

Compound Discoverer 3.3 SP3 Stable Isotope Labeling Tutorial

To familiarize yourself with using the Thermo Scientific™ Compound Discoverer™ 3.3 SP3 application to detect compounds labeled with a stable isotope such as carbon-13, follow the topics in this tutorial. These topics show you how to set up a study and an analysis, process a set of example Xcalibur™ RAW files, review the result file produced by the analysis, and export the results to a Microsoft™ Excel™ spreadsheet.

Note For isotopic labeling experiments, you must use a high resolution accurate mass (HRAM) Thermo Scientific mass spectrometer coupled with a liquid chromatography (LC) inlet to acquire the raw data.

Contents

- [Overview](#)
- [Start the application](#)
- [Check whether the data processing computer can access the external databases](#)
- [Set up a new study and a new analysis](#)
- [Submit the analysis to the job queue](#)
- [Review the analysis results](#)
- [Export the analysis results](#)

Overview

Before begin this tutorial, locate the example files for a stable isotope labeling study and review the tutorial workflow:

- [Locate the example files for this tutorial](#)
- [Tutorial workflow](#)
- [The Help system](#)

Locate the example files for this tutorial

In the Compound Discoverer application, data processing takes place within the study environment. To create a practice study, use the example Xcalibur RAW files that are provided in the following folder on the key-shaped USB drive in the software media kit:

Example Studies\LC\Stable Isotope Labeling

To save space on your data processing computer, you can leave the raw data files on the USB drive provided in the software media.

If you do not have the key-shaped USB drive that comes with the media kit, download the example files from the LSMS Software Download and Licensing Portal.

v To download the example files

1. Go to the following URL: thermo.flexnetoperations.com
The LSMS Software Download and Licensing Portal website opens.
2. Log in.
3. Under Software & Services at the left, click the **Product List** link.
4. On the Product List page, click the **Application - Compound Discoverer** link.
5. On the Product Information page, click the **Compound Discoverer 3.3 SP3** link.

The Product Information page for the Compound Discoverer 3.3 SP3 application contains compressed folders for all the tutorials provided with the application.

- On the Product Download Compound Discoverer 3.3 SP3 page, click the file names of the compressed folders (.zip) that contain the example files of interest.
- Copy the files to a folder on your data processing computer.






File name	File type	File name	File type
Blank_01.raw	RAW file	Ecoli_12C_AcquireX_ID_01.raw	RAW file
Ecoli_12C_01.raw	RAW file	Ecoli_12C_AcquireX_ID_02.raw	RAW file
Ecoli_12C_02.raw	RAW file	Ecoli_12C_AcquireX_ID_03.raw	RAW file
Ecoli_12C_03.raw	RAW file	Ecoli_12C_AcquireX_ID_04.raw	RAW file
Ecoli_13C_01.raw	RAW file	Stable Isotope Labeling.cdResult	Result file (analysis result)
Ecoli_13C_02.raw	RAW file	Stable Isotope Labeling.cdStudy	Study file
Ecoli_13C_03.raw	RAW file		

IMPORTANT For optimal performance, store all your Compound Discoverer study files (.cdStudy) and result files (.cdResult) on a local hard drive, ideally a solid state drive (SSD). Latency, read- and write speeds of external USB-connected hard drives and network drives are typically much slower than internal hard drives.

Because the result file is continuously accessed throughout the entire data processing workflow, processing times can be significantly longer when using external drives. Unlike result files, the application reads the raw data files (input files) only once, at the very beginning of the processing workflow. So, you can store raw data files on an external drive without significantly increasing the processing time.

Tutorial workflow

The typical workflow for a stable isotope labeling analysis includes the following steps.

Step	Task
1	 Start the Compound Discoverer application.
2	 Check the computer's access to the mzCloud™ and ChemSpider™ databases.
3	Use the New Study and Analysis Wizard to do the following: <ol style="list-style-type: none"> Select the study type, create a new study, and select a processing workflow. Add the files that you want to process to the study. Define the sample types for the sample set. Set up the sample groups for the analysis.
4	 Confirm the analysis and start the run.
5	 Open the result file and review, filter, and sort the data.
6	 Sort and filter the data. Then, export the data to a spreadsheet.

The Help system

The Compound Discoverer 3.3 SP3 application provides Help for the views, pages, and dialog boxes.

v To open the Help topic for a specific view, page, or dialog box



- Open the view, page, or dialog box

Start the application


2. On the computer keyboard, press the **F1** key, or equivalent (Fn + F1 keys).

For LC studies, the application also provides a user guide, four tutorials by field of study, and a reporting quick start guide as PDF files.

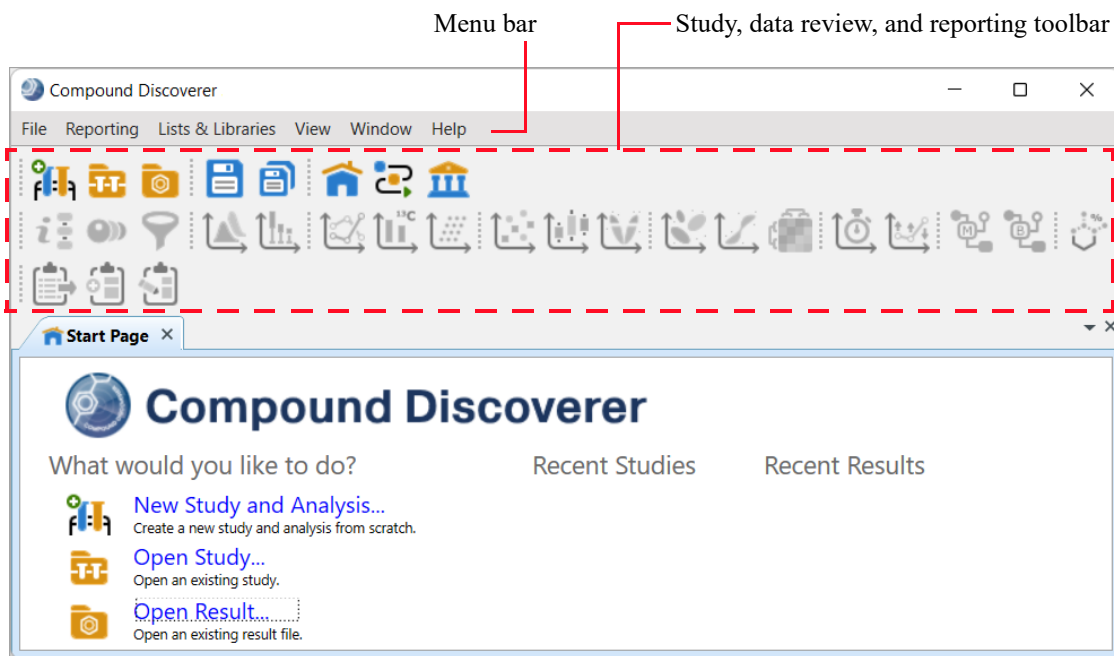
v To start the application

- From the Microsoft Windows™ 10 taskbar, click the **Start** button, , to open the Start menu. Then, choose **Thermo Compound Discoverer 3.3 > Compound Discoverer 3.3**.
- From the Microsoft™ Windows™ 11 taskbar, click the **Start** button, , and click **All Apps**. Then, choose **Thermo Compound Discoverer 3.3 > Compound Discoverer 3.3**.

–or–

- From the computer desktop, double-click the **Compound Discoverer 3.3** icon, .

The application opens to the Start Page.



Check whether the data processing computer can access the external databases

To use any of the processing workflows that use the online databases, such as mzCloud™ and ChemSpider™, your data processing computer must have unblocked access to these databases on the Internet.

v To verify that your computer has access to the external mass spectral databases

1. From the menu bar, choose **Help > Communication Tests**.
2. Click the **mzCloud** tab and click **Run Tests**. When the tests are complete, go to the next step.
3. Click the **ChemSpider** tab and click **Run Tests**.
4. If your computer has an Internet connection, but these tests fail, leave the Communication Test dialog box open and press the **F1** key to open the Help. Then, follow the instructions to troubleshoot the communication failure.

Go to the next topic to “[Set up a new study and a new analysis.](#)”

Set up a new study and a new analysis

Make sure to copy the example files to an appropriate folder on your data processing computer. See “[Locate the example files for this tutorial](#)” on page 1.

Follow these steps to create a new study and a new analysis in the order listed:

1. [Open the New Study and Analysis Wizard](#)
2. [Select the study type, specify the directory folder, and name the new study](#)
3. [Select the processing workflow](#)

Open the New Study and Analysis Wizard


4. Add the input files to the study
5. Specify the sample types
6. Set up the sample groups
7. Customize the processing workflow

In the Compound Discoverer application, you use the New Study and Analysis Wizard to create new studies and set up new analyses.

Note After you create a new study and assign sample types to the input files, you can set up different analyses from within the study.

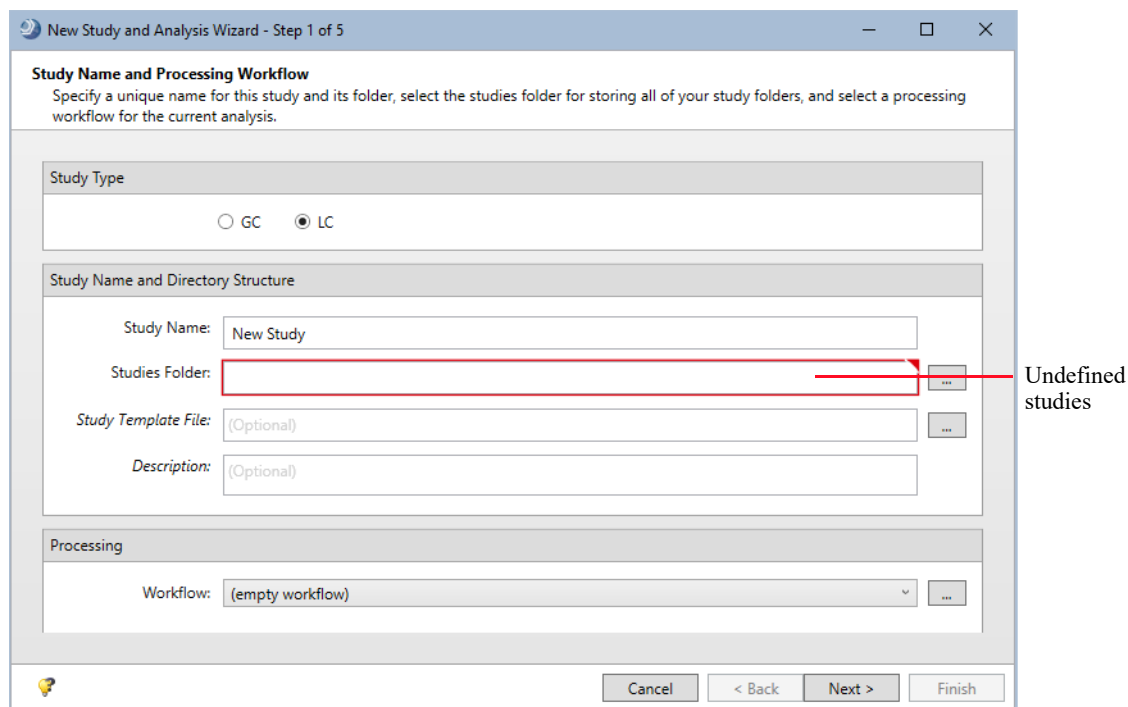
v To open the New Study and Analysis Wizard

Do one of the following:

- From the menu bar, choose **File > New Study and Analysis**.
- From the application toolbar, click the **Create a New Study and Analysis from Scratch** icon, .
- On the Start Page, click the **New Study and Analysis** link in the What Would You Like to Do? area.

The New Study and Analysis Wizard opens to the Study Name and Processing Workflow page. The first time you create a new study, the (top-level) studies folder is undefined. See [Figure 1](#).

Figure 1. Study Name and Processing Workflow page of the wizard



Leave this page of the wizard open and go to the next topic to “[Select the study type, specify the directory folder, and name the new study.](#)”


Select the study type, specify the directory folder, and name the new study

v To select the study type, specify the directory folder, and name the new study

1. In the Study Type area on the Study Name and Processing Workflow page of the wizard ([Figure 1](#)), select the **LC** option if it is not already selected.

The application stores this selection until you change it.

Note There are two types of studies: GC for gas chromatography-mass spectrometry data and LC for liquid chromatography-mass spectrometry data.

2. In the Study Name and Directory Structure area, select the studies directory folder as follows:
 - a. Click the **browse** icon, , next to the Studies Folder box.
The Select Folder dialog box opens.
 - b. Browse to the directory where you want to store your studies.

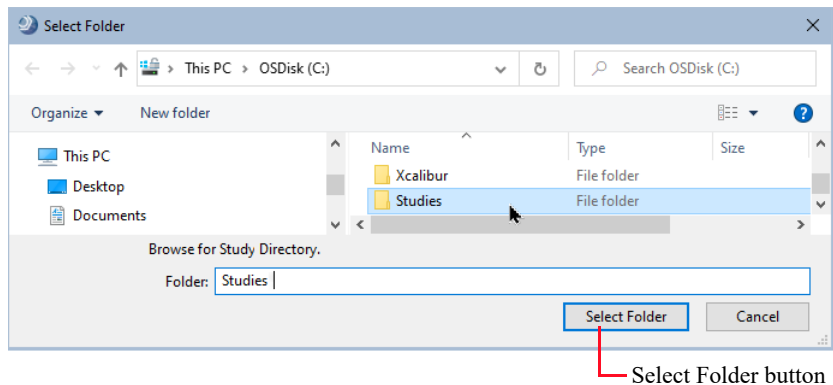
IMPORTANT To avoid excessive processing times, select a directory on your data processing computer. Do not store your studies on an external hard drive.

