Agilent G3772AA MassHunter Analytical Studio Reviewer Quick Start Guide

A guide to get started with MassHunter Analytical Studio Reviewer and the Agilent ChemStation add-on to generate ASR files

Use this quick reference guide as a road map for your first steps with the software, and as a guide through your user information.

What is MassHunter Analytical Studio Reviewer?

Agilent MassHunter Analytical Studio Reviewer is a browser that lets researchers quickly review large amounts of liquid chromatography/mass spectrometry (LC/MS) data in high-throughput labs.

This application speeds decisions in drug discovery and other research areas by providing an intuitive user interface, making it easy to quickly review data, and offering a wide range of reporting options. The data display is customizable to enable review of large amounts of data at a glance.

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The product also includes the Agilent MassHunter ASR File Generator for ChemStation, which lets you convert ChemStation results to MassHunter Analytical Studio Reviewer (ASR) files.

You can also generate ASR files from the Agilent MassHunter Workstation Software - Qualitative Analysis program.

Main features of MassHunter Analytical Studio Reviewer

- Quickly navigate through results files.
- View color-coded results that indicate whether one or more target compounds were detected.
- View color-coded results for sample purity.
- View UV peak purity and MS peak purity.
- Customize the display of data.
- Edit results, including deletion of peaks and change of target compound status (red, green, yellow).
- Generate new MassHunter Analytical Studio Reviewer (ASR) files that reflect any changes to the results.
- Generate configurable Microsoft Word reports without requiring Microsoft Word to be installed.
- Generate configurable PDF reports.
- Export results from batches of data to spreadsheets.
- Print MassHunter Analytical Studio Reviewer reports automatically from Agilent ChemStation software (Figure 1). The report uses report settings that you last saved within MassHunter Analytical Studio Reviewer.

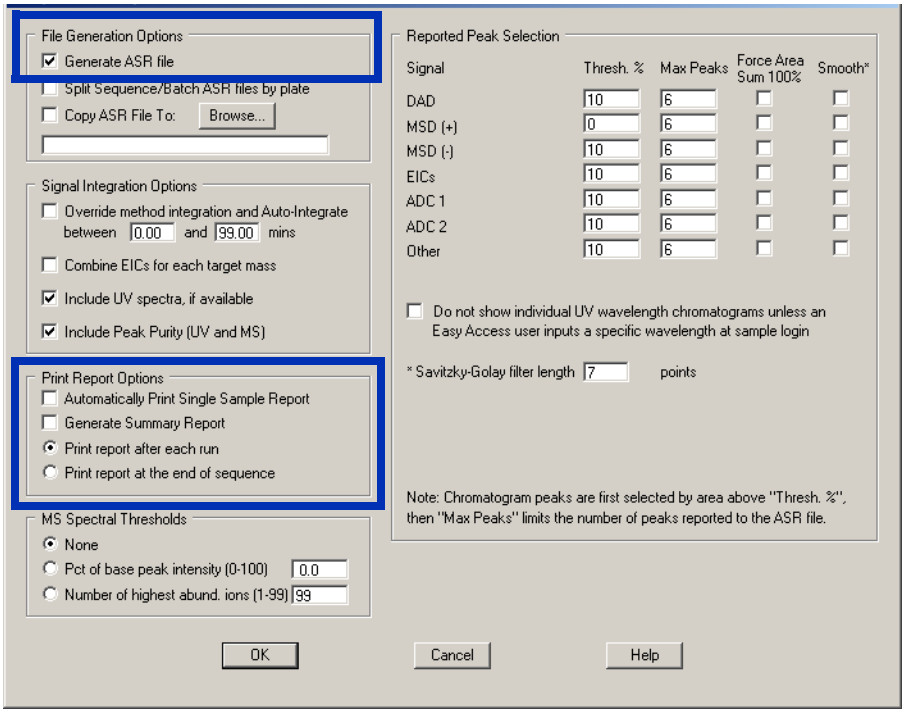


Figure 1 You can set up your ChemStation method to automatically generate an Analytical Studio Reviewer report from ChemStation.

