Agilent Revident LC/Q-TOF

Introduction Workbook

Notices

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Software Revision

This guide is valid for MassHunter 12.0, until superseded.

Instrument Manufacturing

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1 Introduction

About this Training Workbook

This Training Workbook provides instructions on the Agilent Revident LC/Q-TOF systems running MassHunter Data Acquisition 12.0.

For additional information on the software and detailed instructions on the workflow not covered in this workbook, see the Online Help.

This workbook is your introductory guide for the set-up and execution of basic procedures with the LC/Q-TOF and method development workflow. This workbook is divided into chapters, each building upon the last, so we recommend that each chapter is completed in succession. During each chapter, lessons are guided by an Agilent-certified service professional.

By completing this learning event, you'll have an introductory level of experience in the use of an Agilent Revident Q-TOF LC/MS System.

This introduction covers:

- Reviewing hardware components and software procedures
- Performing a checktune
- Acquiring and analyzing a sample
- Performing routine maintenance

How to use this Workbook

This learning experience introduces basic concepts in a learning-by-doing, guided manner. Each chapter uses step-by-step instructions.

Exercises to be completed are marked like this:

Exercise Name

Exercise Instructions

Task steps look like this:

1 Tasks or items needed to complete tasks look like this.

If you are expected to enter any information or if something is important, it is set in italicized type like this:

Type *Blank One* in the field.

If you are expected to press a key on the keyboard or button on the software screen, the key is displayed in bold like this:

Press **Enter**.

Cross references appear in blue:

(For example, Link)

Before You Begin

This introduction workbook is recommended for all participating end users.

- Download the *Agilent Revident Q-TOF LC/MS System User Guide* by scanning the code or navigating to **https://aglt.co/LCMSUserDocs.**
- Use the *Agilent Revident Q-TOF LC/MS System Introduction Workbook* and Introduction Checklist with your Agilent-certified service professional and keep for future reference.

Additional Resources

User Documentation

Data analysis and library management documentation can be found by scanning the code or navigating to **https://aglt.com/DALibMgmtDocs**.

Instrument documentation, step-by-step videos, and more can be found by scanning the code or navigating to **https://aglt.co/LCMSUserDocs.**

Agilent Q-TOF LC/MS Supplies

Use this quick reference list to keep your shelves stocked by navigating to **https://aglt.co/LCQTOFSupplies**

Where to find more information

Agilent Community

To get answers to your questions, join over 10,000 users in the Agilent Community. Review curated support materials organized by platform technology. Ask questions to industry colleagues and collaborators. Get notifications on the latest videos, documents, tools, and webinars relevant to your work.

https://community.agilent.com/

2 Hardware

Overview

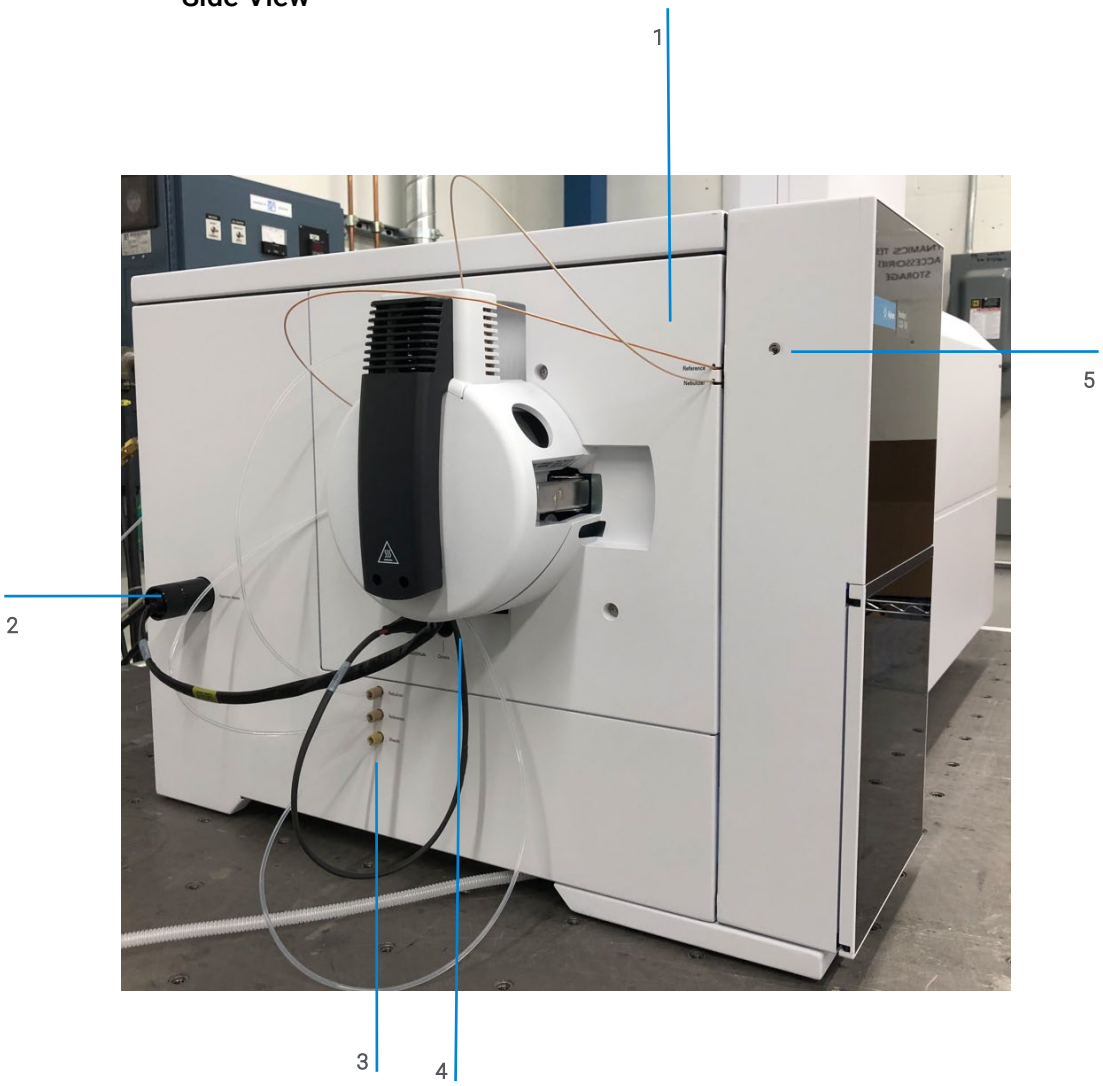
In this section, you'll identify basic hardware components and their locations for the Agilent Revident LC/Q-TOF system.