You can archive your studies on an external hard drive. But, if you need to fully reprocess any of the result files in these studies, move the studies back to a computer that has an installation of the Compound Discoverer application.

During data processing, the application makes a copy of the spectral data in the raw data files and copies this data to the result file, which is located in the folder that has the same name as the study. This processing step is relatively fast, so storing the raw data files on an external hard drive instead of the processing computer does not add a significant amount of time to data processing.

- c. Click **New Folder**.
- d. Name the new folder **Studies**, select it, and then click **Select Folder** (Figure 2).

Figure 2. Select Folder dialog box



Note The first time you create a new study, you must specify the directory (Studies Folder) where you want to store your studies. Thereafter, you can use the same studies folder or create additional studies folders.

3. In the Study Name and Directory Structure area, name the new study in the Study Name box.
For example, type **Stable Isotope Labeling** in the Study Name box.

Note When you create a new study, the application creates a new study folder with the same name and stores the study file (.cdStudy) in the new folder and the new study folder in the specified top-level folder for your studies.

 > This PC > OSDisk (C:) > Studies > Stable Isotope Labeling > Stable Isotope Labeling.cdStudy

Leave this page of the wizard open and go the next topic to [“Select the processing workflow.”](#)

Select the processing workflow

In the Compound Discoverer application, the processing method that interprets the raw data is called a processing workflow (.cdProcessingWF). The application provides defined processing workflows for several applications including stable isotope labeling experiments.

This tutorial uses a defined processing workflow that searches the mzCloud and ChemSpider databases to identify the unlabeled compounds detected in the sample files. It uses the Analyze Labeled Compounds node to detect the isotopologues of these compounds. This workflow also maps compounds to their biological pathways by using the local Metabolika pathway files.

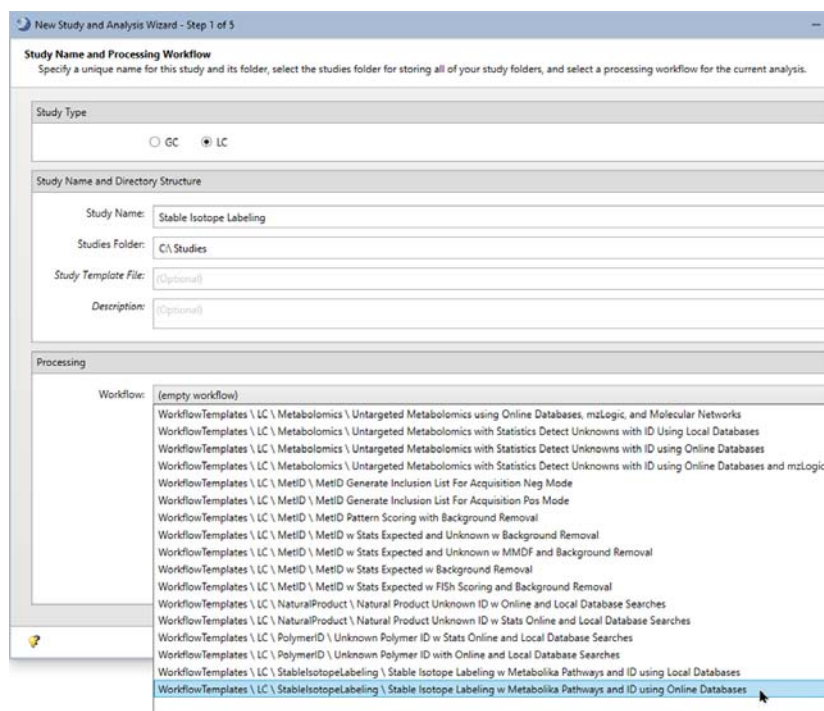
Note If your processing computer does not have Internet access, select the following processing workflow: Stable Isotope Labeling w Metabolika Pathways and ID using Offline Databases.

v **To select the processing workflow**

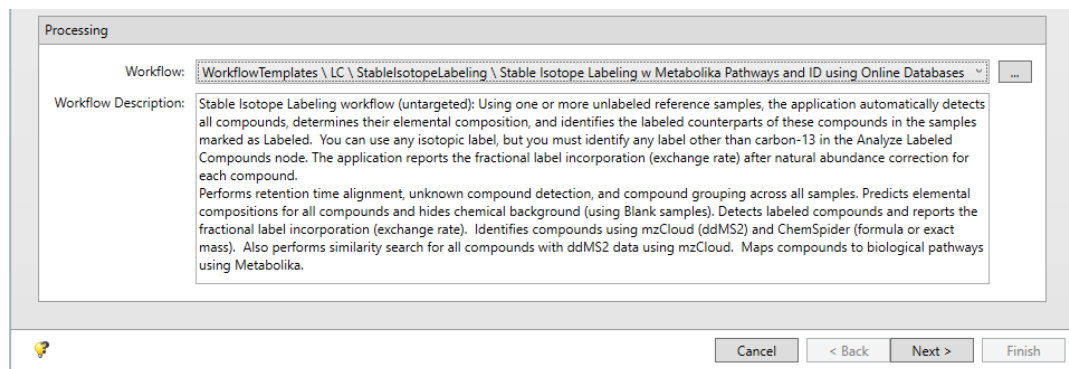
1. In the Processing area on the Study Name and Processing Workflow page of the wizard, select the following processing workflow from the Workflow list:

Workflow Templates \LC\ Stable Isotope Labeling\Stable Isotope Labeling w Metabolika Pathways and ID using Online Databases

Figure 3. Selecting the processing workflow template from the Workflows list



A description of the processing workflow appears in the Workflow Description box.



2. Read the description.

Note When you complete the wizard, the application creates the Stable Isotope Labeling Example.cdStudy file, stores the study file in the Stable Isotope Labeling Example folder, and stores the Stable Isotope Labeling Example folder in the Studies folder.

When you run the analysis in this tutorial, the application stores the result file (.cdResult) in the Stable Isotope Labeling Tutorial folder.

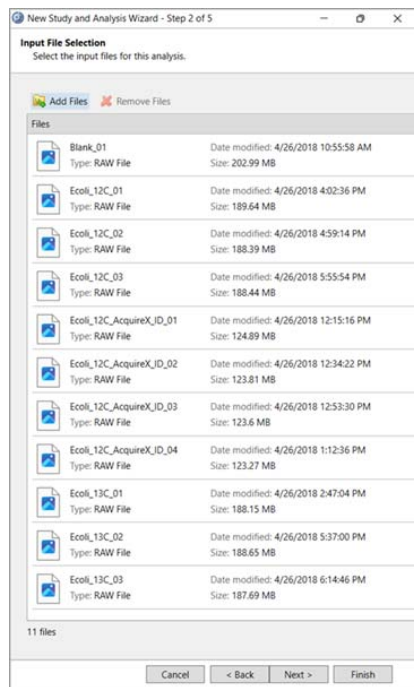
Go to the next topic to [“Add the input files to the study.”](#)

Add the input files to the study

- v **To add input files to the study**
- 1. At the bottom of the Study Name and Processing Workflow page of the wizard, click **Next**. The Input File Selection page opens.
- 2. On the Input File Selection page, click **Add Files**.
- 3. In the Add Files dialog box, browse to the folder where you copied the example RAW files.

Tip The application assigns a file number to each input file in the order you import them (see [Figure 4](#)). The file numbers are useful for tracking the input files in the result file tables.

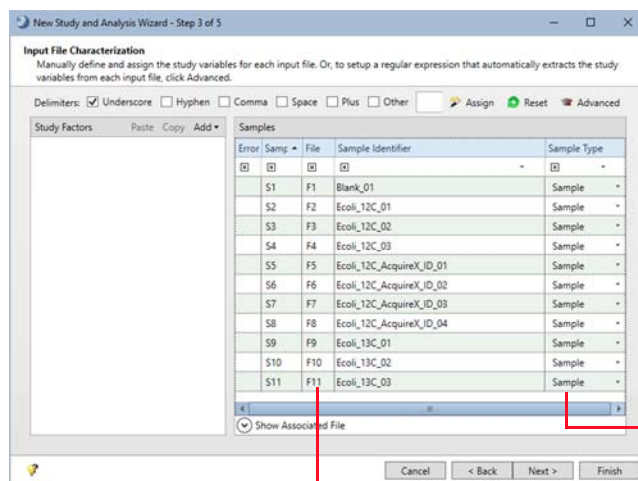
- 4. Select all 11 Xcalibur RAW files in this folder and click **Open**. Imported example files



- 5. Click **Next** to open the Input File Characterization page of the wizard.

[Figure 4](#) shows the newly added samples in the Samples area on the Input File Characterization page of the wizard. By default, the application assigns Sample as the Sample Type to new samples.

Figure 4. Imported files with assigned file numbers



Default sample type

File numbers based on the import

Leave this page of the wizard open and go to the next topic to “Specify the sample types.”

Specify the sample types

To specify the sample types for the example files in this tutorial, do the following in any order on the Input File Characterization page of the wizard:

- [Automatically assign the blank sample type](#)
- [Specify the identification samples](#)
- [Specify the labeled samples](#)

Table 1 describes the sample types for a stable isotope labeling analysis.

Table 1. Sample types

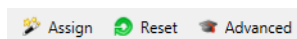
Sample type	The application processes these sample types as follows
Sample	Detects the unlabeled compounds in the sample.
Blank	Marks the background compounds in the entire data set.
Identification Only	Does not report the chromatographic peak areas for the compounds in these samples. Uses the sample's fragmentation scans for component (compound) identification.
Labeled	Determines the isotopic label incorporation.

Automatically assign the blank sample type

v To assign the Blank sample type

Note When you select the appropriate delimiters, the application assigns the Blank sample type to files named Blank or files with Blank in the file name.

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



The application assigns the Blank sample type to the Blank.raw file.

Go to the next topic to identify the samples to be used to identify the compounds in the *unknown* samples.

Specify the identification samples

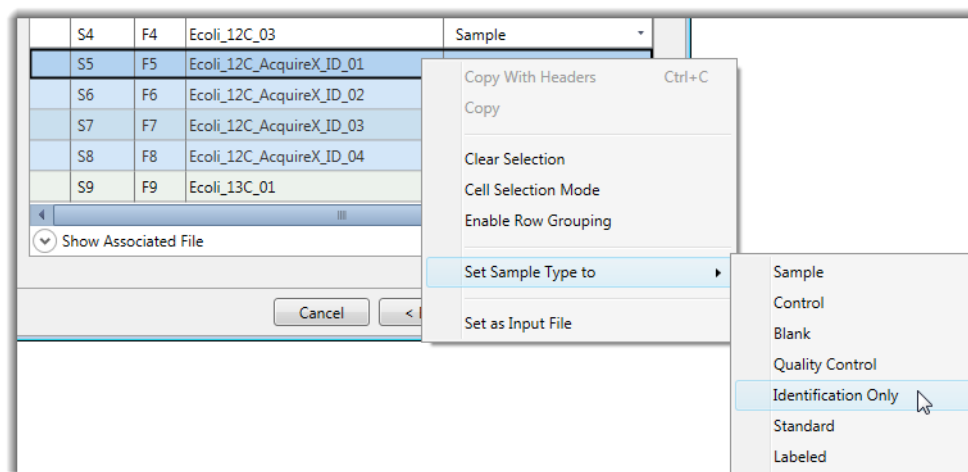
Identification samples must have fragmentation scans. In the example data set, the Acquire_X_ID.raw files contain data-dependent fragmentation scans (acquired within the same acquisition sequence and the same chromatographic conditions as the other data files).

v To specify the samples to use for compound identification

Use the SHIFT key to select the four Acquire_X_ID files. Then, right-click the selected rows and choose **Set Sample Type To > Identification Only** (Figure 5).

Tip To select a row, you can click any column but the Sample Type column.

Figure 5. Defining the samples to be used for Identification Only



Specify the labeled samples

Go to the next topic to identify the labeled samples.

The tutorial data set includes three samples labeled with carbon-13.

v To specify the labeled samples for the detection of labeled compounds

Use the CTRL key to select the files with ¹³C in their file name. Then, right-click the selected rows and choose **Set Sample Type To > Labeled** (see [Figure 6](#) on [page 9](#)).

Figure 6. Defining the labeled samples

Study Definition	Input Files	Samples	Analysis Results	
Error	Samp	File	Sample Identifier	Sample Type
	S1	F1	Blank_01	Blank
	S2	F2	Ecoli_12C_01	Sample
	S3	F3	Ecoli_12C_02	Sample
	S4	F4	Ecoli_12C_03	Sample
	S5	F5	Ecoli_12C_AcquireX_ID_01	Identification Only
	S6	F6	Ecoli_12C_AcquireX_ID_02	Identification Only
	S7	F7	Ecoli_12C_AcquireX_ID_03	Identification Only
	S8	F8	Ecoli_12C_AcquireX_ID_04	Identification Only
	S9	F9	Ecoli_13C_01	Labeled
	S10	F10	Ecoli_13C_02	Labeled
	S11	F11	Ecoli_13C_03	Labeled

Set up the sample groups

v To set up the sample groups for the analysis

1. At the bottom of the Input File Characterization page, click **Next**.

The Sample Groups and Ratios page of the wizard opens. Use this page of the wizard to set up the sample groups and ratios for a differential analysis.

