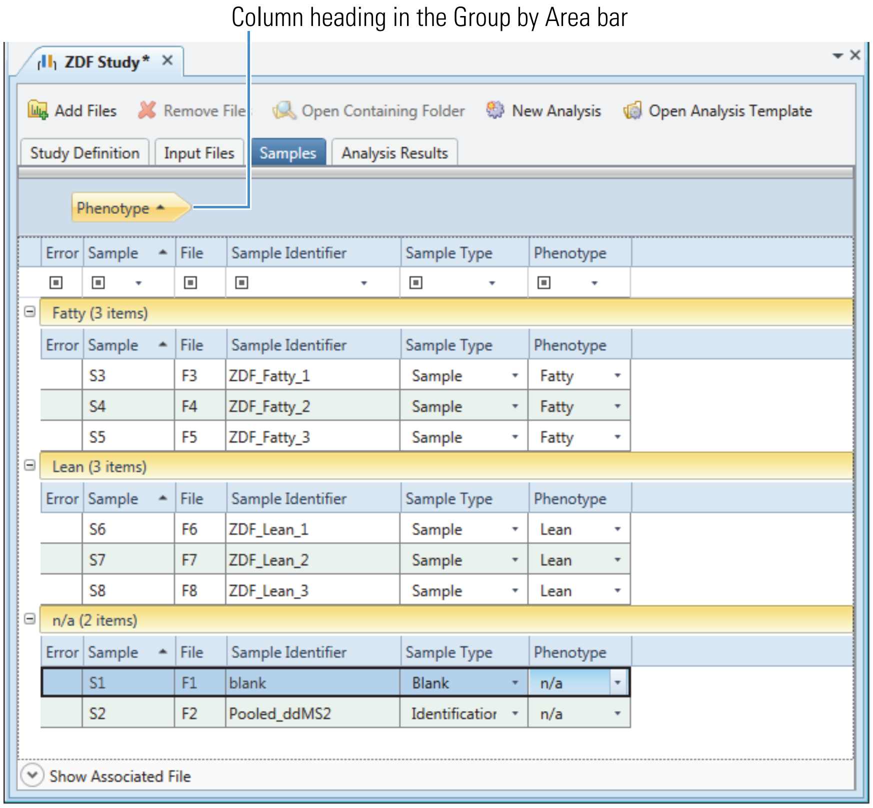


Error	Sample	File	Sample Identifier	Sample Type	Phenotype
	S1	F1	blank	Blank	n/a
	S2	F2	Pooled_ddMS2	Identificatior	n/a
	S3	F3	ZDF_Fatty_1	Sample	Fatty
	S4	F4	ZDF_Fatty_2	Sample	Fatty
	S5	F5	ZDF_Fatty_3	Sample	Fatty
	S6	F6	ZDF_Lean_1	Sample	Lean
	S7	F7	ZDF_Lean_2	Sample	Lean
	S8	F8	ZDF_Lean_3	Sample	Lean

3. To ungroup the table rows, drag the column heading out of the Group by Area bar.

   Figure 166 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 166. Samples table grouped by phenotype



Fatty (3 items)

Error	Sample	File	Sample Identifier	Sample Type	Phenotype
	S3	F3	ZDF_Fatty_1	Sample	Fatty
	S4	F4	ZDF_Fatty_2	Sample	Fatty
	S5	F5	ZDF_Fatty_3	Sample	Fatty

Lean (3 items)

Error	Sample	File	Sample Identifier	Sample Type	Phenotype
	S6	F6	ZDF_Lean_1	Sample	Lean
	S7	F7	ZDF_Lean_2	Sample	Lean
	S8	F8	ZDF_Lean_3	Sample	Lean

n/a (2 items)

Error	Sample	File	Sample Identifier	Sample Type	Phenotype
	S1	F1	blank	Blank	n/a
	S2	F2	Pooled_ddMS2	Identificatior	n/a

4. To turn off the group by row feature, right-click the page and choose **Disable Row Grouping**.

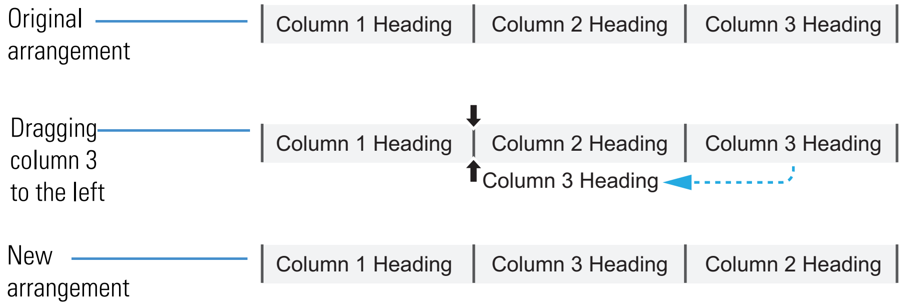
Changing the Position of Table Columns

Use the following procedures to change the position of table columns. Changes to tables in any of the Lists & Libraries views are temporary. You can save the layout changes to a result table by applying the File > Save Result View Layout command.

❖ To change the order of the columns in a library or result table

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 (Figure 167).

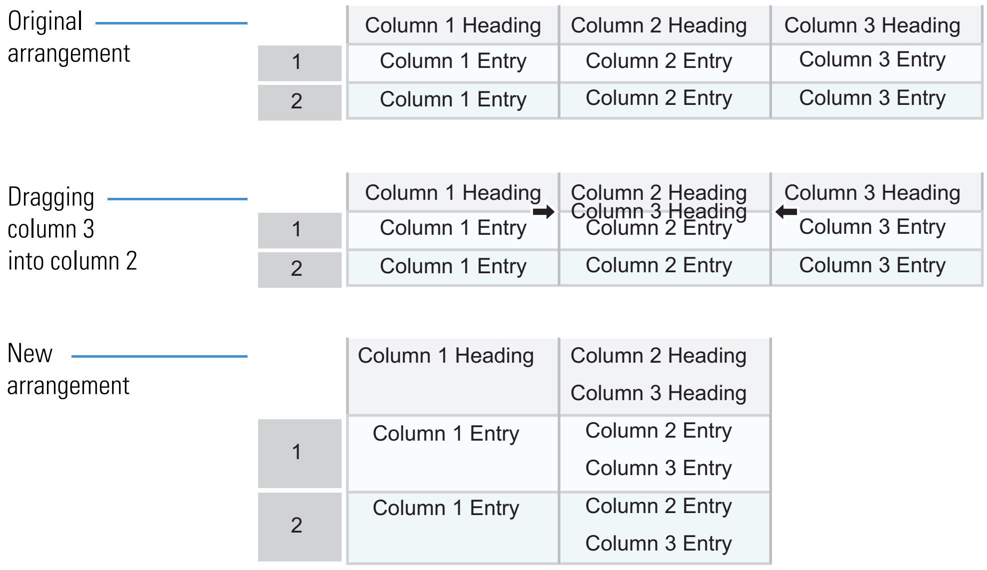
Figure 167. Moving a column to the left



❖ To stack two table columns into one column

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 168).