What's new in B.02.01

- Reporting
  - The Single Sample Report is more flexible in how the report is constructed and has an updated look and feel.
  - Other reports are more consistent with the single sample report where appropriate.
- File Read Performance
  - Read performance of Agilent ASR and Waters RPT files has been significantly improved (typically greater than a factor of 10X).
- User Interface
  - Rapid zooming with X-axis zooming by default, y-axis and x,y-axis zooming are additional options.
  - Improved automatic peak labelling and automated display of relevant peak related information when space is limited.
  - Ability to copy graphics from the MassHunter Analytical Studio Reviewer to a report or presentation.
  - Ability to copy tabular information from the MassHunter Analytical Studio Reviewer to another file, such as a spreadsheet.
  - Freezing of the top chromatogram frame for viewing relative to other chromatogram traces.
  - Improved rescaling of the displayed and reported spectrum in the cases where the processed spectrum is very narrow.
  - Improved baseline display.
- ASR File Generator
  - Single panel setup screen for focused reports.
  - Option to automatically integrate and smooth chromatograms.
  - Composite DAD signals: Total Wavelength and Maximum Absorbance chromatograms are now available.
  - Improved labeling of Extracted Ion Chromatograms to show origin.
  - Flexible improved peak selection by both relative threshold and number of peaks.
  - With Easy-Access, option to hide UV chromatogram if not requested by the user.

Where to find more information

Each of the software components has its own online Help.

MassHunter Analytical Studio Reviewer

Getting Started with Agilent MassHunter Analytical Studio Reviewer

Agilent MassHunter Analytical Studio Reviewer lets you browse your analytical results without the need to purchase and launch full ChemStation software on your desktop.

To start viewing data, see the online Help **Getting Started** instructions to:

- Browse through samples that were analyzed in vials or well-plates.
- View summary results, peak results, and sample details in the Summary pane.
- View chromatograms and mass and UV spectra.
- View chromatographic peak details, including retention times, areas, and which peaks contain target compounds.
- Edit peak data.
- Save edited results as a new ASR file.

The **Getting Started** instructions are on the Welcome page for the online Help.

Online Help Use the online Help for in-depth information not given in the Quick Start. To display online Help, click **Help > Analytical Studio Reviewer Help** or press **F1** on your keyboard.

The online Help is divided into two sections.

- How-to contains step-by-step instructions.
- Reference contains information about menus, toolbars, panes, and dialog boxes.

Find topics of interest through the **Contents**, **Index**, or **Search** tabs.

MassHunter ASR File Generator for ChemStation

Getting Started with Agilent MassHunter ASR File Generator for ChemStation

Agilent MassHunter ASR File Generator for ChemStation is an add-in that lets you convert ChemStation results to an ASR file.

To start exporting ASR files, see the online Help **Getting Started** instructions to:

- Set up a ChemStation method to generate ASR files.
- Generate ASR files manually within ChemStation Data Analysis.
- Generate ASR files automatically by running a method or sequence.

Online Help Use the online Help for in-depth information not given in the Quick Start. To display online Help, in either the Method and Run Control or Data Analysis view, click **ASR > Help**.

The online Help is divided into two sections.

- How-to contains step-by-step instructions.
- Reference contains information about menus and dialog boxes.

Find topics of interest through the **Contents**, **Index**, or **Search** tabs.

MassHunter ASR File Generator for MassHunter Qualitative Analysis

You can export results in ASR format from within the MassHunter Qualitative Analysis program. Refer to the online Help for the Qualitative Analysis program for more information on how to export data files in ASR format, or see "Generating ASR files from MassHunter Workstation (TOF Data)" on page 10.

Installation

System Requirements

- One of the following operating systems:
  - Microsoft Windows XP SP1 or SP2
  - Microsoft Vista
- Microsoft .NET framework version 2.0
- For ChemStation systems, ChemStation version B.03.02 or later

To install Agilent MassHunter Analytical Studio Reviewer

You may install and use Agilent MassHunter Analytical Studio Reviewer software without installing ChemStation or MassHunter Workstation software.

1. Insert the MassHunter Analytical Studio Reviewer installation disk (G3772-60102) into the disk drive.
2. In Windows Explorer, navigate to the **Analytical Studio Reviewer** folder and double-click **Agilent_ASR_Install_G3772_B_02_01.msi**.
3. Follow the instructions on the screen.

To install Agilent MassHunter ASR File Generator for ChemStation

You install this component on a computer that already has ChemStation software. You must also install the Agilent MassHunter Analytical Studio Reviewer on this computer. You can install the two ASR products in either order.