Fill in the Blank:

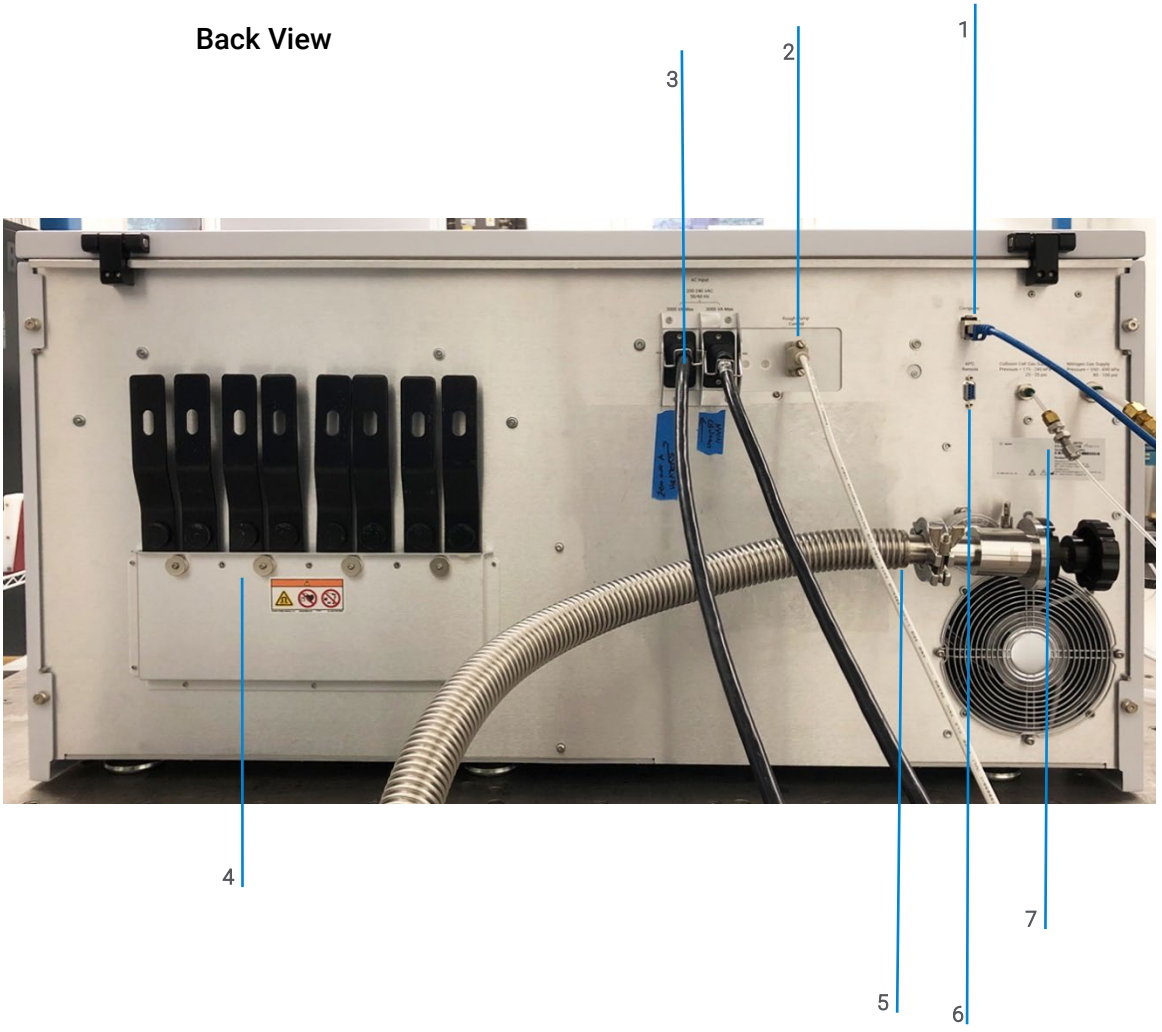
Work with your Agilent Service Engineer and/or use the Agilent Revident Q-TOF LC/MS System User Guide to label the flagged components for your installed instrument(s).

Front view

Side View



Back View



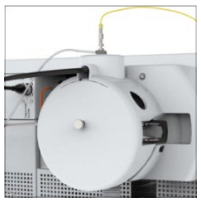
Basic Components

Ionization Source

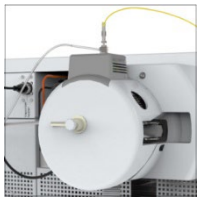
- Agilent liquid chromatography/mass spectrometry (LC/MS) ion sources enable analysis of a wide range of samples quickly and accurately. These easily interchangeable ion sources for Agilent LC/MS systems include the:

- Agilent Jet Stream (Dual AJS) source

- Electrospray Ionization (Dual ESI) source



- Atmospheric Pressure Chemical Ionization (APCI) source



- Multimode source (MMI)

Hardware Introduction

1 List the ionization source in use:

---

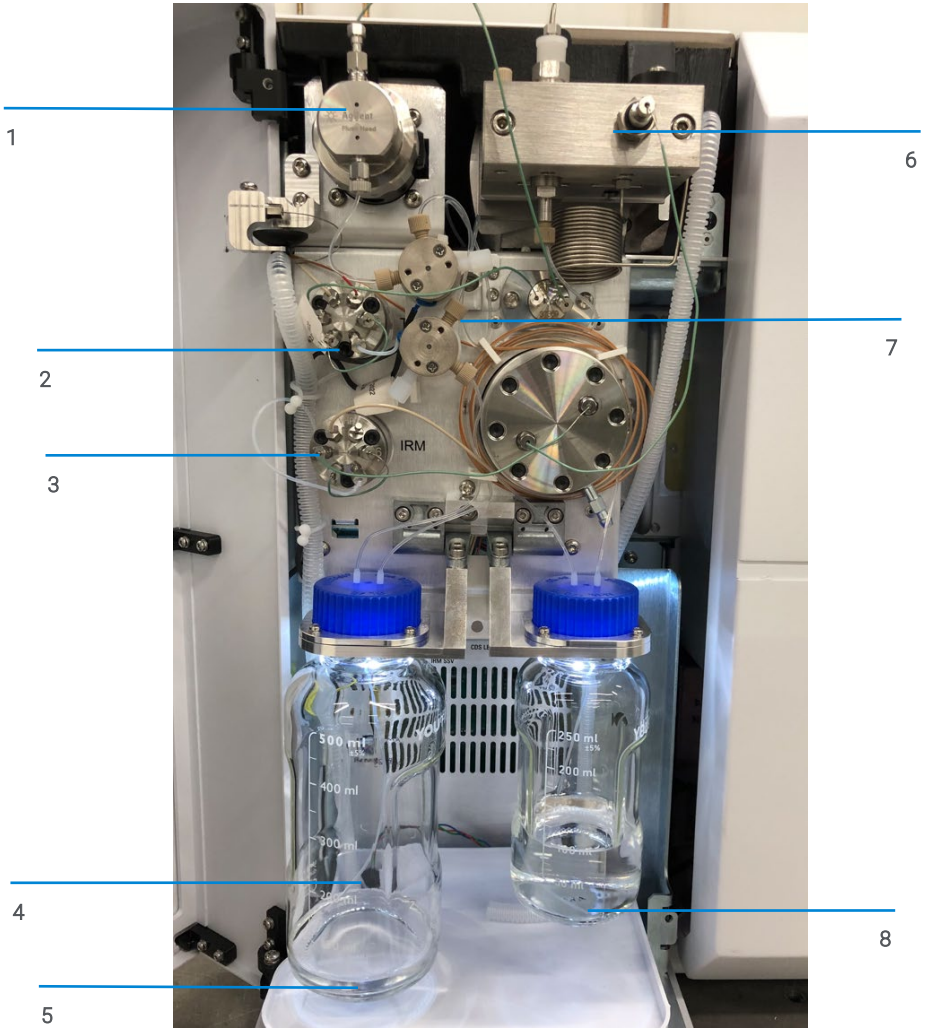
2 It is reviewed on _____ page of the user guide and includes the following parts:

---

3 List the name and part number of the proper tune solution for this system:

Calibrant Delivery System (CDS)/Bottle

The calibrant delivery system (CDS) introduces calibration solution for automated mass calibration of the mass spectrometer, to ensure that the mass accuracy of the system is maintained throughout batch acquisition.