Figure 168. Stacking two columns into one column



Freezing 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, ⊥.

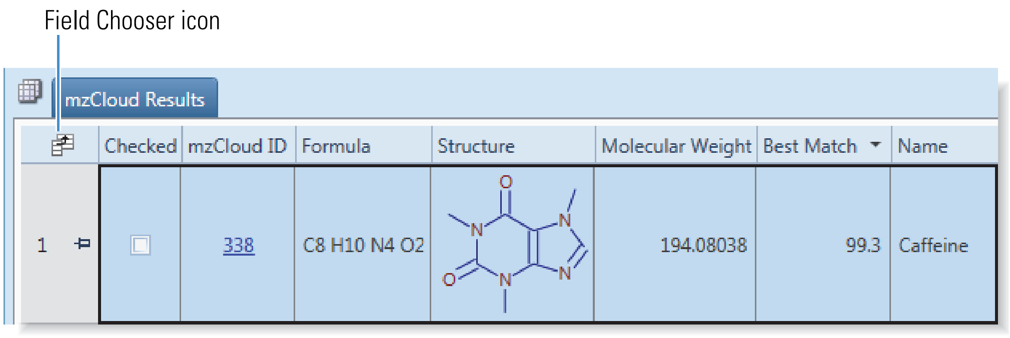
Showing or Hiding Table Columns

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.

❖ To show or hide columns in a library or result table

1. Click the **Field Chooser** icon, ▦, in the upper left corner of the table (Figure 169).

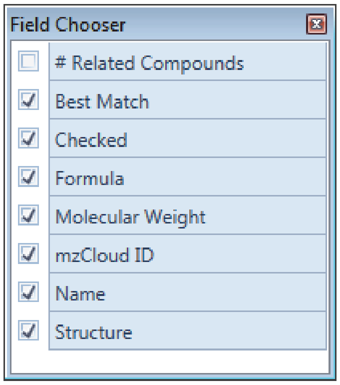
   Figure 169. Field chooser icon in the upper left corner of the mzCloud Results table



	Checked	mzCloud ID	Formula	Structure	Molecular Weight	Best Match	Name
1	☐	338	C8 H10 N4 O2		194.08038	99.3	Caffeine

   The Field Chooser dialog box opens with a list of all of the column headers for the current table in alphabetical order (Figure 170).

Figure 170. Field Chooser dialog box for the mzCloud Results 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.

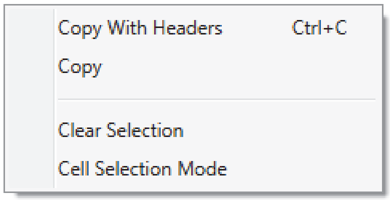
Copying Table Entries to the Clipboard

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.

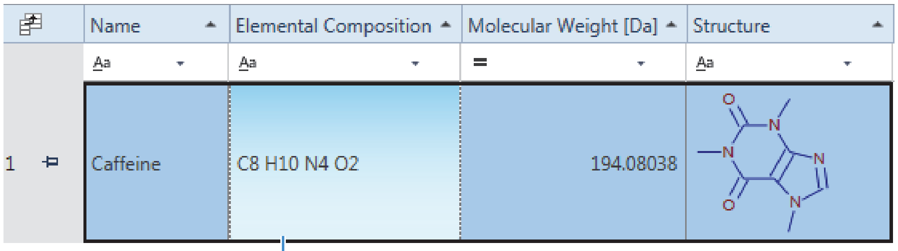
❖ To copy table cells to the Clipboard

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.



	Name	Elemental Composition	Molecular Weight [Da]	Structure
	Aa	Aa	=	Aa
1	Caffeine	C8 H10 N4 O2	194.08038	

Selected table cell

3. Right-click and choose **Copy** from the shortcut menu.

❖ To copy a single 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**.

❖ 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.

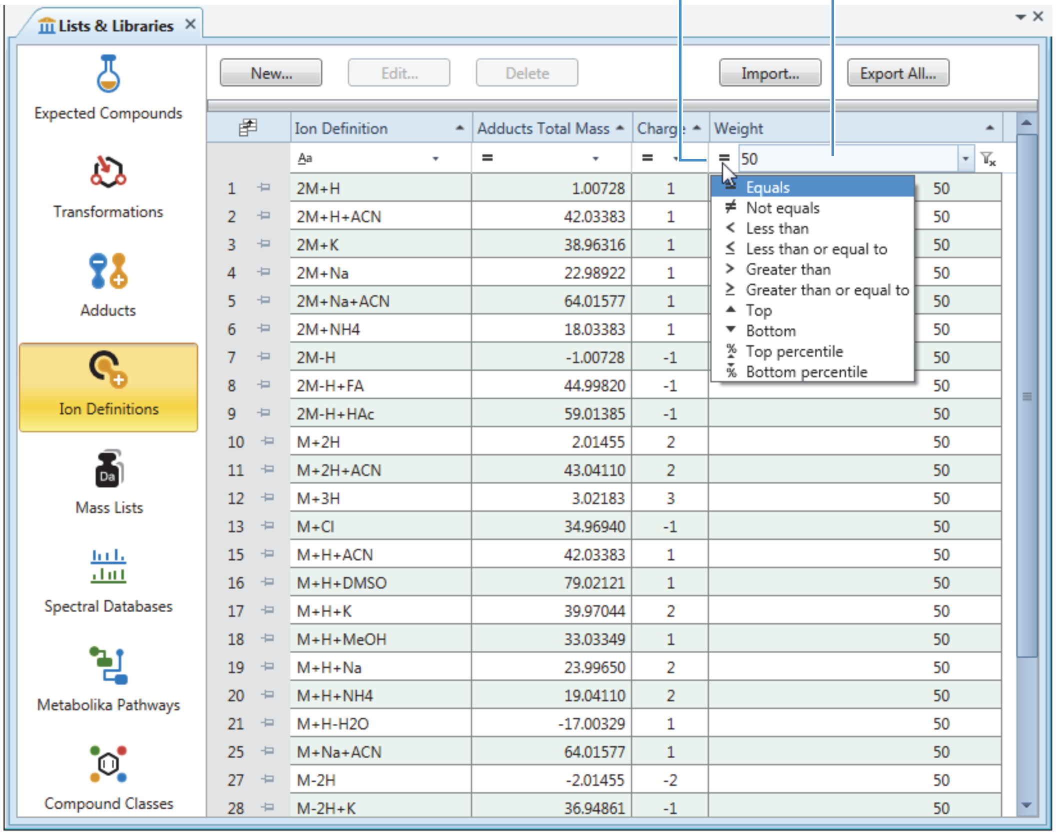
Filtering Tables

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 "Using Result Filters for Data Reduction and Creating Filter Sets" on page 162.