1. Insert the MassHunter Analytical Studio Reviewer installation disk (G3772-60102) into the disk drive.
2. In Windows Explorer, open the folder **ASR File Generator for ChemStation** and double-click **Setup.exe**.
3. Follow the instructions on the screen.

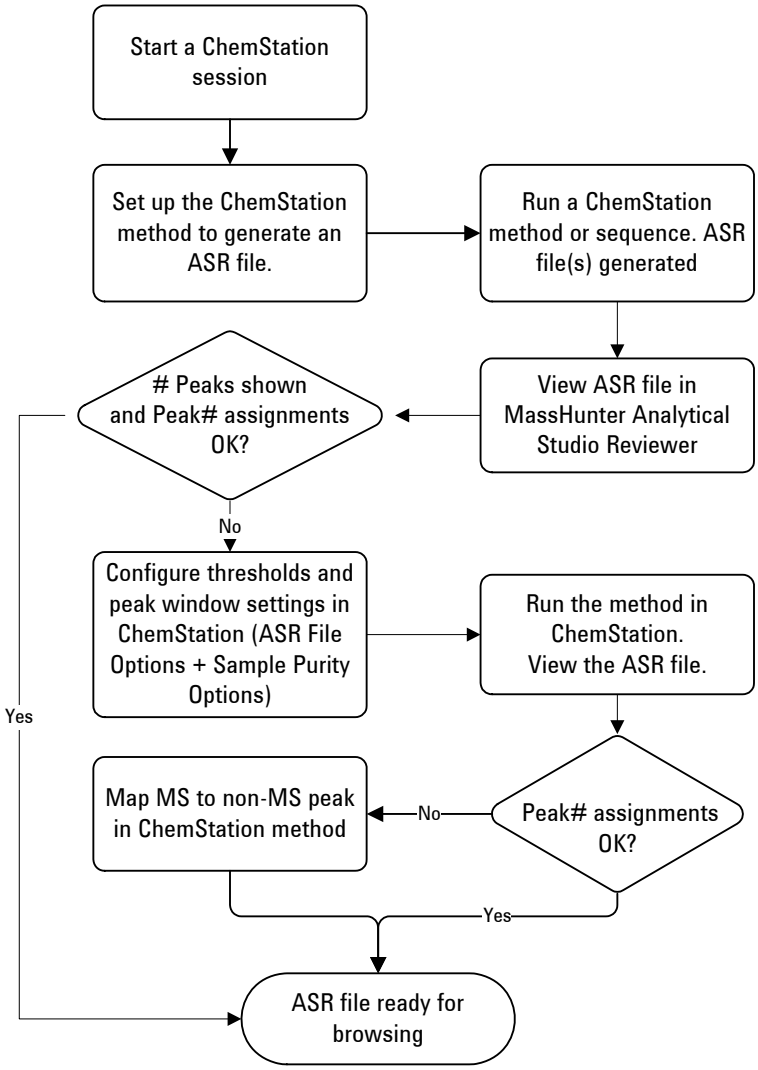
To reinstall either component

1. Remove the current software.
   a. Click **Start > Control Panel**.
   b. Click **Add or Remove Programs**.
   c. Find the program in the list and remove it. For a ChemStation computer, remove either Agilent MassHunter Analytical Studio Reviewer or Agilent MassHunter ASR File Generator for ChemStation.
2. Reinstall the software using the installation instructions above.

Generate ASR files from ChemStation data

Roadmap to generate ASR files from ChemStation data

See the online Help for more information. *Note that you can reprocess existing data to generate ASR files.*



Generating ASR files from MassHunter Workstation (TOF Data)

To generate ASR files interactively

1. On the MassHunter Qualitative Analysis program, analyze data to generate results.
2. Open the data file.
3. Click **File > Export > as ASR**. The Export ASR Options dialog box is opened.
4. Select the file (or files) to export.
5. Click **Qualitative method**.
6. Select whether or not to combine multiple files into one export file. To create one export file, click **Combine into one export file**. To create a separate export file for each data file, click **One export file per data file**. If you selected multiple locations, then you can combine all of the files into one export file if you wish. The option **Combine into one export file** does not append to an export file that already exists.
7. Select either the folder to use when creating the file or type the file name for the export file.
8. Click one of the options under **If export file already exists**.
9. Review the **Peak window** value on the **Settings** tab.
10. Click **OK**.