[Figure 7](#) shows the 11 individual example files with their defined sample types in the Generated Sample Groups pane. Because you have not yet selected the study variables, the samples are not grouped.

Figure 7. Generated sample groups without any study variables

Tip Unlike a typical metabolic flux experiment, this tutorial does not include time as a study variable. For information on how to set up the study factors for a metabolic flux experiment, follow the embedded wizard Help or press the F1 key to access the Help system.

The time points in a flux experiment are the items for a categorical study factor.

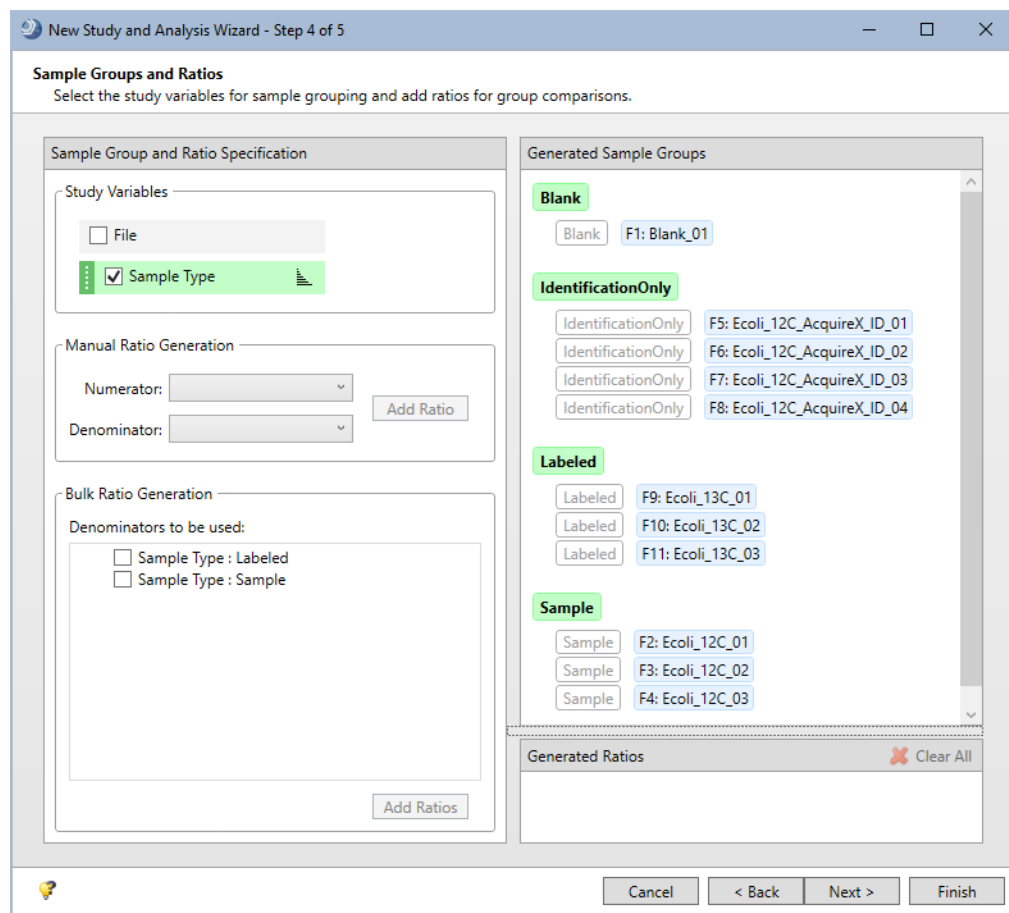
2. In the Study Variables area of the Sample Groups and Ratios page of the wizard, select the **Sample Type** check box.

The sample groups—Blank, Sample, Identification Only, and Labeled—appear in the Generated Sample Groups area (see [Figure 8](#) on [page 10](#)).

Note For the example data set, grouping the samples by sample type makes reviewing the data in the result tables easier.

Tip If you are setting up a metabolic flux study for your own data set, use the Sample Groups and Ratio page to set up the ratios for a differential analysis.

Figure 8. Samples grouped by sample type



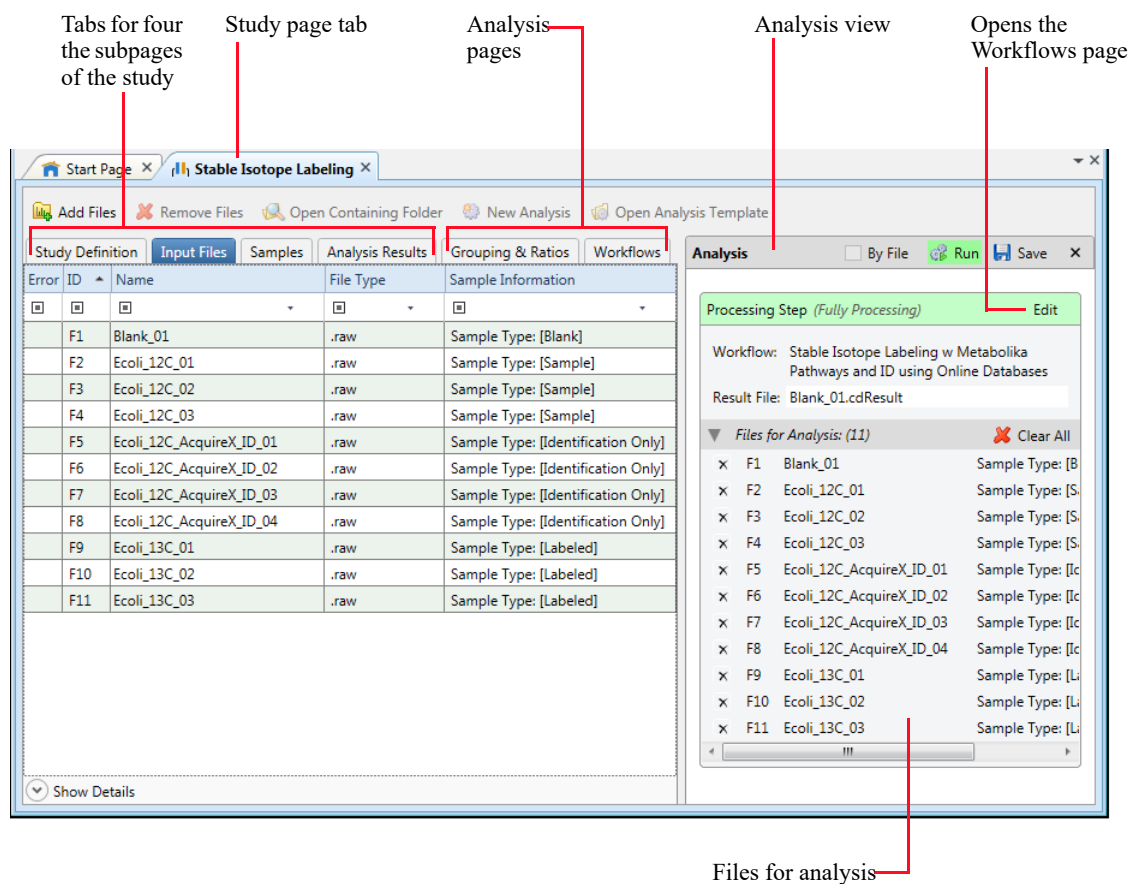
3. At the bottom of the Sample Groups and Ratios page, click **Finish** to save the study and close the wizard.

The study page with its four subpages and the analysis that you set up with the wizard open. See [Figure 10](#).

The Analysis view lists the 11 input files in the example data set. The analysis is set up to combine the processed results from these files into one result file—that is, the By File check box is clear and the file name for the result file is available for editing.

Figure 9 shows the Input Files page of the study and the Analysis view with a list of files for analysis.

Figure 9. Study with an analysis that is ready for processing



Customize the processing workflow

Before submitting the analysis to the job queue, review the processing workflow and make changes as needed.

v To review and customize the processing workflow for this tutorial

1. Click the **Workflows** tab to open the Workflows page of the analysis.

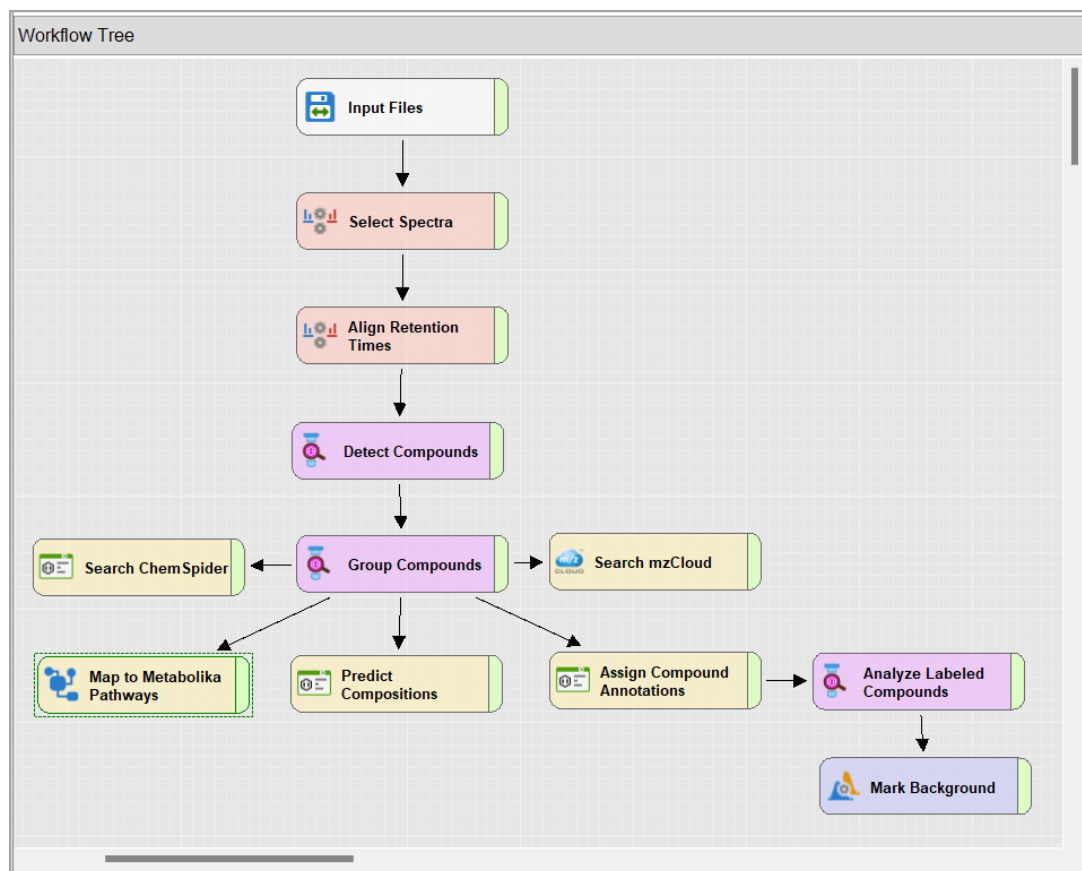
The Workflows page displays the processing workflow that you selected with the wizard.

Tip You can open the Workflows page in two ways:

- Click the **Workflows** tab to the left of the Analysis view.
- Click **Edit** in the Analysis view to the right of Processing Step.

Figure 10 on page 12 shows the processing workflow in the Workflow Tree pane.

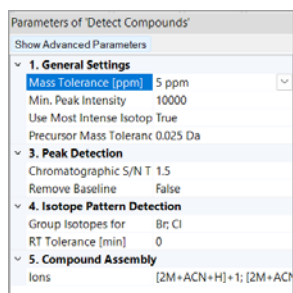
Figure 10. Processing workflow template for a stable isotope labeling experiment



2. To customize the minimum peak intensity for the Detect Compounds node, do the following,
 - a. In the Workflow Tree area on the Workflows page, click the **Detect Compounds** node to select it. A dashed green border appears around the Detect Compounds node.

In addition, the parameters page for the node opens to the left of the Workflow Tree pane. Most of the parameters for the node are set to their default values, but Thermo Fisher Scientific customized a few of the parameters settings for the processing workflow template.

Figure 11. Parameter settings for the Detect Compounds node



3. (Optional) To learn more about the parameter settings for the workflow nodes in the processing workflow template for stable isotope labeling studies, review the settings in [Table 2](#).

Table 2. Processing workflow node settings for the stable isotope processing workflow template (Sheet 1 of 2)

Group Compounds node

In the processing workflow template for stable isotope labeling, the Peak Rating Filter is adjusted as follows:

- Peak rating Threshold is set to 5.
- Number of Files is set to 3.

The Group Compounds node creates the MSn tree that the analysis sends to the search nodes and saves to the result file. The Predict Compositions node uses the MSn tree to match fragments.