Hardware Introduction

1 Practice removing and attaching the calibrant bottle and the internal reference mass bottle.

2 Are the calibrant bottle and the internal reference mass bottle interchangeable? Why?

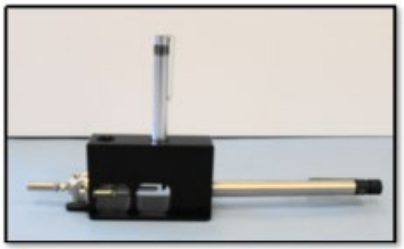
---

3 How often is the calibrant bottle checked and refilled?

Nebulizer

A nebulizer is a device for producing a fine mist of charged droplets that converts a liquid sample into an aerosol for introduction into the vacuum system.

APCI & APPI
Nebulizer



Nebulizer adjustment kit
Use to check the condition and concentricity of the needle, and to adjust the needle position

ESI, MM, & AJS
Nebulizer

View The Needle

1 Find your nebulizer type per the user guide or the document that comes with the kit. List the part number below:

Rough Pump

MS-40+

Locate The Oil Sight

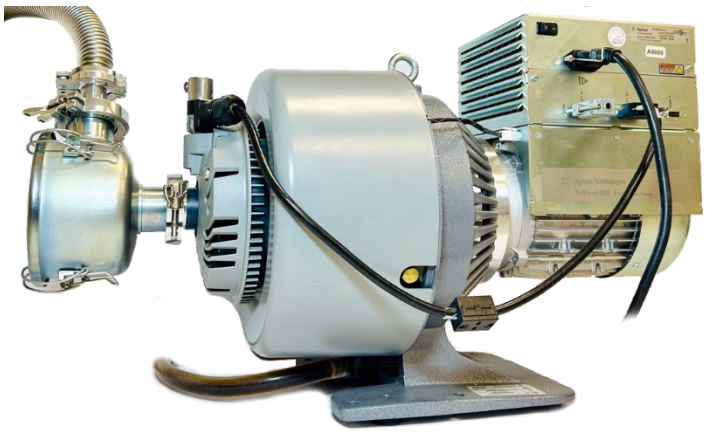
Using the user guide, fill out the following information:

1 The oil level should be _____ the marks for Max and Min.

2 Check that the pump oil is _____ and the color is _____ than amber.

3 If the pump oil is _____ or full of _____ replace it.

TriScroll™ 800 Series V3 Dry Scroll Vacuum Pump



Maintenance Information

Using the user guide, fill out the following information:

1 T or F - The expected interval between maintenance is 13-16 months.

2 T or F – It is acceptable to change the configurations of the connections to the pump after performing maintenance.

3 How often should the HEPA filter be changed?

_____

Waste Bottle from LC pump or Mass Spectrometer

Waste Bottle

1 At what level should you empty the waste bottle?

---

2 Does the waste bottle have a waste line connected? Why is this important to keep in place?

---

3 Software Basics

Overview

The MassHunter Control Panel is the administrative and management center for MassHunter Data Acquisition software:

- Full instrument status information of your entire laboratory.
- Central configuration and administration of users, instruments, and security settings.
- Full system documentation and built-in reports.

You will review:

- Starting the software
- Navigation overview
- Closing the connections
- Creating projects
- Creating and configuring instruments
- Launching instruments
- Offline method editor
- Creating shortcuts

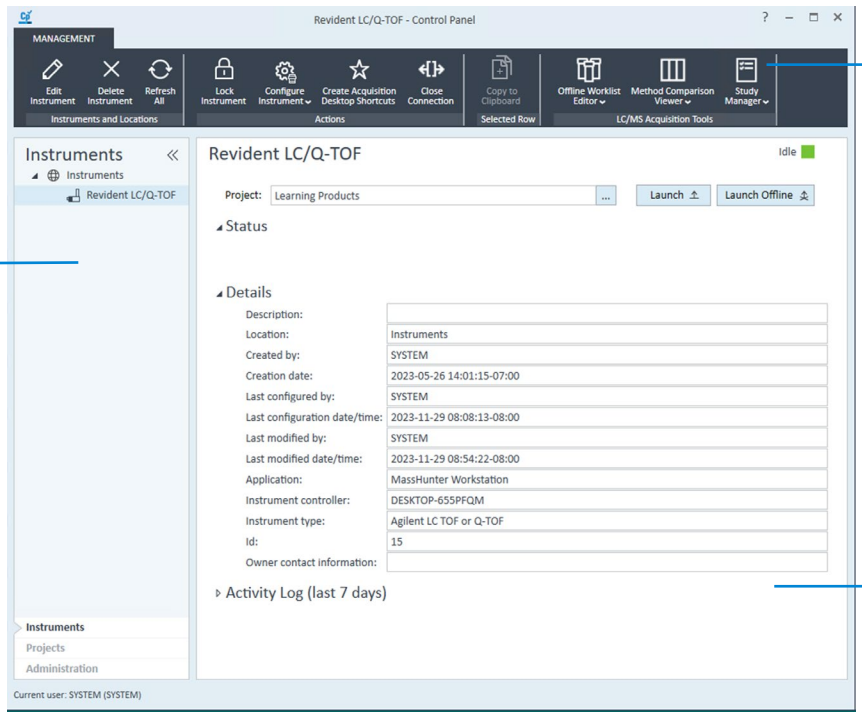
Software Start-Up

1 From the desktop, double-click the **Control Panel** icon

.

2 The navigation pane opens by default and can be minimized or expanded based on your preference.

User Interface and General Navigation



Ribbon

Panes

Instruments – Controls specific instruments.

Projects – Create paths to save project data.

Administration – Add and remove configuration

Main Window

- To minimize the pane, click **<<**. When minimized, the tab currently selected is displayed vertically.
- To expand the pane, click **>>**.

- Drag and drop items in the Instruments and Projects pane. The existing privileges of the instrument or project are not retained when moving. The user must have the proper privileges to perform this function.

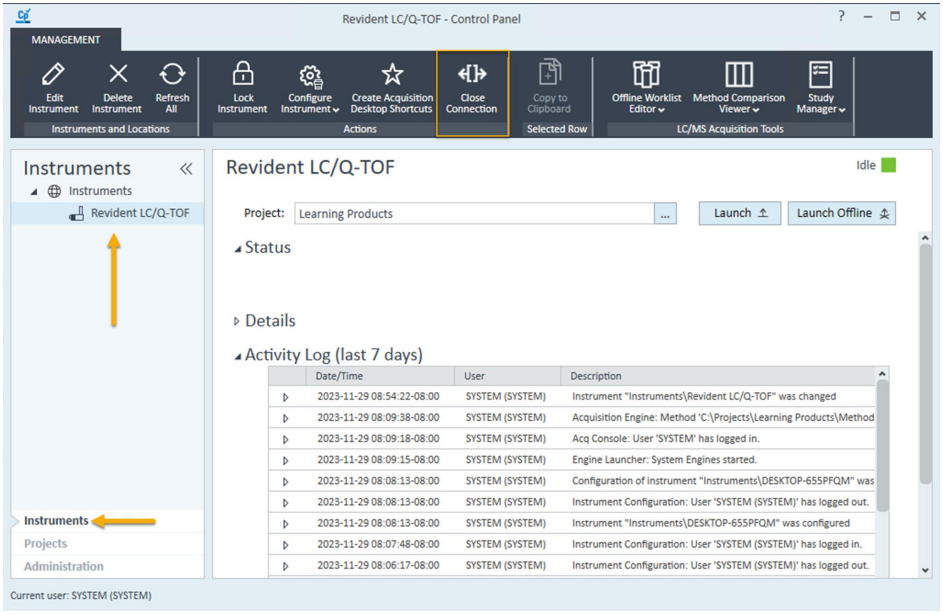
Close Connection

Use the Close Connection function to sever the connection between the instrument and the configured Instrument Controller (AIC or Workstation).