    A file with the extension ASR is created at the folder you selected. You can use this file directly in MassHunter Analytical Studio Reviewer.

To set up a method to use in a worklist

1. Open a data file.
2. Display the **Export > Export List** section in the Method Editor window.
   - Select **Export List** in the **Export** section of the Method Explorer window.
   - Select **Export List** in the Method Item list from the Method Editor Toolbar.
3. Mark the **ASR** check box.
4. Review the other check boxes. Clear the check box if you do not want to export in the specified format.

5 Display the **Export > ASR Options** section in the Method Editor window.

- Select **ASR Options** in the **Export** section of the Method Explorer window.
- Select **ASR Options** in the Method Item list from the Method Editor Toolbar.

6 Click either **Worklist** or **Qualitative method**. If you click **Worklist**, then the data file is exported to the **Worklist** location. This location is specified in the Acquisition program in the **Worklist Run Parameters** dialog box.

If this file already exists, then this file is appended to the end of the existing file. If the **Worklist** button is clicked, then the other options on this tab are unavailable.

7 Select whether or not to combine multiple files into one export file. To create one export file, click **Combine into one export file**. To create a separate export file for each data file, click **One export per data file**. If you selected multiple locations, then you can combine all of the files into one export file if you wish. The option **Combine into one export file** does not append to an export file that already exists.

8 Select either the folder to use when creating the file or type the file name for the export file.

9 Click one of the options under **If export file already exists**. If you click **Overwrite existing export file**, then the file is overwritten every time the method is run. If you click **Auto-generate new export file name**, a new filename is automatically created if the file already exists.

10 Review the **Peak window** value on the **Settings** tab.

11 Display the **Worklist Automation > Worklist Actions** section in the Method Editor window.

- Select **Worklist Actions** in the **Worklist Automation** section of the Method Explorer window.
- Select **Worklist Actions** in the Method Item list from the Method Editor Toolbar.

12 Select **Export** in the **Available actions** list.

13 Double-click **Export** to move it to the **Actions to be run** list. The **Export** action is added at the end of the **Actions to be run** list.

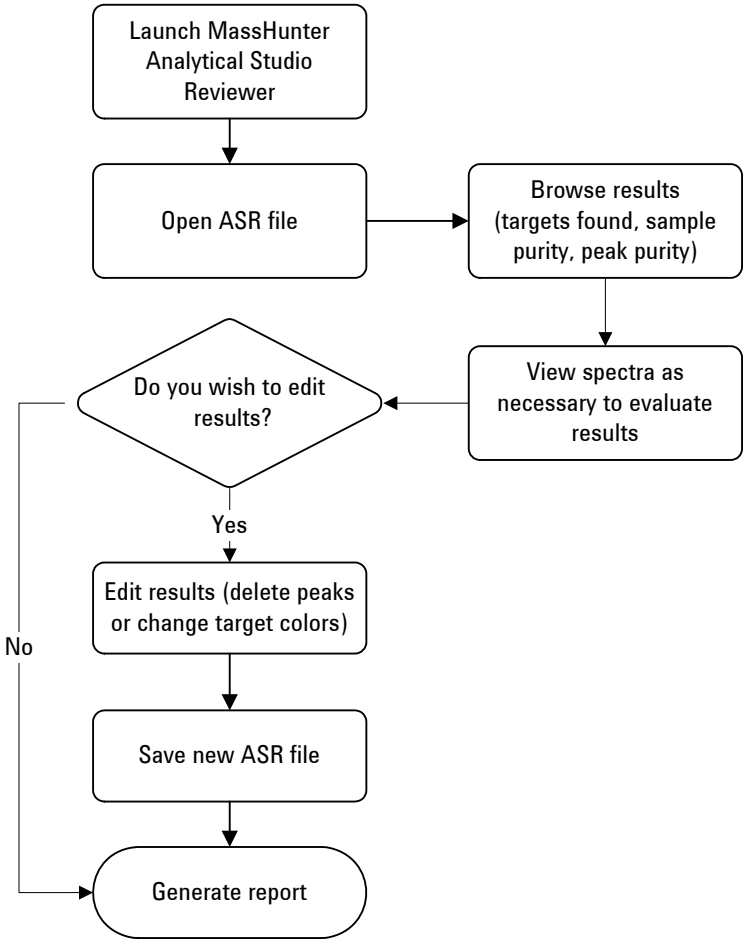
14 Save the method parameters.