Parameters of 'Group Compounds'	
Show Advanced Parameters	
▼ 1. General Settings	
Mass Tolerance	5 ppm
RT Tolerance [min]	0.2
Minimum Valley [%]	10
Align Peaks	False
Preferred Ions	[M+H] ⁺ 1; [M-H] ⁻ 1
Area Integration	Most Common Ion
▼ 2. Peak Rating Contributions	
Area Contribution	3
CV Contribution	10
FWHM to Base Contribu	5
Jaggedness Contribution	5
Modality Contribution	5
Zig-Zag Index Contribu	5
▼ 3. Peak Rating Filter	
Peak Rating Threshold	5
Number of Files	3

The peak rating filter set

Assign Compound Annotations node

For the example data set, do not change the settings.

Parameters of 'Assign Compound Annotations'	
Hide Advanced Parameters	
▼ 1. General Settings	
Mass Tolerance	5 ppm
▼ 2. Data Sources	
Data Source #1	mzCloud Search
Data Source #2	Predicted Compositions
Data Source #3	MassList Search
Data Source #4	ChemSpider Search
Data Source #5	Metabolika Search
Data Source #6	
Data Source #7	
▼ 3. Scoring Rules	
Use mzLogic	True
Use Spectral Distance	True
SFit Threshold	20
SFit Range	20
▼ 4. Reprocessing	
Clear Names	False

Tip If you are working with your own data set and the analysis does not identify the correct isotopologues, consider changing Data Source #1 to a custom mass list for your analytes and reprocessing the analysis.

Table 2. Processing workflow node settings for the stable isotope processing workflow template (Sheet 2 of 2)

Analyze Labeled Compounds node

For the example data set, keep the default settings. For a different data set, enter the appropriate isotope for the Label Element parameter.

Parameters of 'Analyze Labeled Compounds'	
Show Advanced Parameters	
1. Label Settings	
Label Element	[13]C
Max. Exchange	25
Source Efficiency [%]	100
2. Pattern Analysis	
Abundance Integration	Area
Mass Tolerance [ppm]	5 ppm
Intensity Tolerance [%]	30
Intensity Threshold [%]	0.1
Minimum Valley [%]	10
S/N Threshold	3
Min. # Scans per Peak	5
3. General Settings	
Ions to Use	Most Common Ion
Exclude Blanks	True
Mark Irregular Exchange	True
Hide Unprocessed	True
4. Peak Rating Contributions	
Area Contribution	3
CV Contribution	10
FWHM to Base Contribution	5
Jaggedness Contribution	5
Modality Contribution	5
Zig-Zag Index Contribution	5

Customize this setting for your own data set, as
Specifies the maximum number of exchangeable atoms.

The default setting is 25.

If you set this value to 0, the analysis determines the maximum number of exchangeable atoms for

Hides the compounds without formulas in the Compounds table.

Submit the analysis to the job queue

For the example data set and analysis, you can now submit the analysis to the job queue for processing.

Tip If you modified the analysis and the Run button is unavailable, do the following:

- Remedy the issues listed in the Current Workflow Issues pane on the Workflows page.
- If there is a Caution symbol to the right of Edit in the Analysis view, point to it and remedy other analysis errors, for example, no input files in the Files for Analysis area of the Analysis view or missing node connections.

If a prompt appears when you submit the run, open the Grouping & Analysis page of the analysis and select the Sample Type check box to group the input files by sample type.

v To submit the analysis to the job queue

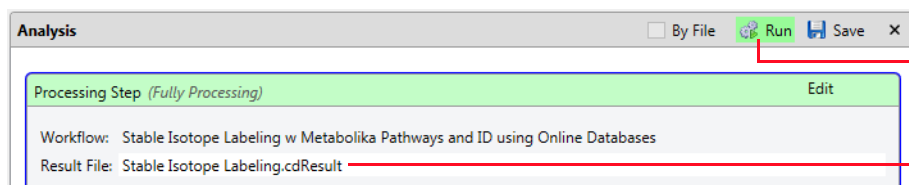
1. To create one result file for the input file set, leave the **By File** check box clear in the Analysis view.

In this analysis (and for most analyses), you compile the processing results from multiple input files into one result file.



By default, the application uses the name of the first input file for the file name of the result file.

2. In the Result File box, rename the result file **Stable Isotope Labeling**.



Available Run command


Result file name

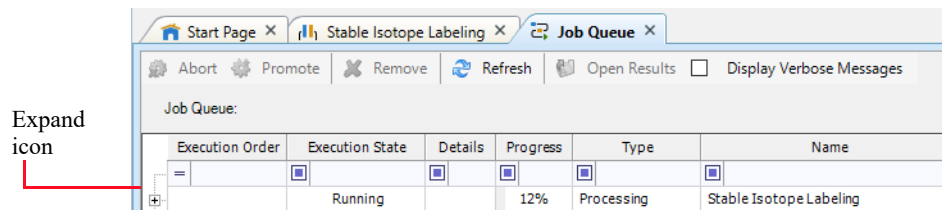
3. Click **Run**.

The Analysis Validation Issues prompt opens with an alert about the lack of a peak rating filter in the Group Compounds node.

4. Click **Ignore**.

The Job Queue page opens.

5. To view the processing messages, click the expand icon, , to the left of the job row.



Note During the run, the Search ChemSpider node generates warning messages, which you can ignore. Warning messages have a yellow background.

6. Leave the Job Queue page open and go to “[Review the analysis results.](#)”

Review the analysis results

To review the analysis results, follow these topics in the order listed:

1. [Open the result file](#)
2. [Review the default layout for the result page and common layout modifications](#)
3. [Apply the Stable Isotope Labeling layout](#)
4. [Review the exchange rates](#)
5. [Review the labeling status](#)
6. [View a trend chart for a single compound or a set of trend lines for multiple compounds](#)
7. [View the distribution of the isotopologues for each compound](#)
8. [View the Metabolika pathways for a compound](#)

For more information about a specific result table or view, select the table or view to make it active, and then press the F1 key. The Compound Discoverer application provides F1 Help for all the views that you access from the View menu and all the result tables.

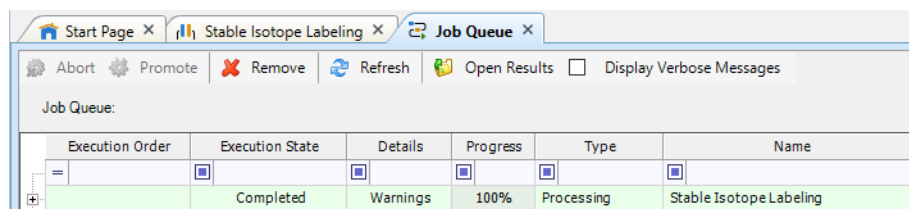
Open the result file

You can open a result file from multiple locations: the Job Queue page, the Analysis Results page of a study, the Compound Discoverer Start Page, or the menu bar.

Note For this tutorial, you can create a result file by setting up and running an analysis with the example data set. Or, you can open the result file—Stable Isotope Labeling—in the same folder where you found the example data set.

- v **To open the result file generated by the analysis**

When the application completes the run, double-click the run on the Job Queue page.



Review the default layout for the result page and common layout modifications

Default layout for the stable isotope labeling analysis

These topics describe the default layout for the result file that the stable isotope labeling analysis generates and some of the common layout modifications that you can make:

- [Default layout for the stable isotope labeling analysis](#)
- [Common layout modifications](#)

The result file opens as a tabbed document with the following layout (numbered in [Figure 12](#) on [page 16](#)):

1. The Chromatograms view appears on the upper left of the page.

The Chromatograms view displays the overlaid and shaded chromatographic peaks for the compound in the first row of the Compounds table.

2. The Mass Spectrum view appears on the upper right of the page.

The Mass Spectrum view displays the MS1 scan in the spectrum tree that is closest to the apex of the compound's chromatographic peak.

The spectrum tree to the left of the spectrum plot includes the MS1 scans and the fragmentation scans for the preferred ions that the MS acquired within the following retention time window:

- The chromatographic peak apex for the selected compound \pm peak width at half maximum (FWHM) –or–
- The Start and end points of the chromatographic peak, as determined by the peak detection algorithm

Note If the data set does not include data-dependent MS2 scans within the retention time window but does include data-independent scans within this window, the spectrum tree includes the data-independent scans.

3. A set of tabbed result tables opens in the bottom half of the page. The Compounds table is the active table.

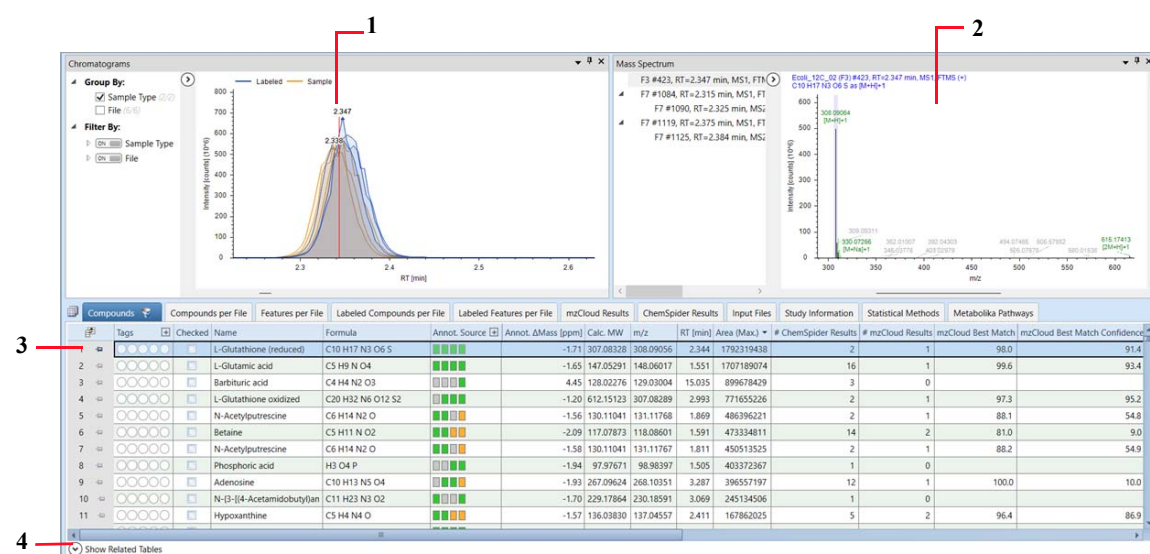
Because the selected processing workflow includes the Mark Background Compounds node and the Analyze Labeled Compounds node, the Compounds tab has a filter icon with a check mark (☑). The compounds that the analysis identified as background compounds are marked as background compounds in both the blank and non-blank samples and are hidden from the table. In addition, the compounds without a formula are hidden from the table.

4. A collapsed area for the related data tables below the main tables.

In the Compounds table, the detected compounds are listed in descending order of the maximum chromatographic peak area [Area (Max.)] across the set of input files. The Chromatograms and Mass Spectrum views are populated with data for the first compound in the table.

[Figure 12](#) shows the factory default layout for the Stable Isotope Labeling.cdResult file.











Figure 12. Default result file layout



Common layout modifications

You can change which columns, tables, and views are visible or hidden. To display the subcolumn headings for columns that contain multiple subcolumns, you must expand the column headers.

Table 3. Common layout modifications

Task	Procedure
Show or hide a table column	Open the Field Chooser for a table by clicking the icon,  , in the upper left corner of the table. To display a column, select its check box. To hide a column, clear its check box.
Show or hide a table	Open the Select Table Visibility dialog box by clicking the icon,  , at the left of the table tabs.
Close a view	Click the close icon,  , in the upper right corner of the view.
Open a view	In the application menu bar, choose View > Specific View . Or, in the toolbar, click the icon for the view.
Expand the header for a column with multiple subcolumns	Click the expand icon,  , to the right of the heading.
Freeze a column to the left side of the table	Right-click the table and choose Enable Column Fixing . Then, click the pin icon to the right of the column heading.
Pin a row to the top of the result table.	Click the pin icon to the right of the row number (unpinned,  , or pinned, )
Sort a result table by a column with numeric or text information.	Click a column header once or twice to sort the rows in ascending order () or descending order (), based on the contents of the column.
Sort a result table by multiple columns.	Click the column header of the primary sort column once or twice to sort the rows in ascending order () or descending order (), based on the contents of the column. Hold down the CTRL key and click the column header of the secondary sort column once or twice to set the sort order.
Reset the result page layout.	From the application menu bar, choose Window > Reset Layout .

Apply the Stable Isotope Labeling layout

The application comes with the factory default layout and two named layouts: Statistics and Stable Isotope Labeling. When reviewing the results of a stable isotope labeling analysis, apply the Stable Isotope Labeling layout.

v To apply the Stable Isotope Labeling layout to the current result file

From the application menu bar, choose **Window > Apply Layout > Stable Isotope Labeling**.

Applying the Stable Isotope Labeling layout does the following to the example result file as shown in [Figure 13](#) on [page 18](#):

- Hides the following main tables:
 - Compounds per File
 - Features per File
 - ChemSpider Results
- Hides the following columns in the Compounds table:
 - #Adducts
 - #Metabolika Pathways
 - Annot. Δ Mass [Da]
 - Annotation MW
 - Avg. Exchange
 - Background
 - FISH Coverage
 - Labeled Compounds per File
 - Labeled Features
 - mzCloud Results
 - Gap Status
 - Metabolika Pathways
 - MS Depth
 - mzCloud Library Matches
 - RT Tolerance [min]
 - Structure
- Opens the Related Tables pane to the Labeled Compounds per File table for the first compound in the Compounds table.
- Opens the Isotopologues Distribution Chart, Trend Chart, and Metabolika Pathways views as tabbed views on the bottom right of the page.
- Selects the Rel. Exchange data property for the Trend Chart view.