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. Figure 171 shows the filter row of an Ion Definitions list where the Ion Definition column contains text entries and the other columns contain numeric entries.

Figure 171. Unfiltered Ion Definitions list



Equals (=) is the default operator for numeric columns.

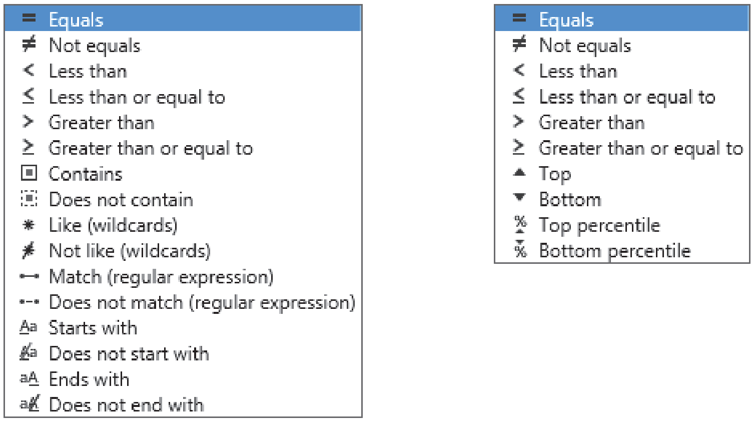
Operand box

	Ion Definition	Adducts Total Mass	Charge	Weight
	Aa	=	=	= 50
1	2M+H	1.00728	1	50
2	2M+H+ACN	42.03383	1	50
3	2M+K	38.96316	1	50
4	2M+Na	22.98922	1	50
5	2M+Na+ACN	64.01577	1	50
6	2M+NH4	18.03383	1	50
7	2M-H	-1.00728	-1	50
8	2M-H+FA	44.99820	-1	50
9	2M-H+HAc	59.01385	-1	50
10	M+2H	2.01455	2	50
11	M+2H+ACN	43.04110	2	50
12	M+3H	3.02183	3	50
13	M+Cl	34.96940	-1	50
15	M+H+ACN	42.03383	1	50
16	M+H+DMSO	79.02121	1	50
17	M+H+K	39.97044	2	50
18	M+H+MeOH	33.03349	1	50
19	M+H+Na	23.99650	2	50
20	M+H+NH4	19.04110	2	50
21	M+H-H2O	-17.00329	1	50
25	M+Na+ACN	64.01577	1	50
27	M-2H	-2.01455	-2	50
28	M-2H+K	36.94861	-1	50

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 (see Figure 172). 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 154 on page 545 and Table 155 on page 546.

Figure 172. Operators for library table entries

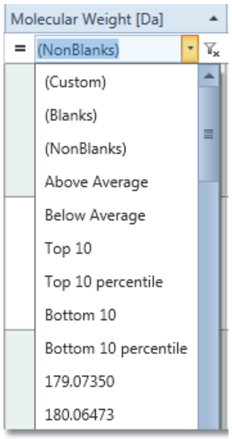


Operator list for text columns (Aa)

Operator list for numeric columns (=)

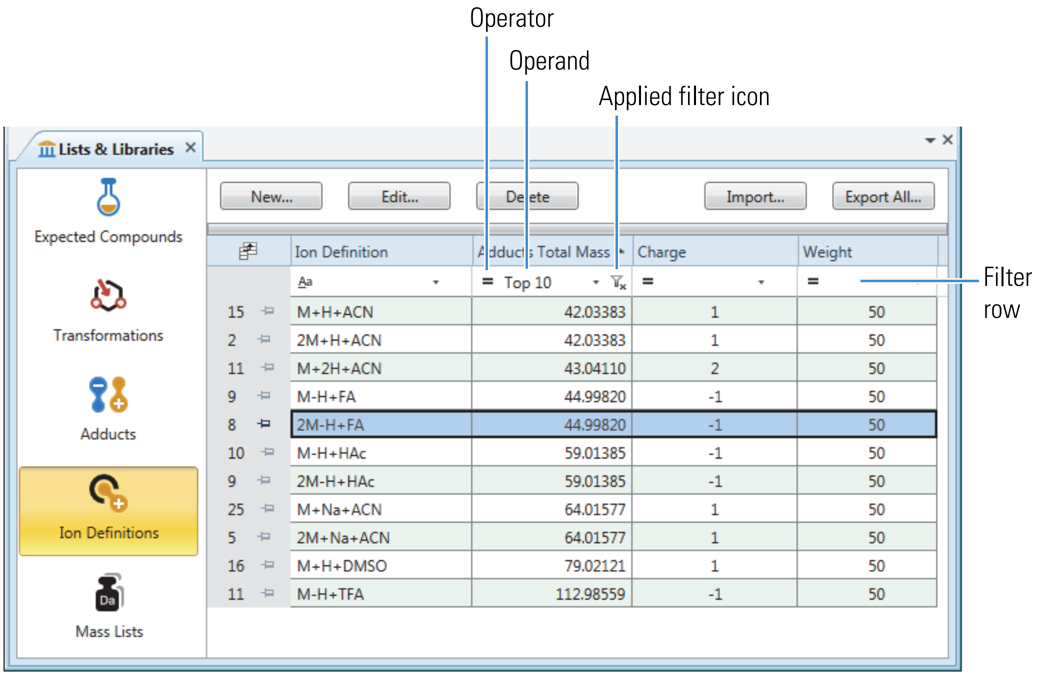
For all columns, the operand list includes the following: Custom, Blanks, NonBlanks, and the column entries. For numerical-entry columns, the operand list also includes the following: Above Average, Below Average, Top 10, Top 10 Percentile, Bottom 10, and Bottom 10 Percentile (see Figure 173). For more information, see Table 153.