You select this method in a worklist. When the Qualitative Analysis method is run during a worklist, the worklist actions are executed.

Reviewing results in MassHunter Analytical Studio Reviewer

Roadmap to review results in MassHunter Analytical Studio Reviewer

See the online Help for more information.



To configure a Plate view for TOF results

For TOF results, you must set up a well-plate configuration to see your samples displayed in a plate format. Otherwise, the software displays your samples in the Vial view. Assuming that you always use the same plate configuration, you need to manually configure the Plate view only once.

1 Click **Tools > Options**.

2 Click the **Container** tab.

3 Mark the check box for **Always use this plate layout**.

4 Establish the appropriate settings to configure your well-plate. See the online Help for more information.

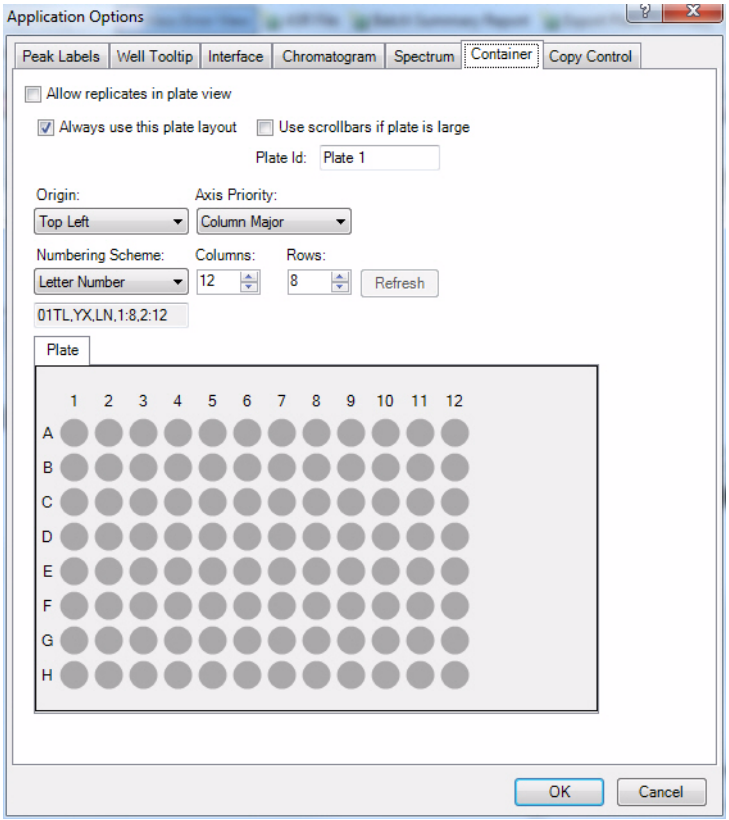


Figure 2 Example of configuring a well-plate so that samples can be displayed in the Plate view

To determine if target compounds were found

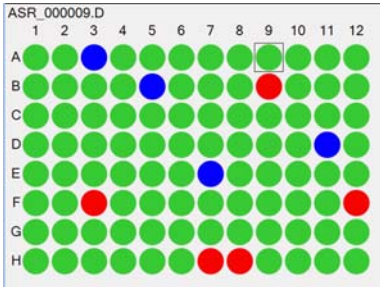


Figure 3 View red, green, and blue color-coding for targets in the Plates/Vials pane

Table 1 Color-coding of target compound results

Color	Meaning	Details for ChemStation results	Details for MassHunter results
	One or more targets found	At least one target ion from a target mass was found and at least one target ion had an intensity that exceeded the **%BPI for Target Confirm** that you set in the Sample Purity Options dialog box in the ChemStation software.	At least one target ion from a target mass was found and at least one target ion exceeds the **Minimum acceptable purity** that you set in the **Options** tab for **Find Compounds by Formula > Find by Formula - Sample Purity** in the MassHunter Workstation software.
	One or more targets found, but with low relative intensity	At least one target ion from a target mass was found, but no target ion had an intensity that exceeded the **%BPI for Target Confirm** that you set in the Sample Purity Options dialog box in the ChemStation software. You may examine the data more closely and edit the color if you decide the target should be green or red. If you edit results, you need to generate a new ASR file to save your changes.	At least one target ion from a target mass was found, but no target ion exceeds the **Minimum acceptable purity** that you set in the **Options** tab in the dialog box for **Find Compounds by Formula > Find by Formula - Sample Purity** in the MassHunter Workstation software.You may examine the data more closely and edit the color if you decide the target should be green or red. If you edit results, you need to generate a new ASR file to save your changes.
	No targets found	No target ions from a target mass were found.	No target ions from a target mass were found.
	No target specified, or no peaks found	No target mass was specified in the ChemStation software, or no peaks were found.	No target mass was specified in the ChemStation software, or no peaks were found.