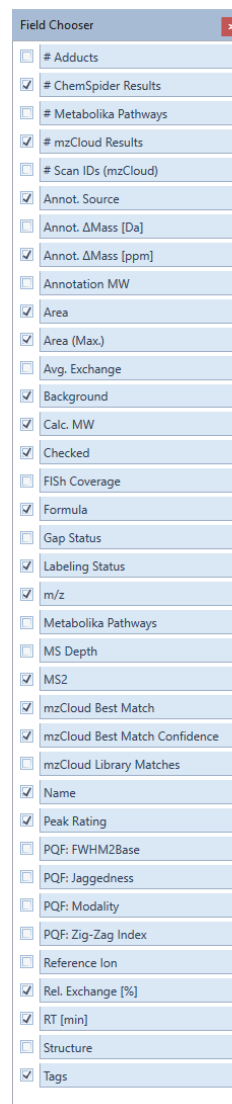
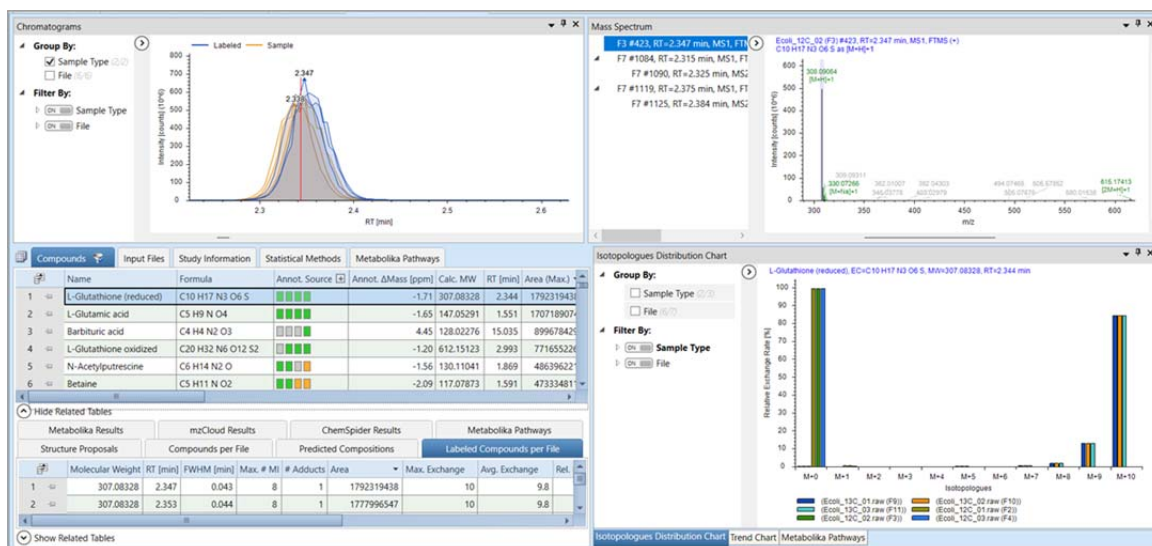


Figure 13. Default layout after applying the Stable Isotope Labeling layout



Review the exchange rates

View the relative exchange rates for a compound across the input file set

The following topics show you how to modify the layout of the result page for easier visualization of the exchange rate columns in the Compounds table:

- [View the relative exchange rates for a compound across the input file set](#)
- [View the exchange rate for each of the compound's isotopologues](#)
- [View the exchange rates for the adducts of a compound](#)

Precondition: You applied the Stable Isotope Labeling layout to the result file as described in “[Apply the Stable Isotope Labeling layout](#)” on [page 18](#).

In this topic, you review the exchange rates for L-glutamic acid. The chromatographic peak for this compound has the second largest maximum area among all the detected compounds, so it sorts to row 2 when the Compounds table is sorted in descending order by the Area (Max). column.

Note The Annotation Source column is hidden in the following figures.

v To view the relative exchange rates for a compound across the input file set

1. In the Compounds table, click the pin icon to the left of L-Glutamic acid in row 2.

Clicking the pin icon to the right of a row number freezes the row to the top of the table.

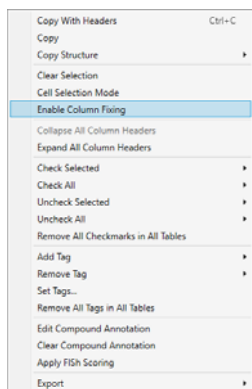
Figure 14. L-glutamic acid frozen at the top of the Compounds table

	Name	Formula	RT [min]	Calc. MW	Area (Max.)	Labeling Status	Annot. Source
2	L-Glutamic acid	C5 H9 N O4	1.551	147.05291	1707189074	■■■■	■■■■
1	L-Glutathione (reduced)	C10 H17 N3 O6 S	2.344	307.08328	1792319438	■■■■	■■■■
3	Barbituric acid	C4 H4 N2 O3	15.035	128.02276	899678429	■■■■	■■■■
4	L-Glutathione oxidized	C20 H32 N6 O12 S2	2.993	612.15123	771655226	■■■■	■■■■

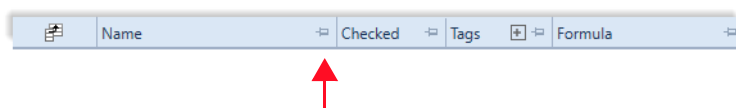
2. In the Compounds table, freeze the Name column at the left of the table as follows:



- a. Right-click the Compounds table and choose **Enable Column Fixing**. See [Figure 15](#).

Figure 15. Shortcut menu for the Compounds table



Pin icons appear to the right of the column headings.



- b. Click the pin icon to the right of the Name column heading (pinned, , and unpinned, )


3. Scroll right to the Rel. Exchange [%] column.
4. To view the input file names in the Rel. Exchange [%] column, click the expand icon () next to the column header. Or, right-click the Compounds table and choose **Expand All Column Headers** to expand all the table column headers.

Figure 16 shows the relative exchange rate for L-glutamic acid in each input file. The relative exchange rate is 98% for the labeled samples and 0% for the unlabeled samples.

Figure 16. Relative exchange rate for L-glutamic acid

Compounds		Compounds per File			Features per File			Labeled Compounds per File			Labeled Features per File			mzCloud Results	
Name	Rel. Exchange [%]									Labeling Sta			Area (Max)	m/z	
	Ecoli_13C_01.raw (F9)*	Ecoli_13C_02.raw (F10)	Ecoli_13C_03.raw (F11)	Ecoli_12C_01.raw (F2)	Ecoli_12C_02.raw (F3)	Ecoli_12C_03.raw (F4)	Ecoli_13C_01.raw (F9)*	Ecoli_13C_02.raw (F10)	Ecoli_13C_03.raw (F11)	Ecoli_12C_01.raw (F2)	Ecoli_12C_02.raw (F3)	Ecoli_12C_03.raw (F4)			
2	L-Glutamic acid	98	98	98	0	0	0	█	█	█	█	█	1707189074	148.06017	
1	L-Glutathione (reduced)	98	98	98	0	0	0	█	█	█	█	█	1792319438	308.09056	
3	Barbituric acid	0	0	0	0	0	0	█	█	█	█	█	899678429	129.03004	
4	L-Glutathione oxidized	98	98	98	0	0	0	█	█	█	█	█	771655226	307.08289	
5	N-Acetylputrescine	93	93	93	0	0	0	█	█	█	█	█	486396221	131.11768	
6	Betaine	0	0	0	0	0	0	█	█	█	█	█	473334811	118.08601	
7	N-Acetylputrescine	93	93	93	1	0	1	█	█	█	█	█	450513525	131.11767	
8	Phosphoric acid							█	█	█	█	█	403372367	98.98397	
9	Adenosine	97	97	97	0	0	0	█	█	█	█	█	396557197	268.10351	
10	N-(3-[(4-Acetamidobutyl)an	81	80	80	0	0	0	█	█	█	█	█	245134506	230.18591	

Name column frozen at the left of the Compounds table

98% relative exchange rate for L-glutamic acid in the three labeled samples (F9, F10, and F11)

View the exchange rate for each of the compound's isotopologues

v To view the exchange rate for each isotopologue of a compound

- In the main Compounds table, select **L-glutamic acid (row 2)**.
 - If you applied the Stable Isotope Labeling layout, the related tables pane is visible and the Labeled Compounds per File table is the active table. See “Apply the Stable Isotope Labeling layout” on page 18.
 - If you fixed the Name column to the left of the table, you can scroll to the right without losing track of which compound you are viewing. See step 2 in “View the relative exchange rates for a compound across the input file set” on page 19.
- Click **Show Related Tables** below the main tables.
- In the related Labeled Compounds per File table, scroll to the Exchange Rate [%] column.
- To view the isotopologues, click the expand icon (⊞) next to the Exchange Rate [%] column heading.

Figure 17 shows the exchange rates in the labeled (F11, F9, and F10) and unlabeled (F2, F3, and F4) samples. The exchange rates for the labeled samples are 92% for the $^{13}\text{C}_5\text{H}_9\text{NO}_4$ isotopologue and 7% for the $^{13}\text{C}_4\text{CH}_9\text{NO}_4$ isotopologue of L-glutamic acid.

The Exchange Rate [%] column contains 25 subcolumns because the analysis specified a maximum exchange of 25 atoms for any of the detected compounds. See “Analyze Labeled Compounds node” on page 14.

Color-coding:

- Irrelevant subcolumns for unprocessed elemental compositions have a gray background.
- Subcolumns for isotopologues have a pink to red background that turns darker as the exchange rate increases.

Figure 17. Exchange Rate and Study File columns in the Labeled Compounds per File table for L-glutamic acid (numbered in clockwise order, starting with 1 at the top right)

No.	Description	No.	Description
1	Unlabeled samples, F2, F3, and F4	4	Exchange rate [%] for all five carbon atoms in L-glutamic acid
2	Labeled samples, F11, F10, and F9	5	Exchange rate [%] for four out of five carbon atoms in L-glutamic acid
3	Blank sample, F1	6	Exchange rate [%] for all no carbon atoms in L-glutamic acid

View the exchange rates for the adducts of a compound

Precondition: Glutamic acid (row 2) is selected in the main Compounds table.

v **To view the exchange rates for the adducts of a compound in a specific input file**

1. In the related Labeled Compounds per File table for glutamic acid, select **F11**, a labeled sample.
2. Click **Show Related Tables** below the Labeled Compounds per File table.
3. In the related tables pane for input file F11, click the **Labeled Features** tab to make it the active table.

This figure shows the relative amounts (by chromatographic peak area) of the labeled adduct ions that the analysis detected for L-glutamic acid in study file F11 (a labeled sample).

Figure 18. Labeled features for L-glutamic acid in study file F11

Review the labeling status


The Labeling Status column in the Compounds table and the Status column in the Labeled Compounds per File table provide information about the quality of the analysis.

- (■) Red—Indicates a contaminating mass in an unlabeled sample.
- (■) Blue—Indicates an irregular exchange rate for a labeled sample.
- (■) Orange—Indicates a low fit between the measured and fitted isotope patterns.
- (■) Gray—Indicates the absence of isotopologues for the detected compound.

A contaminating mass in an unlabeled sample is more problematic than an irregular exchange rate for a labeled sample.

v **To investigate a contaminating mass in an unlabeled sample**

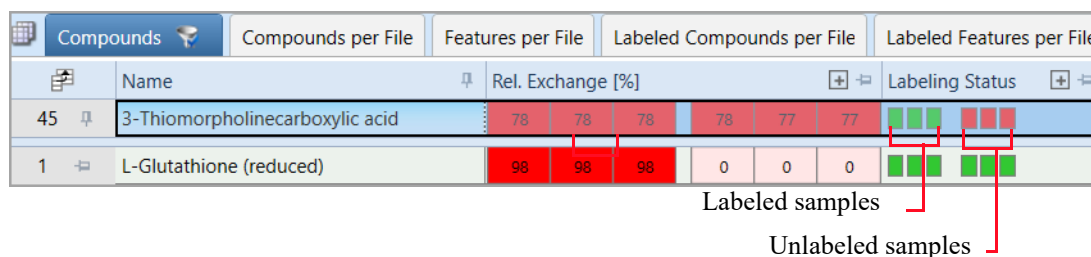
1. In the Compounds table for the example result file, sort the compounds in descending order by Area (Max.). If you fixed L-glutamic acid to the top of the table, sorting the compounds releases it.
2. In row 45, click the pin icon to the left of 3-Thiomorpholinecarboxylic acid to fix this compound to the top of the table.

- Click the expand icon, , for the Labeling Status column.

Because you grouped the samples by sample type (Figure 8), the samples are also grouped by sample type in the Labeling Status column.


The red status for 3-Thiomorpholinecarboxylic acid in the unlabeled samples indicates the presence of a contaminating mass in these samples (F2, F3, and F4).