1 Click **Instruments**.

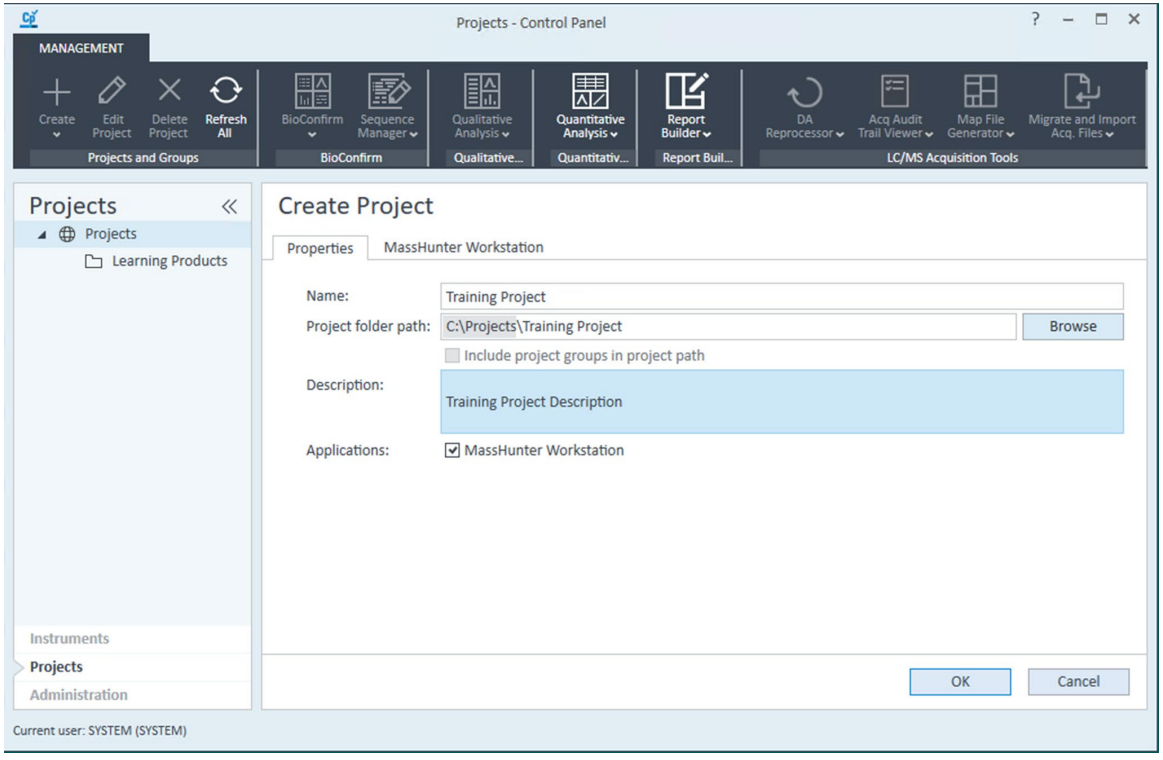
2 Select the instrument to close.

3 Click **Close Connection**.



Creating and Configuring Projects

1. Click **Projects** and select Projects
2. In the Name text box, type *TrainingProject*.
3. In the Project folder path text box, leave the default folder path.
4. In the Description text box, type a description of the project, for this example *Training Project Description*.
5. Click the **MassHunter Workstation** tab and review the available options. Do not change the defaults.
6. Click **OK**.



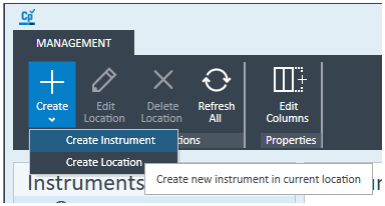
Instruments

Use the Control Panel to connect and control the instruments you want to use with the software.

Create an Instrument

1 Click **Instruments** and select or any location.

2 Click **Create > Create Instrument**.



3 Enter the data required in the Create Instrument pane.

   a Name: *Revident LC/Q-TOF*

   b Instrument Type: **Agilent LC TOF or Q-TOF**

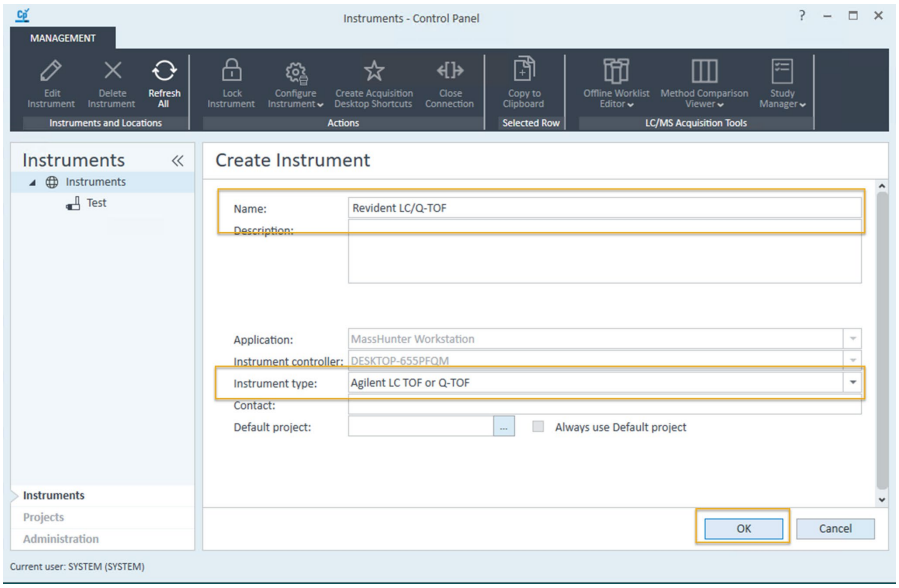
NOTE

Don't select a default project, you'll be prompted to select a project when you launch the instrument.