Figure 173. Operands for numerical-entry columns



After you set up a column filter, the applied filter icon, , appears to the right of the operand box. Figure 174 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 174. Ion Definitions list that is filtered by the adduct mass



	Ion Definition	Adducts Total Mass	Charge	Weight
	Aa	= Top 10	=	=
15	M+H+ACN	42.03383	1	50
2	2M+H+ACN	42.03383	1	50
11	M+2H+ACN	43.04110	2	50
9	M-H+FA	44.99820	-1	50
8	2M-H+FA	44.99820	-1	50
10	M-H+HAc	59.01385	-1	50
9	2M-H+HAc	59.01385	-1	50
25	M+Na+ACN	64.01577	1	50
5	2M+Na+ACN	64.01577	1	50
16	M+H+DMSO	79.02121	1	50
11	M-H+TFA	112.98559	-1	50

Follow these procedures as needed:

- To filter the library entries
- To set up a wild card filter
- To set up a numerical value filter
- To remove an individual filter

❖ To filter the library entries

1. In the filter row, click the operator symbol (**Aa** or =) and select an operator from the list.
2. In the filter row, set up the operand by selecting or typing a value in the operand box.

   After you set up a filter, the applied filter icon, Y_x , appears to the right of the operand box, and the table displays only those rows with entries that fulfill the filter condition.
3. Repeat step 1 and step 2 for each column that you want to filter by.

❖ To set up a wild card filter

1. In the operator list, 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.

❖ To set up a numerical value filter

Do one 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.

❖ To remove an individual filter

Click the filter icon, , to the right of the operand box.

Table 153 describes the available operand selections and the valid typed operand entries for both text and numeric columns.

Table 153. 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. For information about setting up a custom filter, see "Setting Up a Custom Filter" on page 546.

Table 153. Operands for the table columns on a study page or Lists & Libraries view (Sheet 2 of 3)

Operand	Description
(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.
(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 154 on page 545 describes the compatible operators for text entries. Table 155 on page 546 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 154 describes the compatible operators for text entries. Table 155 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.

Table 153. Operands for the table columns on a study page or Lists & Libraries view (Sheet 3 of 3)

Operand	Description
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.
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 154 describes the operators for columns with text entries.

Table 154. 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.
A̸a	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.
aA̸	Does not end with	Displays the text entries that do not end with the selected or typed operand.

Table 155 describes the operators for columns with numeric entries.

Table 155. 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.

Setting Up a Custom Filter

To set up a single condition filter for a library table, follow the instructions in “Filtering Tables” on page 539.

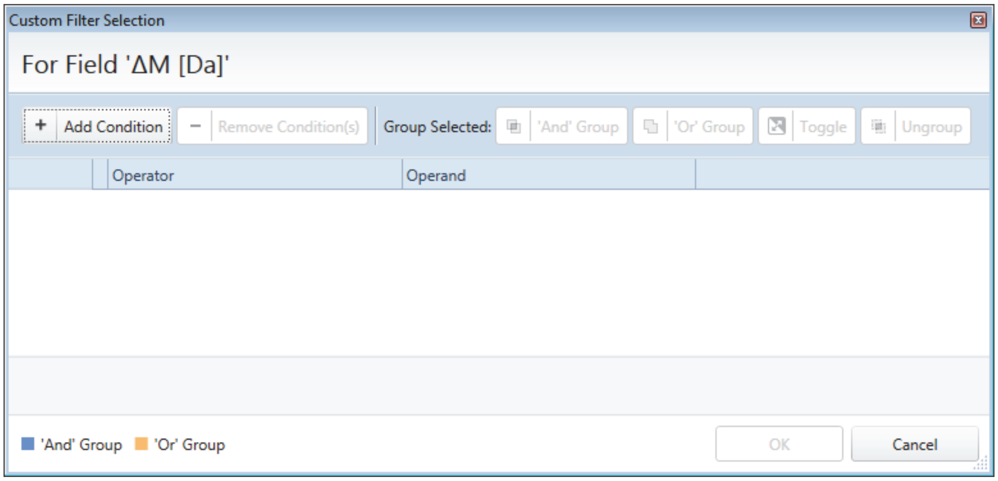
These procedures describe how to set up a library table filter with more than one condition by using the Custom Filter Selection dialog box.

❖ To open the Custom Filter Selection dialog box

Select **(Custom)** from the operand list for a table column.

The Custom Filter Selection dialog box opens (Figure 175).

Figure 175. Custom Filter Selection dialog box with no conditions



❖ To create new conditions

1. Do the following for each condition that you want to add to a group:

   a. Click **Add Condition**.

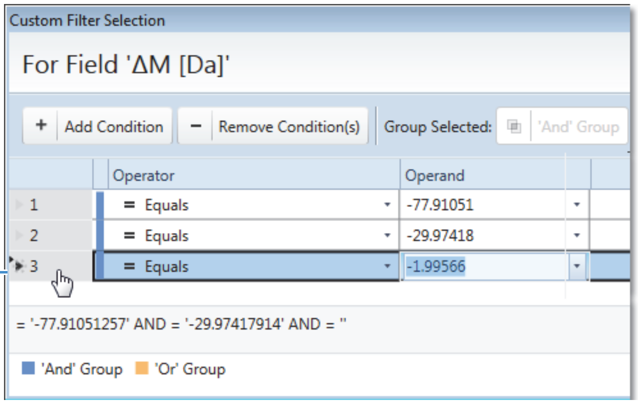
      A new table row appears.

   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.

2. To add the last condition to the group, click its row number (Figure 176).

   Figure 176. Clicking the row number in the last row to add the row to the group



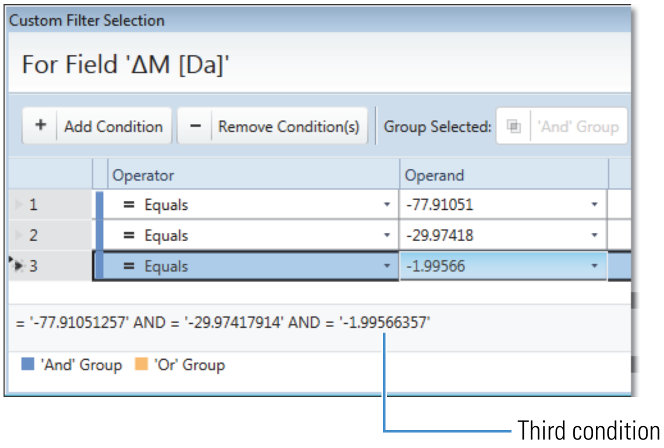
	Operator	Operand
1	= Equals	-77.91051
2	= Equals	-29.97418
3	= Equals	-1.99566

= '-77.91051257' AND = '-29.97417914' AND = ''

Click the row number.

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 177). A vertical blue bar to the left of the condition rows indicates an AND group.