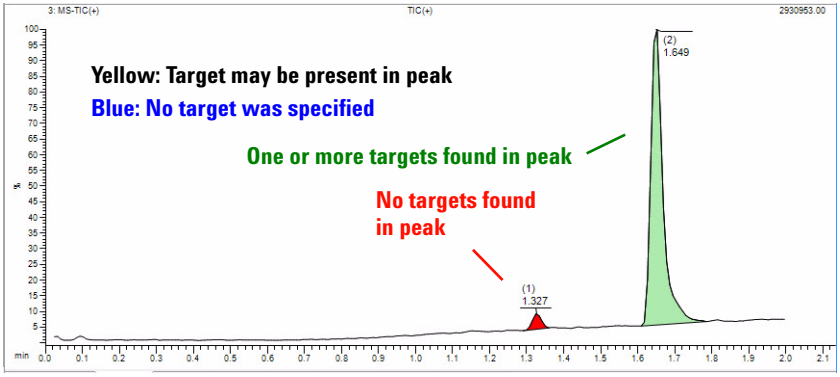


Figure 4 View the chromatograms in the Summary pane to see which peaks contain targets. For green peaks, view tabular **Peak Results** to see which target is in each peak. (See Figure 5.)

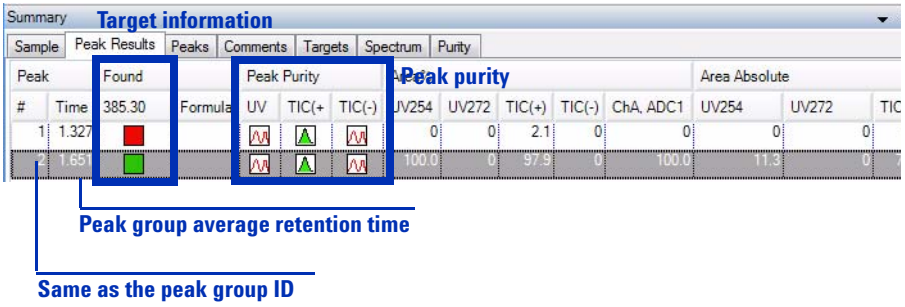


Figure 5 View color-coded targets in the **Peak Results** tab, which shows the results for a peak group

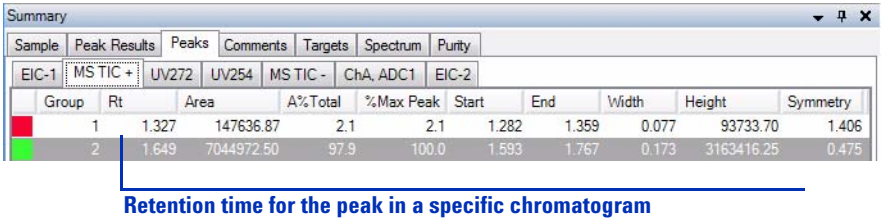


Figure 6 View color-coded targets in the **Peaks** tab in the Summary pane

To assess the purity of your sample

- Click the button to turn on the **Purity View**. The color-coding then changes. 