4 Click **OK**.

5 Click **…** to select the **TrainingProject** project from the Select Project dialog box.

6 Click **OK**. The instrument is displayed in the navigation pane.

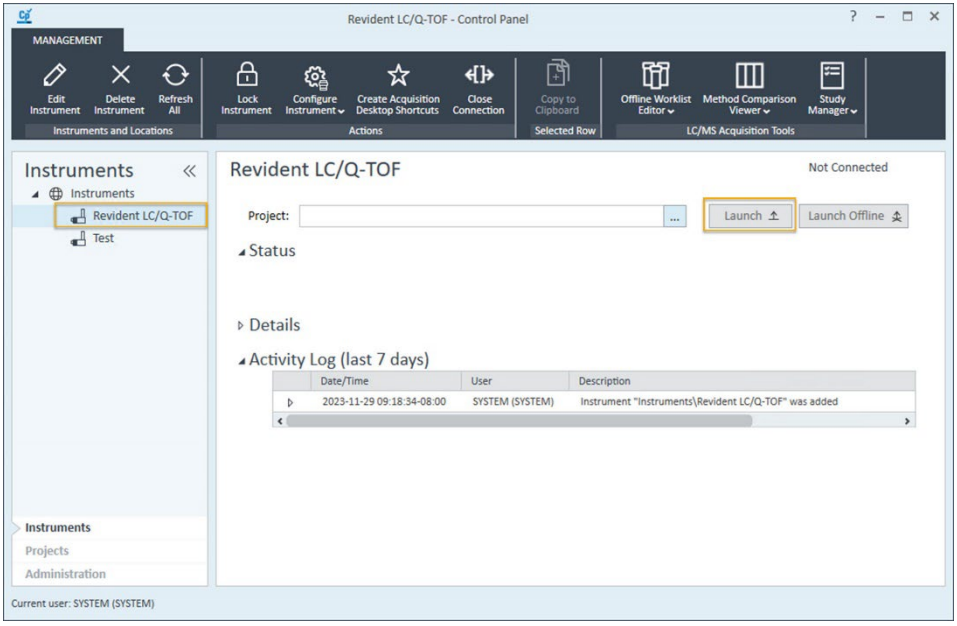

Instruments - Control Panel
MANAGEMENT
Edit Instrument
Delete Instrument
Refresh All
Instruments and Locations
Lock Instrument
Configure Instrument
Create Acquisition Desktop Shortcuts
Close Connection
Actions
Copy to Clipboard
Selected Row
Offline Worklist Editor
Method Comparison Viewer
Study Manager
LC/MS Acquisition Tools
Instruments
Instruments
Test
Instruments
Projects
Administration
Create Instrument
Name:
Revident LC/Q-TOF
Description:
Application:
MassHunter Workstation
Instrument controller:
DESKTOP-655PFQM
Instrument type:
Agilent LC TOF or Q-TOF
Contact:
Default project:
Always use Default project
OK
Cancel
Current user: SYSTEM (SYSTEM)

Launching an Instrument

Once you've added an instrument, launch the instrument to begin acquisition from the instrument table or the instrument details page or launch an instrument directly from your desktop shortcut.

1 Click **Instruments** and select an instrument from the left panel.

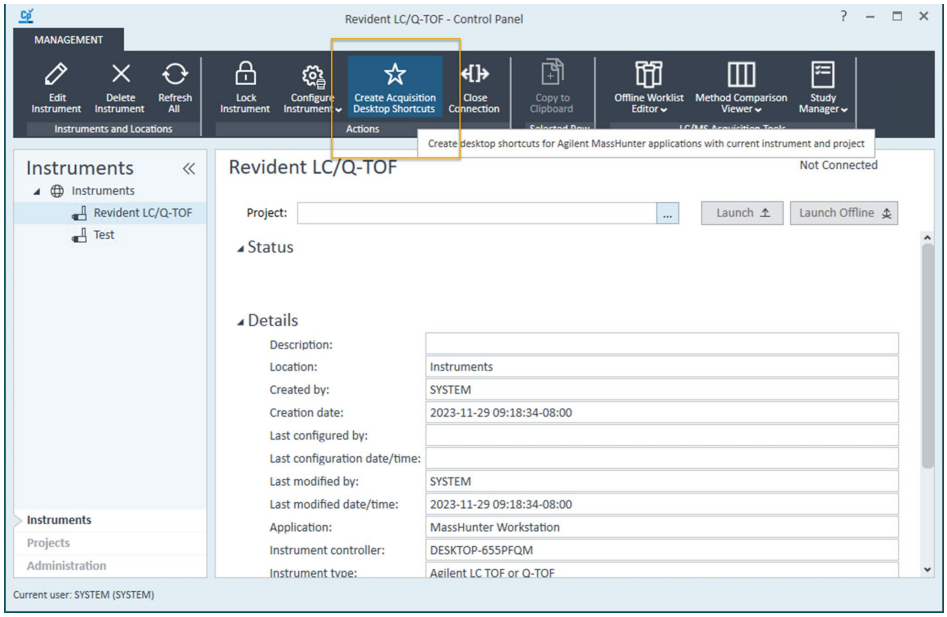
2 In the instrument windows, click the **Launch** button.



Create an instrument shortcut:

1 In the Control Panel, click Instruments and select the **Revident LC/Q-TOF** or **local instrument name.** Verify that the correct Project is selected.

2 Click **Create Acquisition Desktop Shortcuts** in the Actions group on the ribbon. Two icons are added to the desktop with the name of the instrument and whether it is online or offline.



4 Tune MS

Overview

When the LC/MS Q-TOF is used as a detector for the LC, a mass spectrum is associated with each data point in the LC chromatogram. To obtain high quality, accurate mass spectra, the LC/MS Q-TOF must be optimized to:

- Maximize sensitivity.
- Maintain acceptable resolution.
- Ensure accurate mass assignment

What is tuning in LC/MS?

Tuning is the process of adjusting the LC/MS Q-TOF parameters to achieve the optimized goals listed above.

Tuning acts as a diagnostic tool to indicate the service or cleaning requirements of the spectrometer; it provides a chronicle of system performance, and the matching of fragments from a known calibration compound to adjust the mass axis so it agrees with the expected mass assignments.

What is the difference between Tunes?

Mass Calibration performs a TOF mass calibration on the Active Instrument Mode, which is displayed in the Systems Settings panel. Run Mass calibration on a daily basis, at a minimum weekly. During normal operation, it lasts approximately 5 minutes.

A checktune is run each day an analysis is performed. A checktune can be used to determine if the tuning mix ion masses are properly assigned and if the response or sensitivity of these ions is within expectations. In other words, A checktune performs a single profile scan of the tune masses and compares the peak widths and mass axes with target values to make sure they are correct before you start your acquisition. Checktune is performed in either positive or negative ionization mode, or both.

Perform an autotune monthly, after preventative maintenance or if you find a problem with checktune. Periodically run an autotune to ensure that the mass spectrometer is working correctly. Autotune is performed in negative and/or positive ionization.

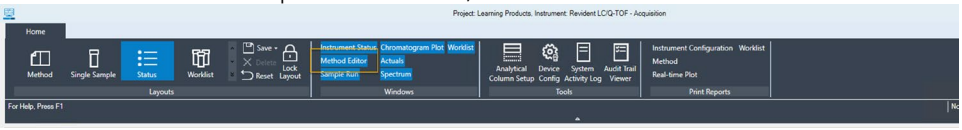
Frequent tuning, automated or manual, is not required. Once tuned, the LC/MS Q-TOF is stable. Tuning should be needed no more often than monthly, weekly at most.

Wait ~12 hours after pumpdown before tuning or operating your LC/MS Q-TOF system. The analyzer takes about 12 hours to reach thermal equilibrium. Tune files that are created, or data that is acquired, before the LC/MS Q-TOF system is at thermal equilibrium may have incorrect mass assignments and other inaccuracies.