Figure 177. Group filter with three conditions and the AND group operator



	Operator	Operand
1	= Equals	-77.91051
2	= Equals	-29.97418
3	= Equals	-1.99566

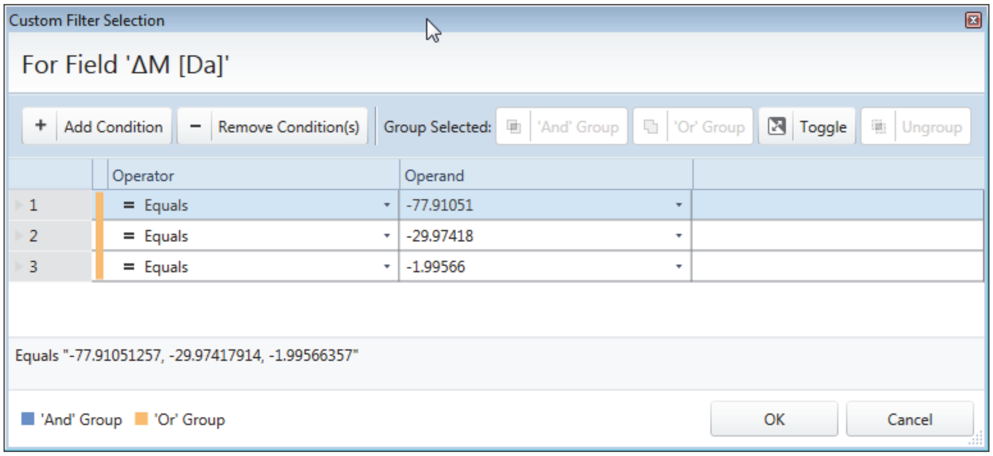
= '-77.91051257' AND = '-29.97417914' AND = '-1.99566357'

❖ 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 178).

Figure 178. Group filter with three conditions and the OR group operator



	Operator	Operand
1	= Equals	-77.91051
2	= Equals	-29.97418
3	= Equals	-1.99566

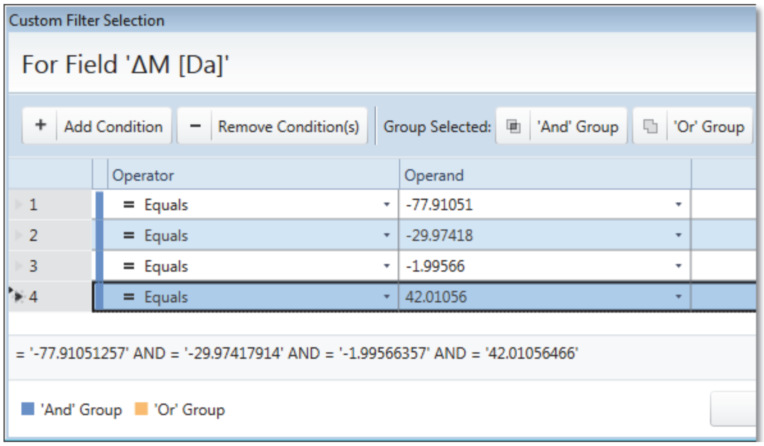
Equals "-77.91051257, -29.97417914, -1.99566357"

❖ To add an overlapping group to the filter

1. 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 179).

Figure 179. Selection of two noncontiguous rows



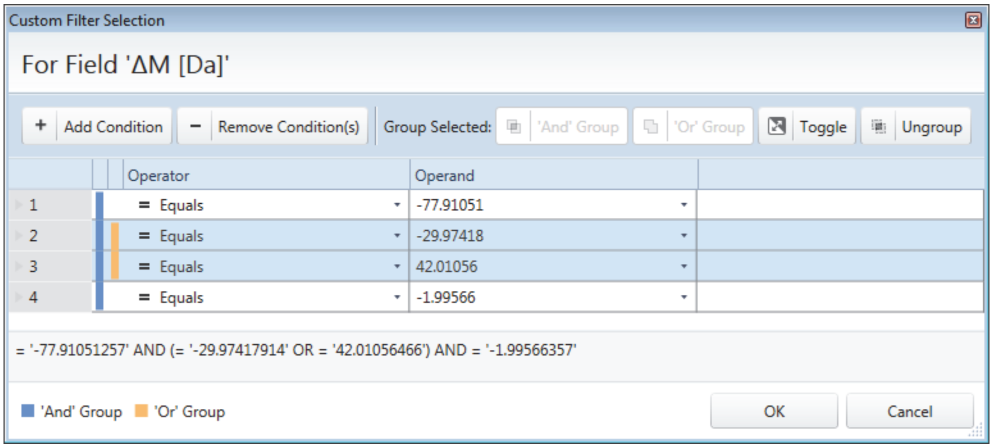
	Operator	Operand
1	= Equals	-77.91051
2	= Equals	-29.97418
3	= Equals	-1.99566
4	= Equals	42.01056

= '-77.91051257' AND = '-29.97417914' AND = '-1.99566357' AND = '42.01056466'

2. 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 180).

Figure 180. A set of filter conditions with two groups



	Operator	Operand
1	= Equals	-77.91051
2	= Equals	-29.97418
3	= Equals	42.01056
4	= Equals	-1.99566

= '-77.91051257' AND (= '-29.97417914' OR = '42.01056466') AND = '-1.99566357'

3. To remove conditions from a group, select the conditions and click **Ungroup**.

❖ 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.

❖ To close the dialog box without applying the filter

Click **Cancel** and select **Yes** at the prompt.

Table 156 describes the features of the Custom Filter Selection dialog box.

Table 156. 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 154 on page 545 for a list of the operators for the text entry columns. See Table 155 on page 546 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 153 on page 542 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.	

Testing 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.

Follow these topics to test and troubleshoot the application's access to the online mass spectrum databases.

Contents

❖ **To test and troubleshoot the application's access to the online databases**

1. Run the communication tests (see "Running the Communication Tests" on page 552).

   If the communication tests succeed, the application has access to the online databases.

2. If a communication test fails, do the following as needed:

   - If only the mzCloud communication test fails, check the Date and Time settings on the processing computer (see "Setting the Correct Time and Time Zone on the Processing Computer" on page 555).
   - If the Check Subscription 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 and individual subscription, and then enter, test, and save your account credentials in the BioCyc User Login view (see "Setting Up a BioCyc Account or Subscription" on page 456).

  - If any of the other communication tests also fail, check the access to the URLs for the online databases (see "Checking the URLs for the Online Databases in Your Browser" on page 553).

    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 needed:

   - 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 "Compound Discoverer" or "Compound Discoverer Server" from accessing the URLs. The application uses the following protocol: http port 80 and .
   - If a proxy setting is blocking access, see "Specifying the IP Address of the Proxy Server" on page 554.