Figure 19. 3-Thiomorpholinecarboxylic acid (row 45) in the Compounds table (with the Name and Labeling Status columns frozen at the left)



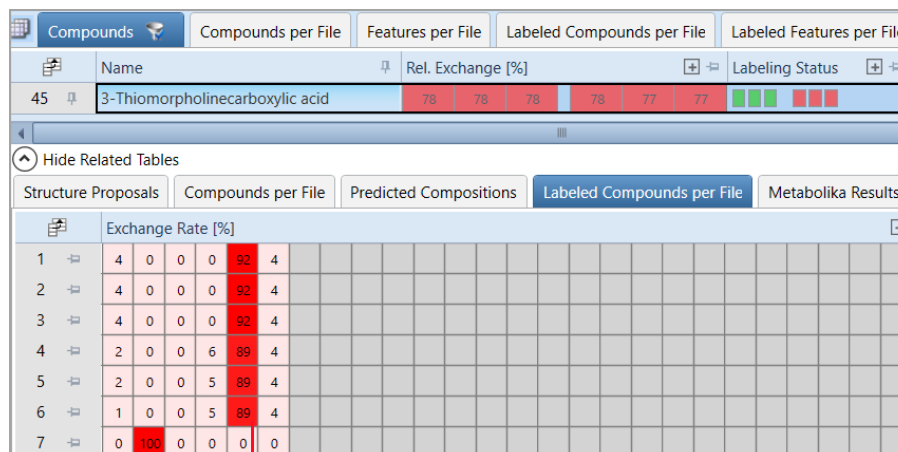
Compounds		Compounds per File	Features per File	Labeled Compounds per File	Labeled Features per File			
Name	Rel. Exchange [%]	Labeling Status						
45	3-Thiomorpholinecarboxylic acid	78	78	78	78	77	77	Labeling Status (red)
1	L-Glutathione (reduced)	98	98	98	0	0	0	Labeling Status (green)

Labeled samples
Unlabeled samples

- In the related Labeled Compounds per File table for 3-Thiomorpholinecarboxylic acid, do the following:
 - Right-click the table and choose **Enable Column Fixing**. Then, click the pin icon for the Exchange Rate [%] column.
 - Click the expand icon, , for the Exchange Rate [%] column.

This figure shows the exchange rate for 3-Thiomorpholinecarboxylic acid in its related Labeled Compounds per File table. The Exchange Rate [%] column shows that the contaminating mass is possibly a compound with a mass of M+4.

Figure 20. Labeled Compounds per File table for 3-Thiomorpholinecarboxylic acid



Name	Rel. Exchange [%]	Labeling Status
45	3-Thiomorpholinecarboxylic acid	78, 78, 78, 78, 77, 77

Exchange Rate [%]	
1	4 0 0 0 92 4
2	4 0 0 0 92 4
3	4 0 0 0 92 4
4	2 0 0 6 89 4
5	2 0 0 5 89 4
6	1 0 0 5 89 4
7	0 100 0 0 0

The false exchange rate of four carbon-13 atoms for an unlabeled compound was probably caused by a contaminating mass of M + 4.

View a trend chart for a single compound or a set of trend lines for multiple compounds

When you apply the Stable Isotope Labeling layout, the Trend Chart view opens as a hidden view below the Isotopologues Distribution Chart view.

Use the Trend Chart view to compare the relative exchange rate [%] for each compound by input file, sample group, or study variable (for example, the time points in a metabolic flux study). When you select a single compound in the Compounds table, you can view its distribution as a box-and-whiskers plot or as a trend line plot. When you select multiple compounds in the Compounds table, the application automatically displays the distribution for each compound as a trend line plot.

Note The example data set does not include metabolic flux samples.

Tip Apply the Stable Isotope Labeling layout if you have not already applied it or if you closed some of the views. To apply the Stable Isotope Labeling layout, choose **Window > Apply Layout > Stable Isotope Labeling** from the menu bar.

v **To view a box-and-whiskers plot for L-glutamic acid**

1. To sort the main Compounds table in descending order by area, click the Area (Max.) column heading. For the example data set, L-glutamic acid sorts to the top of the table.

2. In the Compounds table, select **L-Glutamic Acid** (row 2).

3. In the set of tabbed views to the right of the result table, click the **Trend Chart** tab.

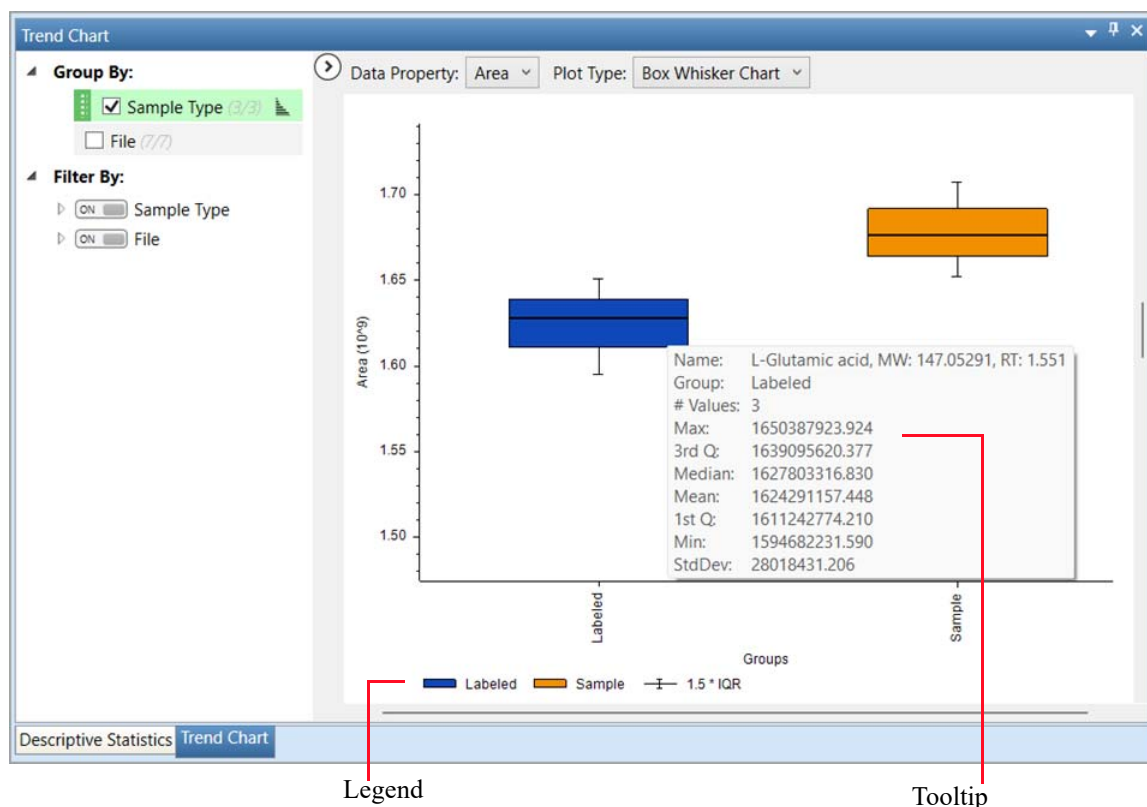
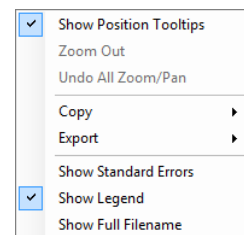
By default, the Trend Chart view displays a box-and-whiskers plot for the relative exchange rate per group (labeled and sample).

4. Right-click the chart and choose **Show Legend**.

The legend appears below the chart.

5. To display a tooltip with descriptive statistics, point to a box or a whisker.

This figure shows the box-and-whiskers plot for L-glutamic acid with the samples grouped by sample type.



View the distribution of the isotopologues for each compound

Use the Isotopologues Distribution Chart view to visualize the distribution of the isotopologues for a compound.

v **To view the distribution of the isotopologues for a compound**

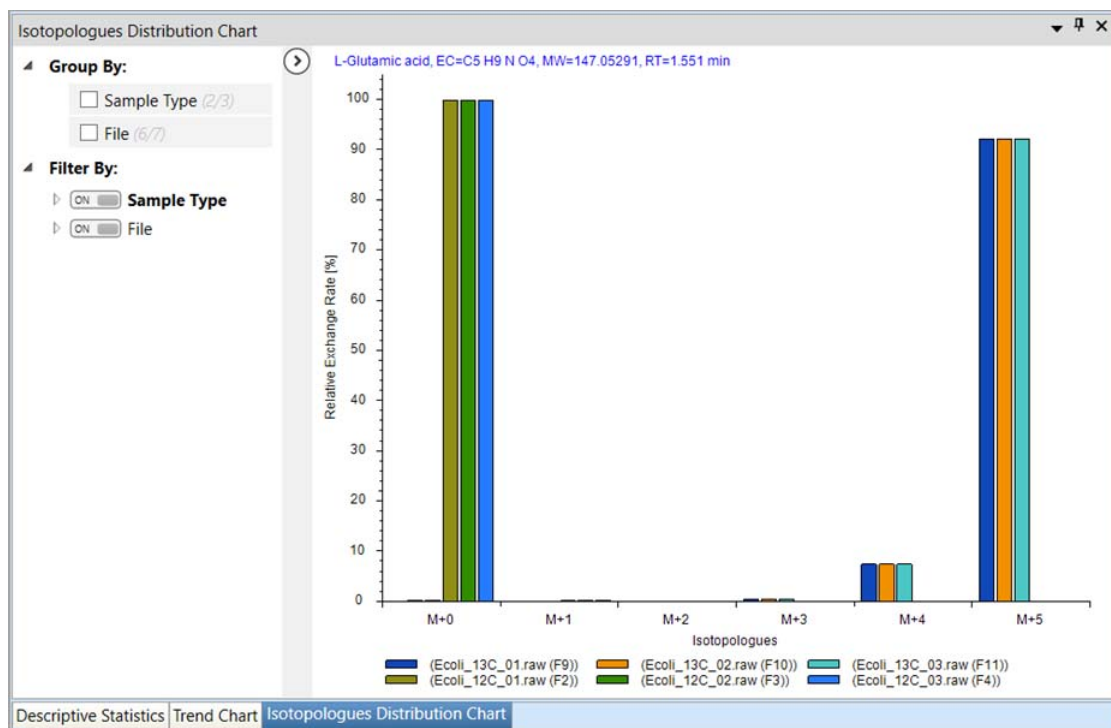
1. Apply the Stable Isotope Labeling layout to the result file (see [“Apply the Stable Isotope Labeling layout”](#) on page 18).

The Isotopologues Distribution Chart view opens to the right of the result tables.

2. In the Compounds table, select a compound of interest.

[Figure 21](#) shows the distribution for L-glutamic acid with no sample grouping.

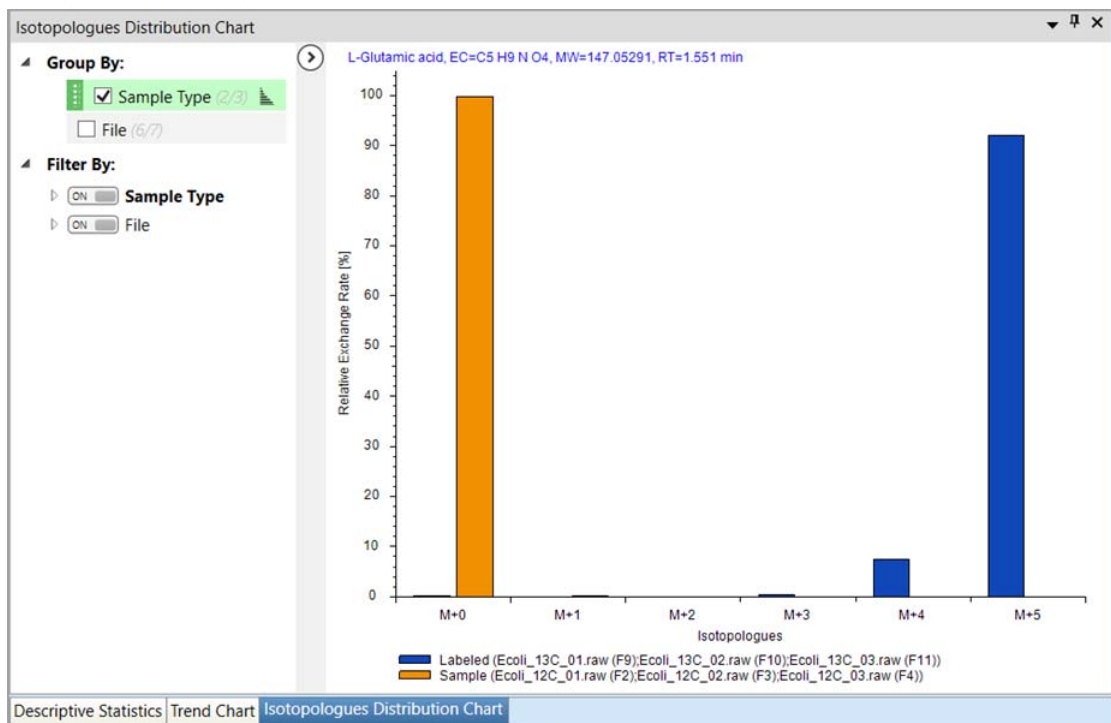
Figure 21. Isotopologues Distribution Chart view showing L-glutamic acid with no sample grouping



- To group the samples by Sample Type, under Group By, select the **Sample Type** check box.

Figure 22 shows the isotopologue distribution for L-glutamic acid with the samples grouped by sample type.