Mass Calibration

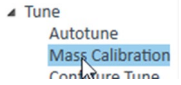
Mass calibration is run with the following ion sources: ESI, AJS ESI, and APCI.

3 In MassHunter Data Acquisition window, click **Method Editor**.



4 Click the **MS Q-TOF** tab.

5 Click **Tune > Mass Calibration** in the left pane.



6 Click **Tune control**.

7 Select **Mass Calibration**.

8 Click Mass calibration/Checktune.

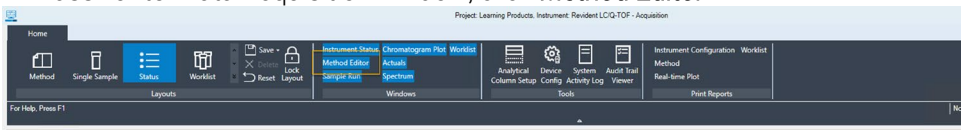
9 When the tune completes, review the report.

10 Click Tune control in the toolbar to release control of the instrument.

Checktune

A checktune is run with the following ion sources: ESI, AJS ESI, and APCI.

1 In MassHunter Data Acquisition window, click Method Editor.

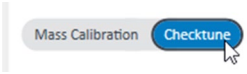


2 Click the MS Q-TOF tab.

3 Click **Tune > Mass Calibration** in the left pane.

4 Click **Tune control**.

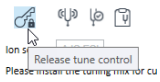
5 Select **Checktune**.



6 Click Mass calibration/Checktune.

7 When the tune completes, review the report.

8 Click Tune control in the toolbar to release control of the LC/Q-TOF instrument.



Review a Tune Report

Generate a detailed tune report

1 Click the MS Q-TOF tab.

2 Click the Tune > Autotune section in the left pane.

3 Click **Tune control**.

4 Click Tune Reports in the toolbar in the Autotune Section.

5 Select the tune report to view and click View tune reports. If no reports are available, then run either a mass calibration, checktune, or autotune first.

6 Click to release control of the instrument.

NOTE

Only the polarities that were last calibrated or tuned appear in the tune reports saved with the data files. Prior detailed tune reports are accessed through the autotune section or mass calibration section.

Example Report

Q-TOF system tune Mass Calibration Report

Q-TOF system tune Mass Calibration Report

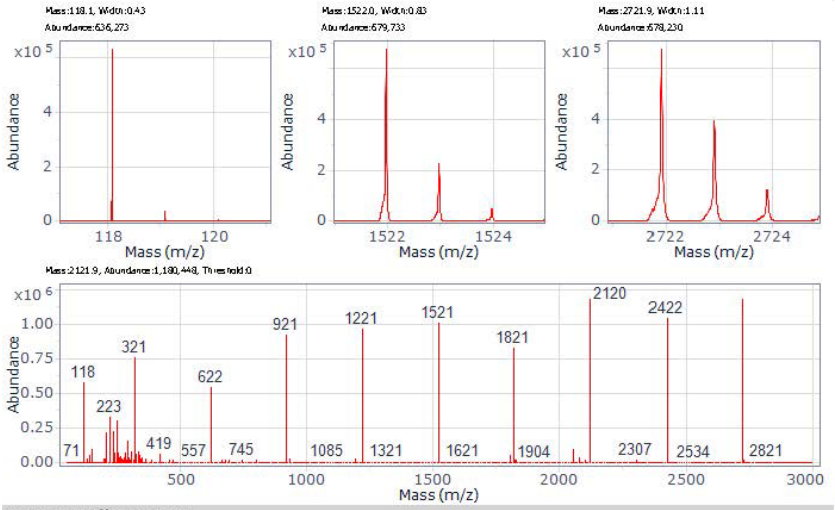
Agilent

Instrument Information

MS Model	G6575A	**Run Date**	2024-02-15T01:27:41+08:00
Serial Number	SG2341Z101	**Check Date**	2024-02-15T03:01:23+08:00
Instrument Mode	Q-TOF system tune	**Firmware Rev**	1.0.151
Mass Range	Standard (3200 m/z)	**TCD Version**	5.0.749
Source Type	Dual AJS ESI	**Slicer Mode**	High Resolution (Position 1)
Polarity	Both	**Overall Result**	Completed

Positive Polarity Results

Tof results



TOF Mass Calibration Data

Theoretical	Actual	Time	Abundance	Calibration Abundance	Resolution	Primary Residuals	Corrected Residuals
118.086255	118.086255	32,568.564844	584,809	614,780	35,344	-5.69	0.00
322.048121	322.048123	53,005.872266	754,388	749,437	50,227	-0.83	0.01
622.028960	622.028942	73,200.215625	552,086	560,613	57,159	-0.05	-0.03
922.009798	922.009832	88,859.862500	919,503	641,592	62,812	0.27	0.04
1,221.990636	1,221.990653	102,118.236719	974,434	715,109	65,754	0.30	0.01
1,521.971475	1,521.971379	113,826.551563	1,012,128	683,970	67,148	0.15	-0.06
1,821.952313	1,821.952366	124,427.430469	828,327	680,924	67,223	0.09	0.03
2,121.933152	2,121.933192	134,185.954688	1,180,448	680,611	66,813	-0.06	0.02
2,421.913990	2,421.913952	143,275.806250	1,045,959	603,713	65,676	-0.14	-0.02
2,721.894828	2,721.894834	151,818.107813	1,179,732	678,146	65,987	-0.01	0.00

Page 1 of 6

Scheduling a Tune

Schedule a mass calibration, checktune, or autotune so that a tune is run automatically at specified times.

1 To display the Method Editor window, click **Method Editor** in the Windows section on the Ribbon. Or, click the **Method** layout on the Ribbon.

2 In the Method Editor window, select the **MS Q-TOF** tab.

3 Select the **Tune > Autotune** section.

4 Click **Tune control**. in the toolbar to lock control of the instrument. You can't start a single sample run or a worklist when Tune has control of the instrument.

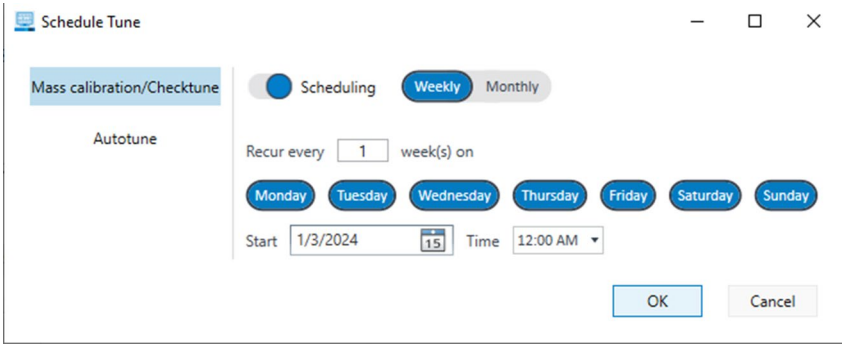
5 Click **Schedule tune** in the toolbar.

6 Select **Mass calibration/Checktune** in the left pane. The right pane shows the information for scheduling a checktune.

7 Click the **Scheduling** slider to switch on Scheduling.

8 Select **Weekly** for this exercise.

9 Select a day of the week and a Start date and time to indicate how often to schedule the checktune.

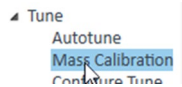


10 Click **OK**.

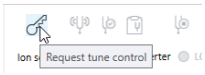
.