Running 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

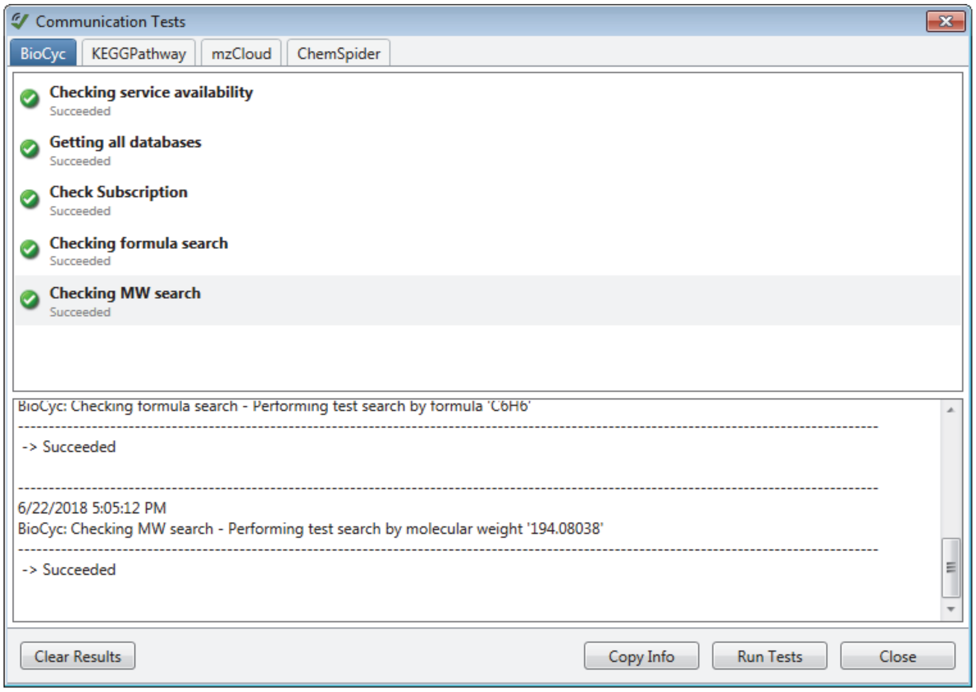
1. From the menu bar, choose **Help > Communication Tests**.

   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 181 shows the communication tests in progress.

Figure 181. BioCyc communication tests



Checking service availability
Succeeded

Getting all databases
Succeeded

Check Subscription
Succeeded

Checking formula search
Succeeded

Checking MW search
Succeeded

```
BioCyc: Checking formula search - Performing test search by formula 'C6H6'
------------------------------------------------------------------------------------------------------------
 -> Succeeded

------------------------------------------------------------------------------------------------------------
6/22/2018 5:05:12 PM
BioCyc: Checking MW search - Performing test search by molecular weight '194.08038'
------------------------------------------------------------------------------------------------------------
 -> Succeeded
```

4. If the tests are successful, your computer has access to the required databases on the Internet. If only the mzCloud test fails, check the Date and Time settings for the processing computer ("Setting the Correct Time and Time Zone on the Processing Computer" on page 555). If any of the other tests also fail, check the access to the URLs in your browser (see "Checking the URLs for the Online Databases in Your Browser" on page 553).

Checking the URLs for the Online Databases in Your Browser

Table 157 lists the URLs for the online mass spectrum databases. If a communication test fails, test the URL for the affected database.

Table 157. URLs of online mass spectrum databases (Sheet 1 of 2)

Database	URL
mzCloud Identity	https://identity.mzcloud.org/
	https://www.mzcloud.org/Services/MzCloudApiV1.svc
	https://www.mzcloud.org/Services/MzCloudApiLightService.svc
ChemSpider	http://www.chemspider.com
	http://chemspider.com/MassSpecAPI.asmx
	http://chemspider.com/Search.asmx

Table 157. URLs of online mass spectrum databases (Sheet 2 of 2)

Database	URL
KEGG: Kyoto Encyclopedia of Genes and Genomes	http://www.kegg.jp/
	http://rest.kegg.jp
BioCyc	https://biocyc.org/
	https://biocyc.org/web-services.shtml

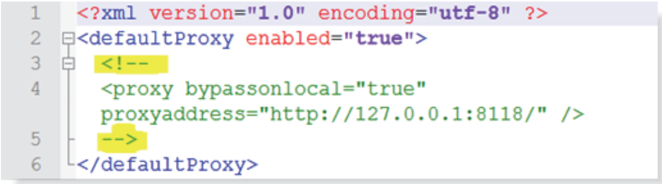
Specifying the IP Address of the Proxy Server

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 3.0\bin\Config.
2. Open the **Proxy.config** file in Notepad.
3. Remove the text that is highlighted in yellow in Figure 182—that is, remove the XML comment delimiters: <!-- and -->.

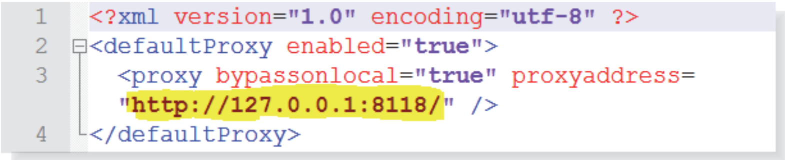
   Figure 182. Proxy configuration setting with XML comment delimiters

```
<?xml version="1.0" encoding="utf-8" ?>
<defaultProxy enabled="true">
  <!--
  <proxy bypassonlocal="true"
  proxyaddress="http://127.0.0.1:8118/" />
  -->
</defaultProxy>
```

4. Replace the text that is highlighted in yellow in Figure 183 with your company proxy address.

   Figure 183. Default proxy address highlighted in yellow

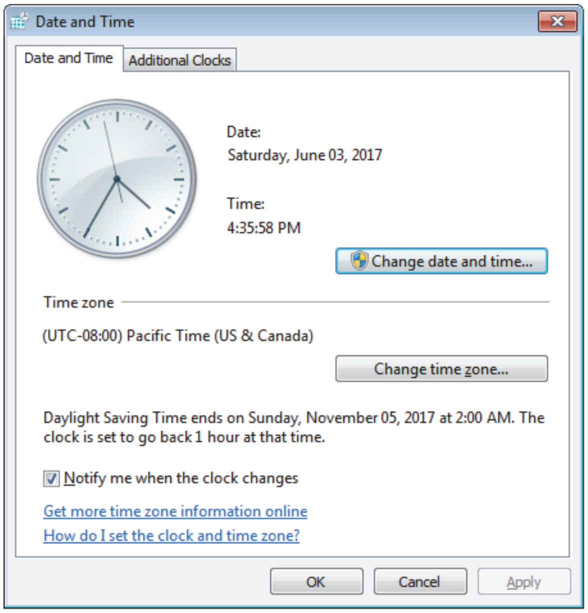
```
<?xml version="1.0" encoding="utf-8" ?>
<defaultProxy enabled="true">
  <proxy bypassonlocal="true" proxyaddress=
  "http://127.0.0.1:8118/" />
</defaultProxy>
```

Setting 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. For the Windows 7 operating system, open the Control Panel. In the View By list, select **Category**, and then choose **Clock, Language, and Region** > **Date and Time**.