Figure 22. Isotopologues Distribution Chart view showing L-glutamic acid with samples grouped by sample type



View the Metabolika pathways for a compound

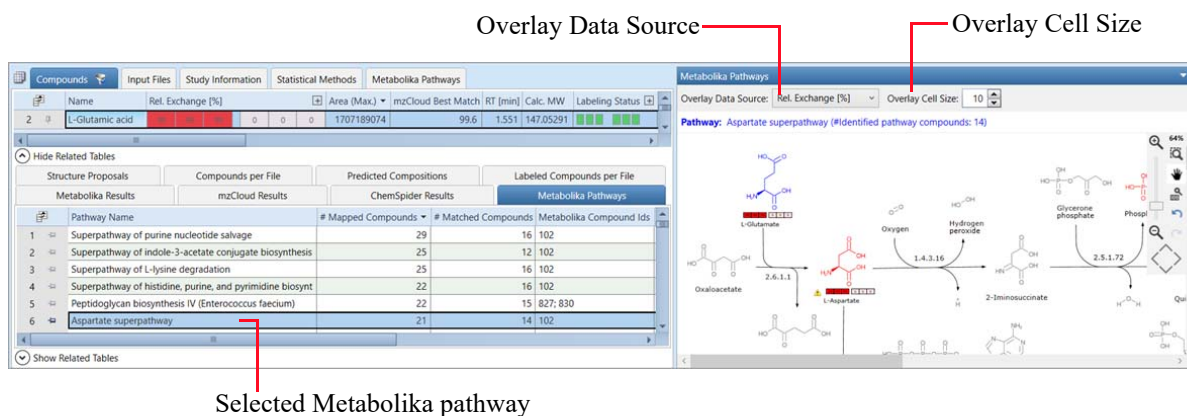
The Map to Metabolika Pathways node (in the selected processing workflow) returns a set of mapped pathways for each detected compound.

v To view the Metabolika pathways that include a selected compound

- Apply the Stable Isotope Labeling layout to the result file (see “Apply the Stable Isotope Labeling layout” on page 18).
The Isotopologues Distribution Chart, Trend Chart, and Metabolika Pathways views open as tabbed views on the bottom right of the page. The related tables pane opens below the main tables pane.
- Close some of the views as follows:
 - In the lower right quadrant, close the Isotopologues Distribution Chart view and the Trend Chart view by clicking their **Close** icons, . Leave the Metabolika Pathways view open.
 - In the upper portion of the window, close the Chromatograms and Mass Spectrum views by clicking their **Close** icons, .
- Right-click the Compounds table and choose **Collapse All Column Headers**.
- Sort the Compounds table by the Area (Max.) column in descending order.
- In the Compounds table, select **row 2** (L-glutamic acid) in the example result file.
- To view a Metabolika pathway that includes L-glutamic acid, do the following:
 - In the related tables pane for L-glutamic acid, click the **Metabolika Pathways** tab to make it the active table.
 - For this tutorial, scroll down to **row 6**—the **Aspartate superpathway** and select it.

This figure shows the selection of row 6 in the Metabolika Pathways table for L-glutamic acid. The mapped pathway appears in the Metabolika Pathways view at the right of the result tables. The Stable Isotope Labeling layout automatically selects the Rel. Exchange [%] column as the overlay data source with an overlay cell size of 10 pixels.

The mapped pathway appears in the Metabolika Pathways view at the right of the result tables. The Stable Isotope Labeling layout automatically selects the Rel. Exchange [%] column as the overlay data source with an overlay cell size of 10 pixels.



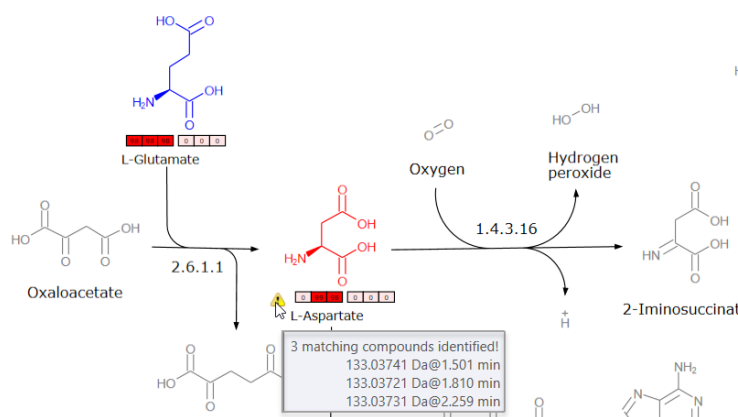
Overlay Data Source Overlay Cell Size

Selected Metabolika pathway

- To view the Metabolika Pathways view below the result tables instead of to their right, drag the view by its title bar until it aligns with the alignment tool's down arrow at the bottom of the page.
- Release the mouse button.
The structure for the compound that you selected in the Compounds table is blue, the structures for other detected compounds are red, and the structures for undetected compounds in the pathway are black.
- To enlarge the overlaid data, increase the value in the Overlay Cell Size box (Range: 6 to 30 pixels in width).
- To view the file name for a specific value, point to the value.

This figure shows the selected Metabolika pathway with an overlay of the relative exchange [%] data for the selected compound—L-glutamate. The overlay cell size is 20 pixels. A Caution symbol next to a compound indicates that the analysis found multiple matches.

9. To view information about the matching compounds for a structure with multiple matches, point to the Caution symbol.



10. To keep only the appropriate explanation for the structure, mark the incorrect explanation as a background compound as follows:

- In the second pane of related tables, open the related Compounds table for the selected Metabolika pathway.
- Fix the Name column to the leftmost column of the table. See “Common layout modifications” on page 17.
- Sort the related table by the Calc. MW column in ascending order.
- Open the Field Chooser dialog box for the related Compounds table and select the check box for the Background column.

The Background column appears in the related Compounds table.

- To mark the two L-Aspartic acid (with lowest abundance and mzCloud best match score) as a background compound, select its check boxes in the Background column.

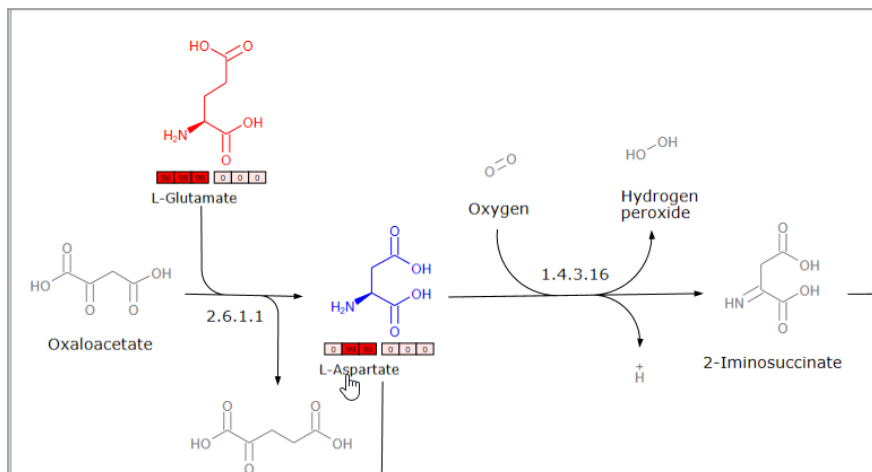
Name	Calc. MW	Background	mzCloud Best Match	Area (Max.)	RT (min)	Metabolika Compound Ids
(2S,4S)-4-hydroxy-2,3,4,5-tetrahy...	87.04778	<input type="checkbox"/>		734921	1.663	239
L-(+)-Methionine	49.05078	<input type="checkbox"/>	98.0	44639565	2.383	246
L-Glutamic acid	47.05291	<input type="checkbox"/>	99.6	1707189074	1.551	102
L-Lysine	46.10530	<input type="checkbox"/>	80.7	19991960	1.398	240
DL-Glutamine	46.06892	<input type="checkbox"/>	99.1	62242865	1.514	101
Homocysteine	35.03526	<input type="checkbox"/>	87.4	974979	1.795	232
L-Aspartic acid	33.03741	<input type="checkbox"/>	99.9	7656003	1.501	237
L-Aspartic acid	33.03731	<input checked="" type="checkbox"/>	80.8	1821917	2.259	237
L-Aspartic acid	33.03721	<input checked="" type="checkbox"/>	95.1	3739744	1.810	237
Succinic acid	119.07639	<input type="checkbox"/>		646077	3.193	38

Calc. MW sorted in ascending order

Checkboxes to select in the Background column with respect to their mzCloud best match score

Caution symbol indicating structure with multiple matches

In the Metabolika pathways view, the Caution symbol below the structure disappears, but the structure remains red.



Export the analysis results

To create a report for your records, filter the Compounds table to display only the compounds of interest, and then export the results using the appropriate format.

Follow these procedures to filter the Compounds table and export the results:

1. Use the [Result Filters](#) view to select compounds of interest
2. Select columns that you want to export
3. Export the results to a spreadsheet

Use the Result Filters view to select compounds of interest

The analysis detected a few thousand compounds, including over one thousand compounds that it marked as background compounds or compounds without a formula. To reduce the number of compounds to export, filter the table or select the check boxes for the compounds of interest.

Note Pointing to the Compounds tab or the scroll bar for the Compounds table displays a tooltip with the number of visible compounds and the total number of compounds that the analysis detected.

Compounds	Compounds per File	Features per File	Labeled Compounds per File
<input type="checkbox"/> Compounds grouped by molecular weight and retention time 1293 of 1937 items shown (644 filtered out)			

Do the following in the order listed:

1. Filter the Compounds table by the selected items
2. Filter the Compounds table by the relative exchange rate
3. Filter the Compounds table by the best mzCloud match

v To filter the Compounds table by the selected items

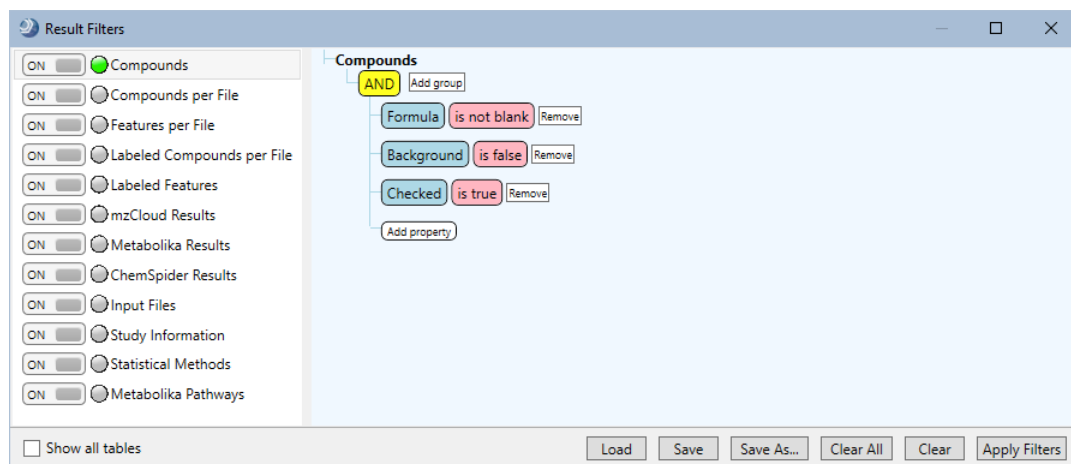
1. If the Compounds table is not the active table, click its tab to make it active.
2. Manually select the check boxes for the compounds of interest.
3. From the menu bar, choose **View > Result Filters**.

Because the processing workflow included the Mark Background Compounds node and the Analyze Labeled Compounds node, the Compounds table is currently filtered by two properties—Background and Formula.

4. Click **Add Property** and select **Checked**.

Filter the Compounds table by the selected items

This figure shows the filter set.



5. Click **Apply Filters**.

The Compounds table displays only the selected compounds.

6. To undo the Checked filter, click **Remove** to its right. Then, click **Apply Filters** again.

Now that you have removed the Checked filter, the Compounds table contains the original set of compounds.

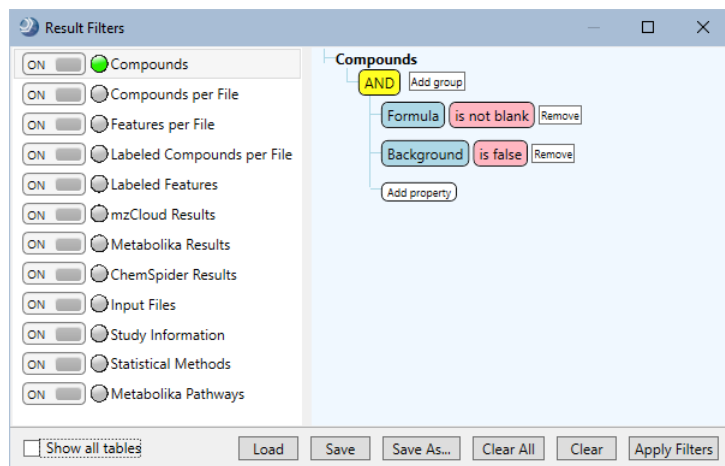
Go to the next topic to “[Filter the Compounds table by the relative exchange rate.](#)”

- v **To filter the Compounds table by the relative exchange rate of each compound**

1. Click the **Compounds** tab for the main Compounds table to make it the active table.
2. From the application menu bar, choose **View > Result Filters**.