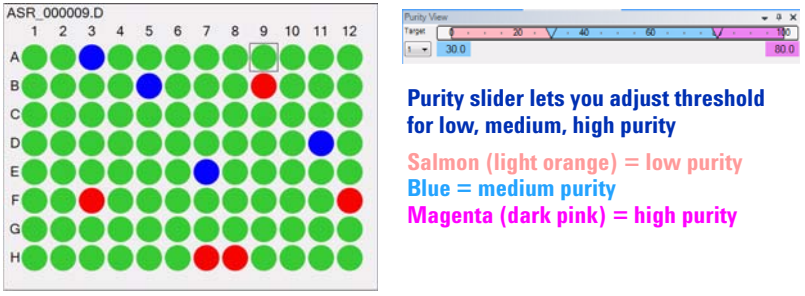


Figure 7 View salmon, blue, and magenta color-coding in the Plate/Vials pane

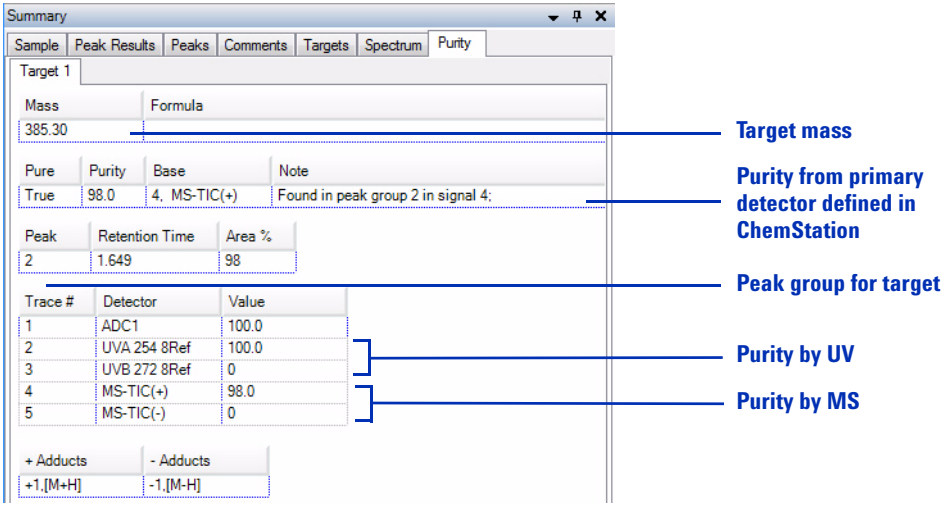


Figure 8 For ChemStation data, view results (for multiple targets, if present) in the **Purity** tab in the Summary pane

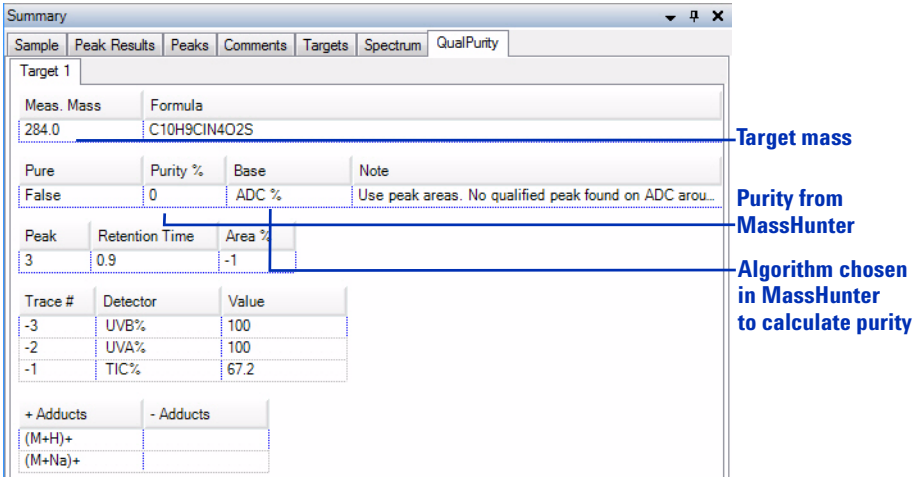


Figure 9 For MassHunter Workstation data, view results (for multiple targets, if present) in the **QualPurity** tab in the Summary pane

To assess the purity of a chromatographic peak

MassHunter Analytical Studio Reviewer can report two kinds of purity:

- *Sample purity*, which looks at all the integrated chromatographic peaks for a given analysis and calculates the purity of the target compound as an area percent
- *Peak purity*, which looks only at a given chromatographic peak and describes how pure that peak is. Peak purity can have two values — the purity calculated from the UV signal and the purity calculated from the MS signal. Peak purity is a unique feature of the Agilent ChemStation. This measurement is not available for TOF ASR files.

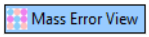
You view peak purity in the **Peak Results** tab within the Summary pane, as shown in Figure 5. To interpret the icons for peak purity, see Table 2.