Date:
Saturday, June 03, 2017

Time:
4:35:58 PM

Time zone
(UTC-08:00) Pacific Time (US & Canada)

Daylight Saving Time ends on Sunday, November 05, 2017 at 2:00 AM. The clock is set to go back 1 hour at that time.

☑ Notify me when the clock changes

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.

Contents

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.

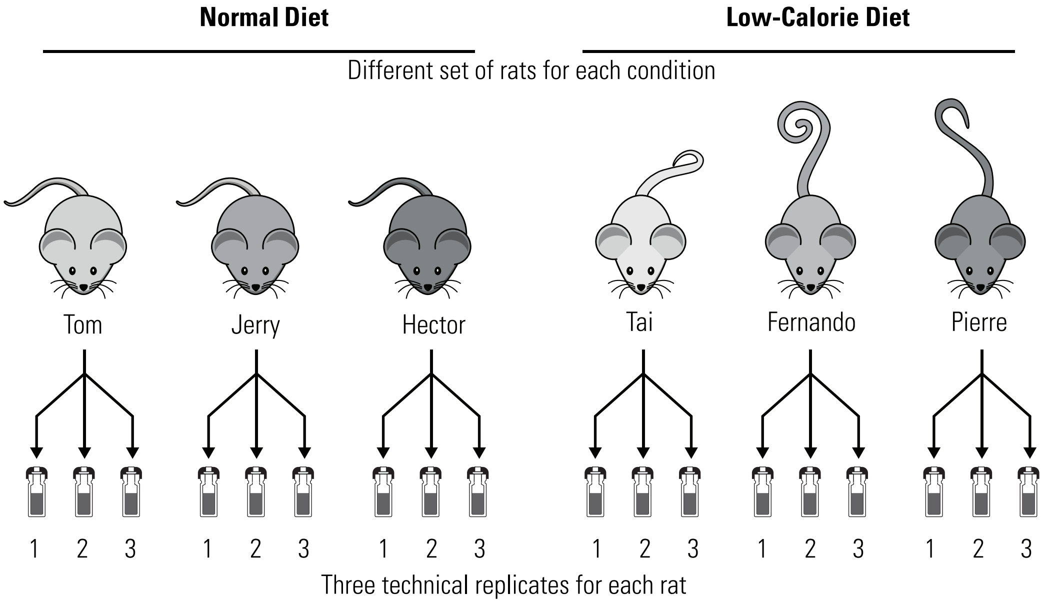
You can add only one biological replicate factor to a study. The application treats study factors nested under a biological replicate factor as technical replicates.

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).

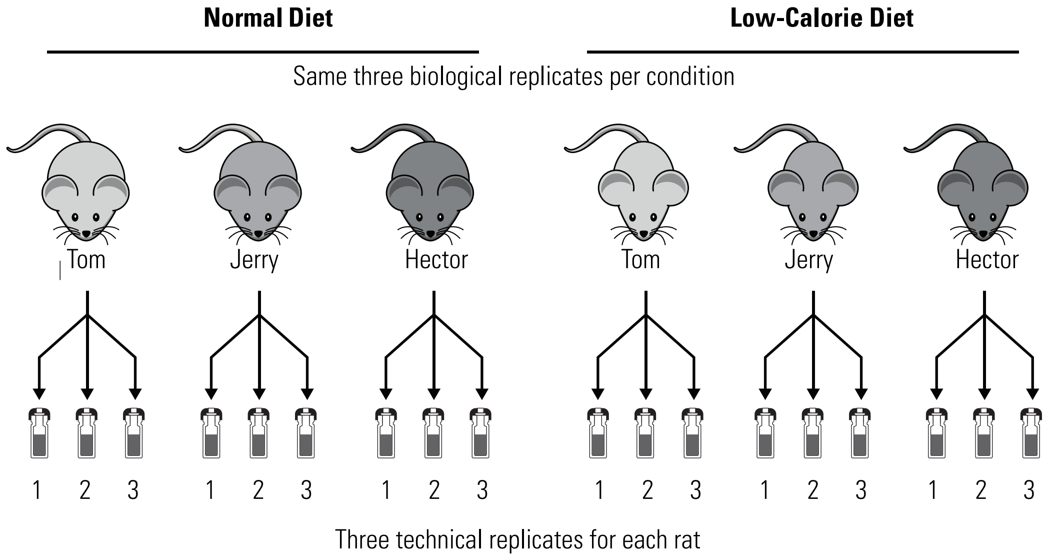
In non-nested experiments, different sets of biological replicates are used for each condition. Figure 184 shows a non-nested experiment where replicate samples are taken from two sets of rats under two conditions. Tom, Jerry, and Hector are fed a normal diet; and Tai, Fernando, and Pierre are fed a low-calorie diet.

Figure 184. 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 185 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 185. Nested design with the same three rats under two dietary conditions

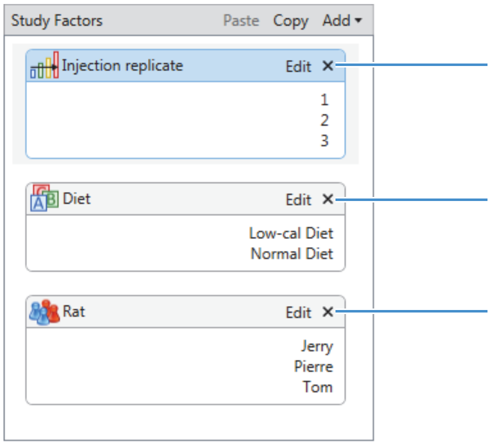


To set up the comparison ratios for a nested design with technical replicates, add the following study factors:

- 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 186 shows the study factors for the experiment shown in Figure 185.