Stop checktune

1 Click the Tune > Mass Calibration section in the left pane.



2 Click Tune control. in the toolbar.



3 Select **Checktune**.

4 Click Mass calibration/Checktune.

5 Before the tune completes, click Stop Tune.

5 Using Methods

Overview

MassHunter Data acquisition methods include the parameters for each component associated with your instrument.

The Method Editor Window

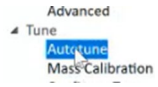
1 Launch the acquisition software: select **OpenLab Control Panel > Instruments** (bottom-left corner) > **your instrument** > click **Launch**. Alternatively, if available double-click the desktop shortcut.

2 In the Windows section, select **Method Editor**.

The Method Editor window opens in the Main Window.

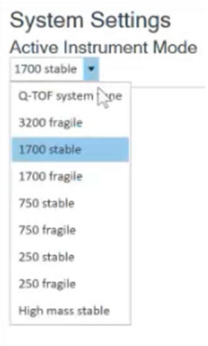
Set the Active Instrument Mode

1 Click **Tune > Autotune** in the left pane.



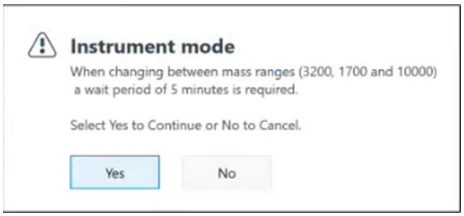
2 Click **Tune control**.

3 Select **Active Instrument Mode** drop-down.



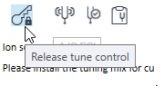
4 Select **1700 Stable** .

5 Select Yes.



Wait for the system to stabilize.

6 Click Release tune control in the toolbar to release control of the TQ instrument.



Set Up and Run an Acquistion Method

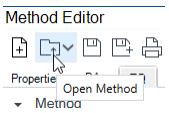
Working with the Default Method

Once an analysis has been created or opened, the default.m method is available to start from or apply a previously created method. The default method represents a good starting point for method development.

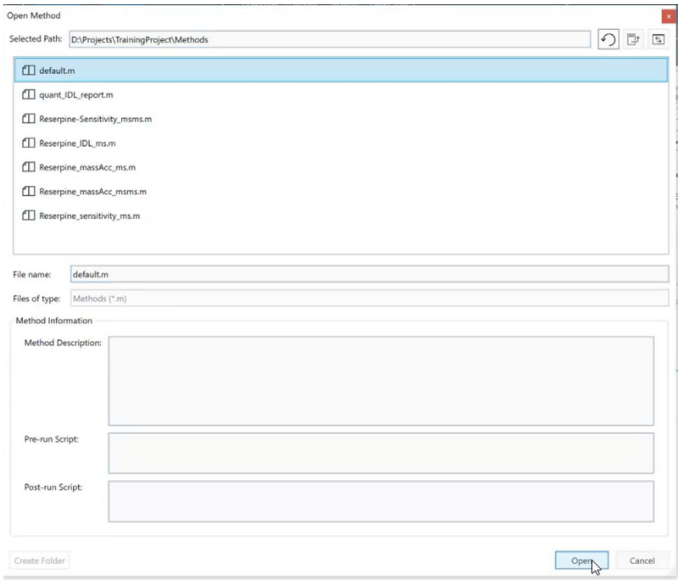
Load the default method

1 In the Method Editor window, click the MS-QTOF tab.

2 Click Open Method to review the methods available.



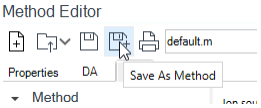
3 Select **default.m** and click **Open**.



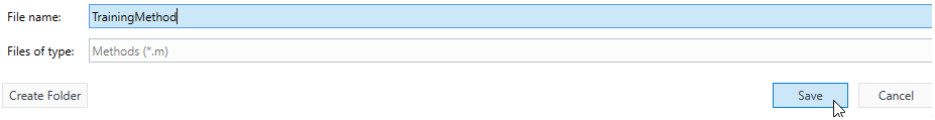
4 Under Method, review all default Method subsections listed below.

- **a** Acquisition - Set Q-TOF acquisition parameters.
- **b** Source - Set source parameters for the instrument.
- **c** Chromatograms - Specify plots to display in the Chromatogram Plot window during the run.

5 Click **Save As Method**.



6 Enter a **File name,** for this example *TrainingMethod,* then click **Save**.



NOTE

After modifying or viewing a method using the drop-down list, you must apply the method to send the parameters to the instruments.

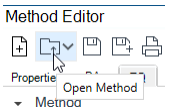
7 Click **Apply**.

Set up a Scan Method

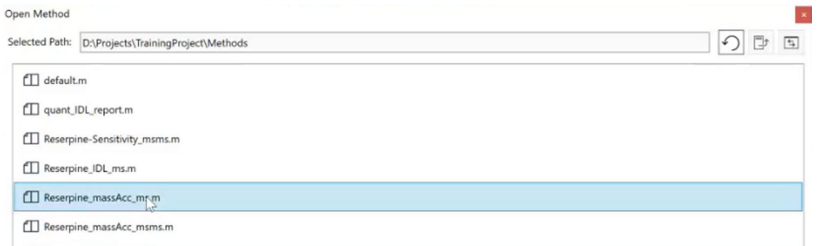
Load an existing method and Save As new method

In this exercise, you will use an existing method (the scan checkout method used during installation) to see if there is a signal for Reserpine at m/z 609 within the spectrum.

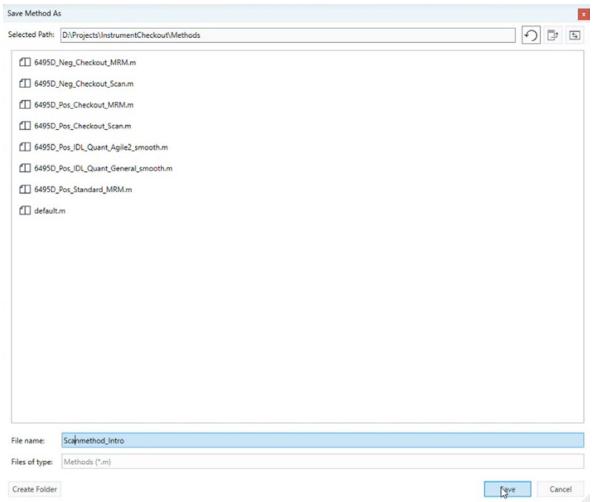
1 Click **Open Method** to review the methods available.



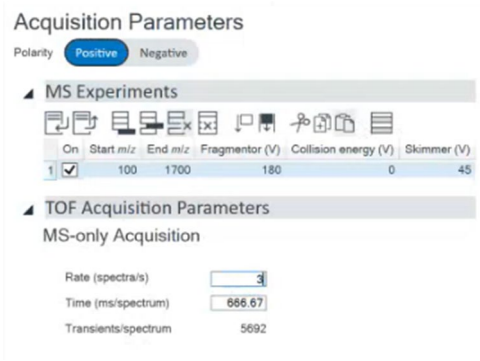
2 Select the checkout method used in installation, for example „Reserpine_massAcc_ms.m" and click **Open**. The method loads into the Method Editor.