Table 2 Peak purity icons

Purity icon	Meaning for MS*	Meaning for UV
	Pure One component found	Pure
	Not pure Two components found	N/A (not used for UV)
	Not pure More than two components found	Not pure

* Click the MS peak purity icon for a list of the ions

To assess mass error for TOF results

- Click the button to turn on the **Mass Error View**. The color-coding then changes. 

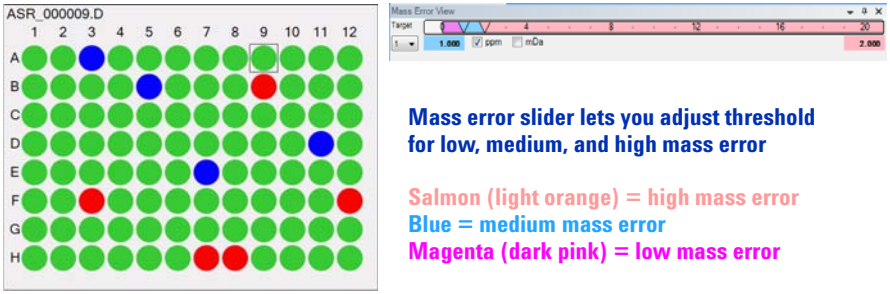


Figure 10 View salmon, blue, and magenta color-coding in the Plate/Vials pane

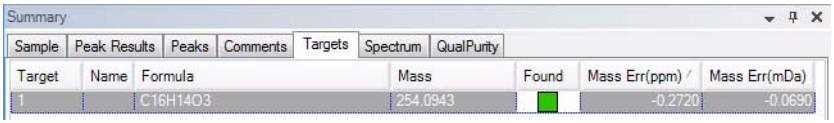


Figure 11 View results (for multiple targets, if present) in **Targets** tab in the Summary pane. (For some ASR files, this information is also listed in the **Compound Screen** or **Elemental** tab under the **Spectrum** tab.)

To edit data and save the results

- To enable editing, click **Tools > Options** and mark the check box in the **Editing** tab.
- To see peak colors within chromatograms, click **Tools > Options**. In the **Peak Labels** tab, mark the check box for **Fill peak region**.
- To save changes when you are done with edits, click ASR File.

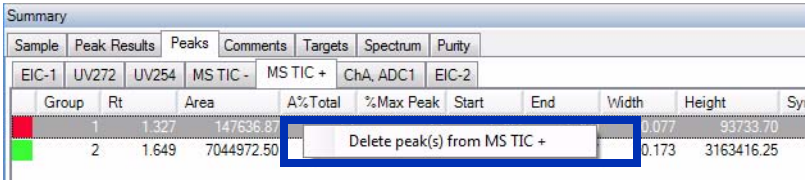


Figure 12 Select a row in the **Peaks** tab in the Summary pane, then right-click

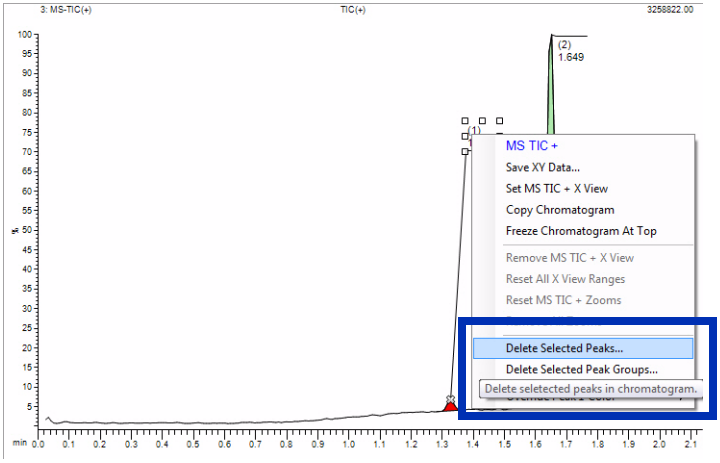


Figure 13 Select a peak number, then right-click

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In this book

This book contains:

- What is MassHunter Analytical Studio Reviewer?
- Where to find online Help
- How to install the software
- How to generate ASR files in the Agilent ChemStation and Agilent MassHunter Qualitative Analysis applications
- Roadmap to review results in MassHunter Analytical Studio Reviewer
- Getting started information for basic tasks

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