Figure 186. Study factors for the nested design experiment



Numerical factor

Categorical factor

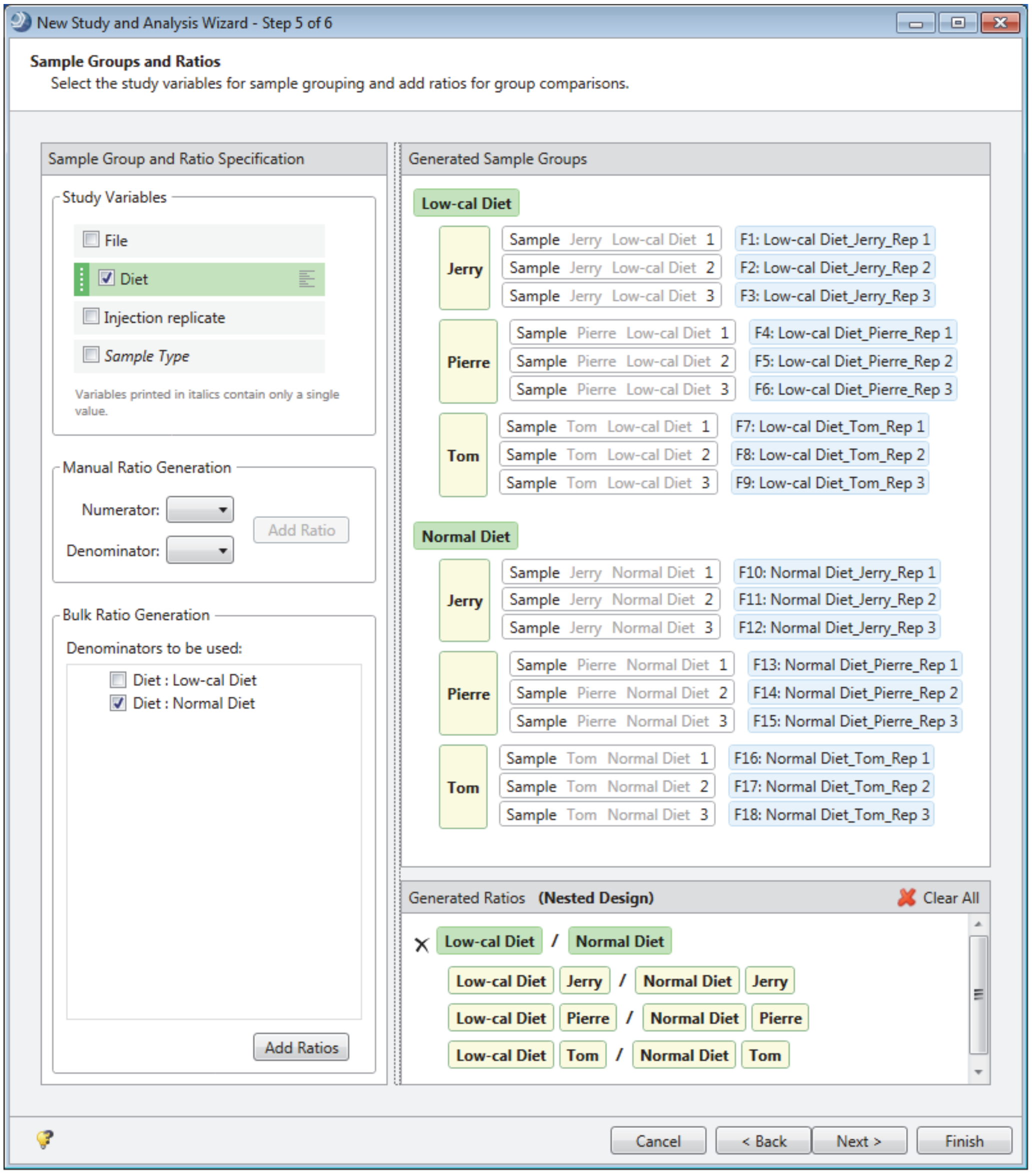
Biological Replicate factor

Figure 187 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 187. Nested design example



New Study and Analysis Wizard - Step 5 of 6

Sample Groups and Ratios

Select the study variables for sample grouping and add ratios for group comparisons.

Sample Group and Ratio Specification

Study Variables

☐ File
☑ Diet
☐ Injection replicate
☐ *Sample Type*

Variables printed in italics contain only a single value.

Manual Ratio Generation

Numerator:
Denominator:
Add Ratio

Bulk Ratio Generation

Denominators to be used:

☐ Diet : Low-cal Diet
☑ Diet : Normal Diet

Add Ratios

Generated Sample Groups

Low-cal Diet

Jerry
Sample Jerry Low-cal Diet 1 — F1: Low-cal Diet_Jerry_Rep 1
Sample Jerry Low-cal Diet 2 — F2: Low-cal Diet_Jerry_Rep 2
Sample Jerry Low-cal Diet 3 — F3: Low-cal Diet_Jerry_Rep 3

Pierre
Sample Pierre Low-cal Diet 1 — F4: Low-cal Diet_Pierre_Rep 1
Sample Pierre Low-cal Diet 2 — F5: Low-cal Diet_Pierre_Rep 2
Sample Pierre Low-cal Diet 3 — F6: Low-cal Diet_Pierre_Rep 3

Tom
Sample Tom Low-cal Diet 1 — F7: Low-cal Diet_Tom_Rep 1
Sample Tom Low-cal Diet 2 — F8: Low-cal Diet_Tom_Rep 2
Sample Tom Low-cal Diet 3 — F9: Low-cal Diet_Tom_Rep 3

Normal Diet

Jerry
Sample Jerry Normal Diet 1 — F10: Normal Diet_Jerry_Rep 1
Sample Jerry Normal Diet 2 — F11: Normal Diet_Jerry_Rep 2
Sample Jerry Normal Diet 3 — F12: Normal Diet_Jerry_Rep 3

Pierre
Sample Pierre Normal Diet 1 — F13: Normal Diet_Pierre_Rep 1
Sample Pierre Normal Diet 2 — F14: Normal Diet_Pierre_Rep 2
Sample Pierre Normal Diet 3 — F15: Normal Diet_Pierre_Rep 3

Tom
Sample Tom Normal Diet 1 — F16: Normal Diet_Tom_Rep 1
Sample Tom Normal Diet 2 — F17: Normal Diet_Tom_Rep 2
Sample Tom Normal Diet 3 — F18: Normal Diet_Tom_Rep 3

Generated Ratios **(Nested Design)** Clear All

× **Low-cal Diet** / **Normal Diet**
Low-cal Diet **Jerry** / **Normal Diet** **Jerry**
Low-cal Diet **Pierre** / **Normal Diet** **Pierre**
Low-cal Diet **Tom** / **Normal Diet** **Tom**

Cancel | < Back | Next > | Finish

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