The Result Filters view opens as a floating window. Because the processing workflow included the Mark Background Compounds node and the Analyze Labeled Compounds node, the filter for the Compounds table already includes a filter for background compounds and a filter for compounds without a formula.

This figure shows the default filters for the example result file.



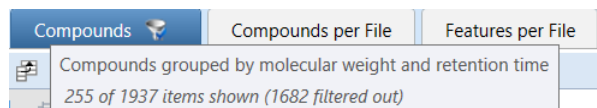
3. On the right side of the Result Filters view, set up filters for the relative exchange rate as follows:
 - a. Click **Add Property**, and then select **Rel. Exchange [%]** from the list.
 - b. In the pink relation list, select **Is Greater Than or Equal To**.
 - c. In the value box next to the relation list, type **98**.
 - d. In the pink condition list, select **In File**.
 - e. In the Green sample list, select one of the labeled input files.
 - f. Repeat steps [step 3a](#) through [step 3e](#) to add a filter for all three labeled input files.

This figure shows the filter set.



4. Click **Apply Filters**.

The applied filter set reduces the number of visible rows in the Compounds table to 255.

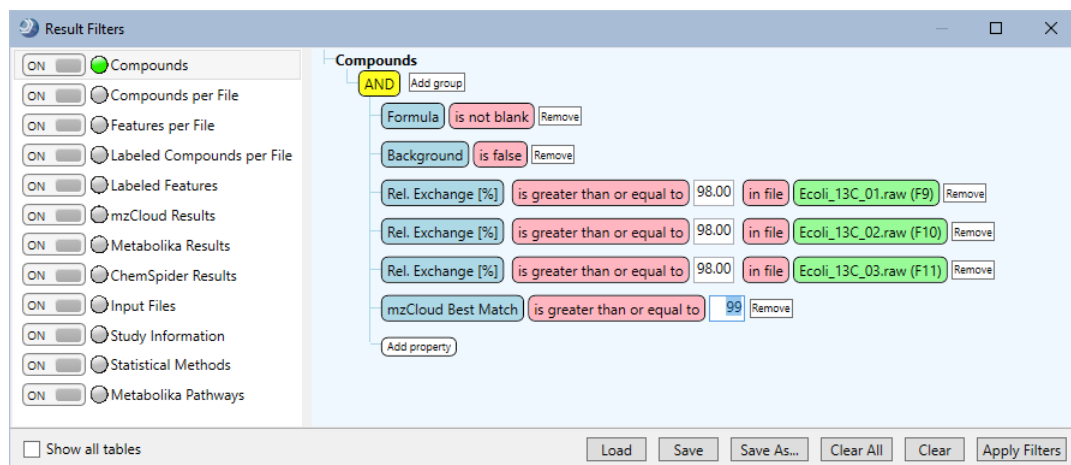


Leave Result Filters view open and go to the next topic to filter the remaining visible compounds by their best mzCloud match scores.

Precondition: The Compounds table in the example result file is filtered by the exchange rate as described in “[Filter the Compounds table by the relative exchange rate](#)” on page 28.

v **To filter the Compounds table by the best mzCloud match**

1. Open the Result Filters view if it is not open.
2. Click **Add Property** below the last Rel Exchange [%] filter.
3. In the dropdown property list, select **mzCloud Best Match**.
4. In the pink dropdown conditions list to the right, select **Is Greater Than or Equal To**.
5. In the value box, type **99**.




6. Click **Apply Filters**.

The Compounds table is now reduced to nine compounds.

Filter the Compounds table by the best mzCloud match

Compounds		Compounds per File	Features per File	Labeled Compounds per File	Labeled Features per File	mzCloud Results	
	Name	mzCloud Best Match	Labeling Status	Calc. MW	m/z	Area (Max)	RT [min]
1	L-Glutamic acid	99.6	■■■■■■■■	147.05291	148.06017	1707189074	1.551
2	L-Tyrosine	99.1	■■■■■■■■	181.07360	182.08085	165576844	2.943
3	L-Valine	99.6	■■■■■■■■	117.07871	118.08599	117224443	2.190
4	DL-Glutamine	99.1	■■■■■■■■	146.06892	147.07619	62242865	1.514
5	L-Valine	99.5	■■■■■■■■	117.07876	118.08604	21930487	2.109
6	L-Aspartic acid	99.9	■■■■■■■■	133.03741	134.04468	7656003	1.501
7	2'-Deoxyadenosine	99.9	■■■■■■■■	251.10163	252.10890	6858505	3.402
8	Y-L-Glutamyl-L-glutamic acid	99.3	■■■■■■■■	276.09560	277.10287	2673558	1.959
9	Adenosine 3'5'-cyclic monophosphate	99.4	■■■■■■■■	329.05233	330.05961	2330900	3.411


7. Close the Result Filters view by clicking the **Close** icon, , in the upper-right corner.

Go to the next topic to “[Export the results to a spreadsheet.](#)”

Select columns that you want to export

For the stable isotope labeling analysis, the Compounds table contains up to 37 visible table columns. With the Stable Isotope Labeling layout applied, the Compounds table contains 19 visible table columns. See the Field Chooser dialog box in the following topic: “[Apply the Stable Isotope Labeling layout](#)” on [page 18](#).

v **To select the table columns that you want to export to a spreadsheet file**

1. Click the **Field Chooser** icon, , for the Compounds table.
2. In the Field Chooser dialog box, clear the check boxes for the columns that you do not want to export to a spreadsheet file. For this tutorial, clear all the check boxes except the following five columns:

Name, Area (Max), Calc. MW, Formula, and RT

3. Close the Field Chooser dialog box.

Preconditions: The Compounds table is filtered by a relative exchange rate of greater than or equal to 98% and an mzCloud Best Match of greater than or equal to 99% and contains only two compounds and only six columns.

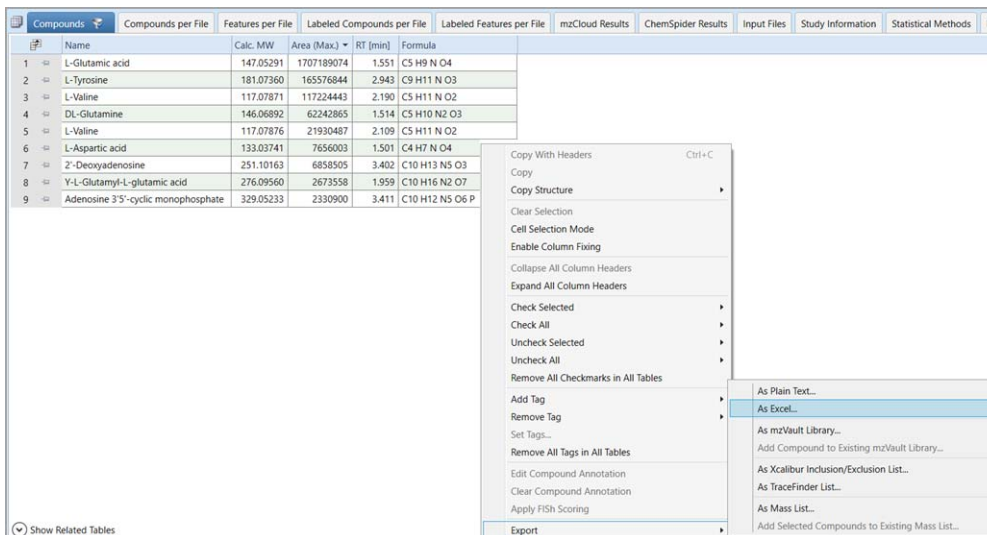
Note If you have not already filtered the Compounds table and reduced the number of visible table columns, see these topics:

- [Filter the Compounds table by the relative exchange rate](#)
- [Filter the Compounds table by the best mzCloud match](#)
- [Select columns that you want to export](#)

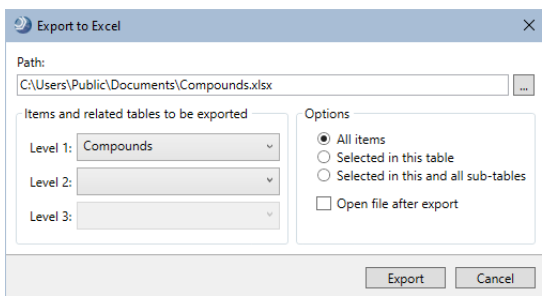
Export the results to a spreadsheet

v **To create a report by exporting the results to a spreadsheet**

1. Sort the Compounds table in descending order by the Area (Max) column.
2. To export the filtered and sorted results, do the following:
 - a. Right-click the Compounds table and choose **Export > As Excel**.



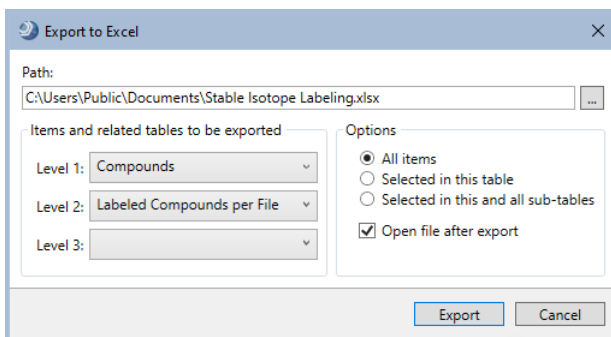
The Export to Excel dialog box opens.



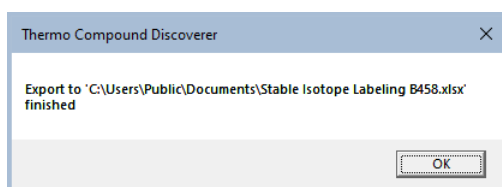
- b. In the Path box, change the file name and the location of the spreadsheet file as appropriate by clicking the browse icon, selecting the storage folder, naming the file, and clicking **Save**.

The dialog box remembers the last folder location you selected. The default file name is the table name.

- c. In the Items and Related Tables to be Exported area, do the following:
 - Do not change the Level 1 selection of the Compounds table.
 - In the Level 2 list, select **Labeled Compounds per File**.
- d. In Options area, select the **All Items** option and the **Open File After Export** check box.



- e. Click **Export**.
- f. At the status prompt, click **OK**.



The Excel spreadsheet opens (Figure 23).

This spreadsheet shows the exported Compounds table.

Figure 23. Excel spreadsheet with three compounds and the labeled compounds per file for each of the three compounds

1	2	A	B	C	D	E
1		Name	Calc. MW	Area (Max.)	RT [min]	Formula
2		L-Glutamic acid	147.05291	1707189074	1.551	C5 H9 N O4
11		L-Tyrosine	181.0736	165576844.2	2.943	C9 H11 N O3
19		L-Valine	117.07871	117224442.9	2.19	C5 H11 N O2
27		DL-Glutamine	146.06892	62242865.36	1.514	C5 H10 N2 O3
36		L-Valine	117.07876	21930487.18	2.109	C5 H11 N O2
44		L-Aspartic acid	133.03741	7656003.228	1.501	C4 H7 N O4
53		2'-Deoxyadenosine	251.10163	6858504.558	3.402	C10 H13 N5 O3
61		Y-L-Glutamyl-L-glutamic acid	276.0956	2673558.107	1.959	C10 H16 N2 O7
69		Adenosine 3'5'-cyclic monophosphate	329.05233	2330899.628	3.411	C10 H12 N5 O6 P

Expand icon

- To view the Compounds per File table for a compound, click the expand icon, to the left of the compound. The Labeled Compounds per File table for the compound expands below the compound.

1	2	A	B	C	D	E	F	G	H	I	J
1		Name	Calc. MW	Area (Max.)	RT [min]	Formula					
2		L-Glutamic acid	147.05291	1707189074	1.551	C5 H9 N O4					
3			Molecular Weight	RT [min]	FWHM [min]	Area	Rel. Excha	Max. # MI	# Adducts	Status	Max. Exch Stud
4			147.05291	1.551	0.029	1707189074	0.02493	3	1	No warnings	5 F2
5			147.05291	1.552	0.028	1676360986	0.033327	3	1	No warnings	5 F3
6			147.05291	1.55	0.028	1651966882	0.033768	3	1	No warnings	5 F4
7			147.05291	1.55	0.028	1650387924	98.19491	5	1	No warnings	5 F10
8			147.05291	1.549	0.027	1627803317	98.2005	5	1	No warnings	5 F11
9			147.05291	1.55	0.027	1594682232	98.33903	4	1	No warnings	5 F9
10			147.05291	1.558	0.024	87259.56661		0	1	No warnings	5 F1
11		L-Tyrosine	181.0736	165576844	2.943	C9 H11 N O3					
19		L-Valine	117.07871	117224443	2.19	C5 H11 N O2					
27		DL-Glutamine	146.06892	62242865.4	1.514	C5 H10 N2 O3					
36		L-Valine	117.07876	21930487.2	2.109	C5 H11 N O2					
44		L-Aspartic acid	133.03741	7656003.23	1.501	C4 H7 N O4					
53		2'-Deoxyadenosine	251.10163	6858504.56	3.402	C10 H13 N5 O3					
61		Y-L-Glutamyl-L-glutamic acid	276.0956	2673558.11	1.959	C10 H16 N2 O7					
69		Adenosine 3'5'-cyclic monophosphate	329.05233	2330899.63	3.411	C10 H12 N5 O6 P					

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