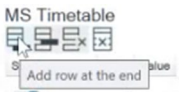
3 Click **Save as Method**, enter *Scanmethod_Intro* for the file name. Click **Save**.



4 Select **Method > Acquisition**, then under Acquisition Parameters, review the acquisition settings, noting Start m/z and End m/z. UnderTOF Aquisition Parameters, set the Rate to 3.



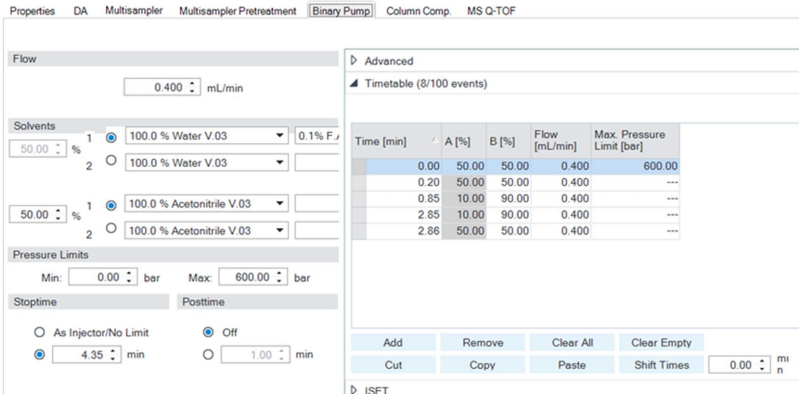
5 Under MS Timetable, click **Add a row at the end** twice.



6 Set the Start time (min) and Value as shown below.

7 Click to enable **Post-run diverter position**.

8 Click **Pump/Sampler/Column Comp settings.** to review the settings programmed for the LC pump, noting the flow rate.



9 To send the current parameters shown in the Method Editor window to the LC and MS instruments, click **Apply**.

Running Methods

Using a Method

In this exercise, you will acquire data using MassHunter Data Acquisition software and then use MassHunter Qualitative Analysis software to identify a precursor ion for Reserpine.

1 Place the Vial 4 100 pg / µl checkout sample; prepared during the system checkout, into a vial location of the sampler and note the location.

2 In the main window, click the Sample Run tab to display the Sample Run window.

3 In the Sample Run window, specify the following information:

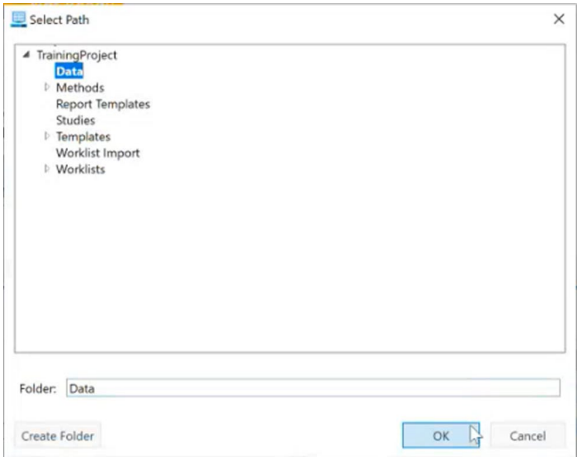
a Sample Name: Sample 1
Sample Position: Vial 4 (or applicable position)

b Sample Injection Volume: Select As Method to use the volume specified in the method applied in the last step.

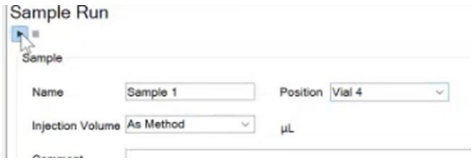
c Data File Name: Introduction_Scan_001.d

NOTE (optional) Select Auto Increment to automatically increment the file name if that file exists

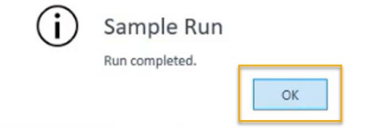
d Data File Path: Set to D:\Projects\TrainingProjectData. Create a folder if necessary.



4 Click Start Sample Run.



5 Click OK when the run completes.



Monitor the Status Windows

As data is being acquired, use the instrument status monitors and online signal displays available in the Instrument Status and Real-time Plot Panes to observe changes in modules.

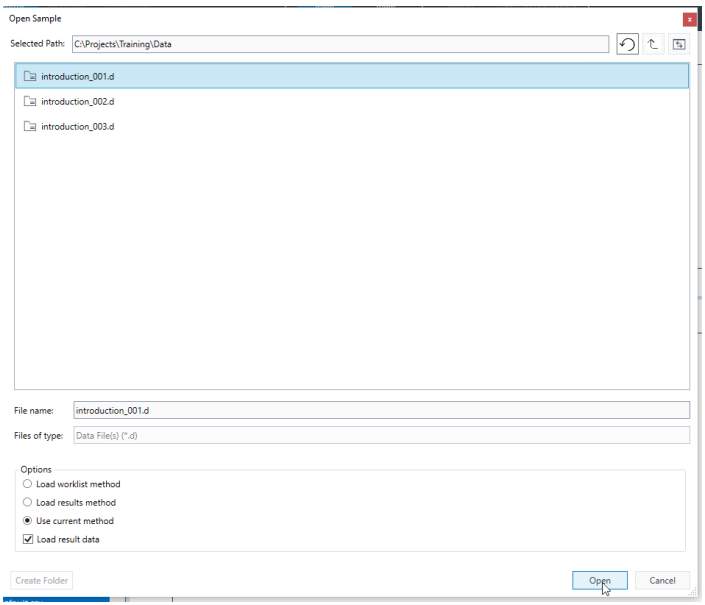
1 View the Chromatogram Plot and note the retention time for Reserpine.

2 Observe the Spectrum window while the samples runs. Discuss with your Agilent-certified service professional the changes observed over time.

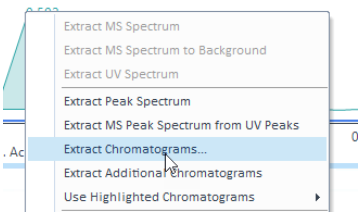
Review the data using Qualitative Analysis

1 From Control Panel, click the Qualitative Analysis icon in the Ribbon and select **Start Qualitiative Analysis** or double click the shortcut icon on the desktop, if available.

2 From the Home tab, click the Open icon . In the Open Data File window, browse to the data file directory used earlier (Data), select the data file to review, and click **Open**.

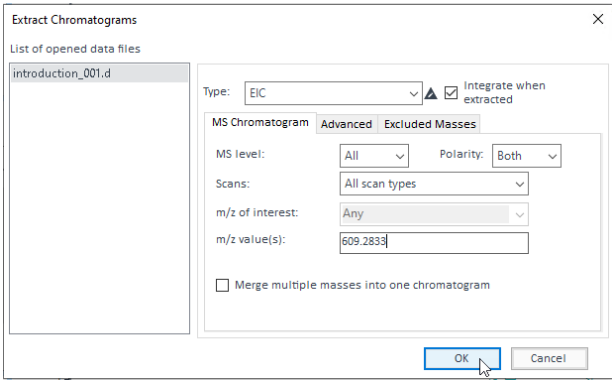


3 In the Chromatogram Results window, right-click and select **Extract Chromatograms...** from the menu.

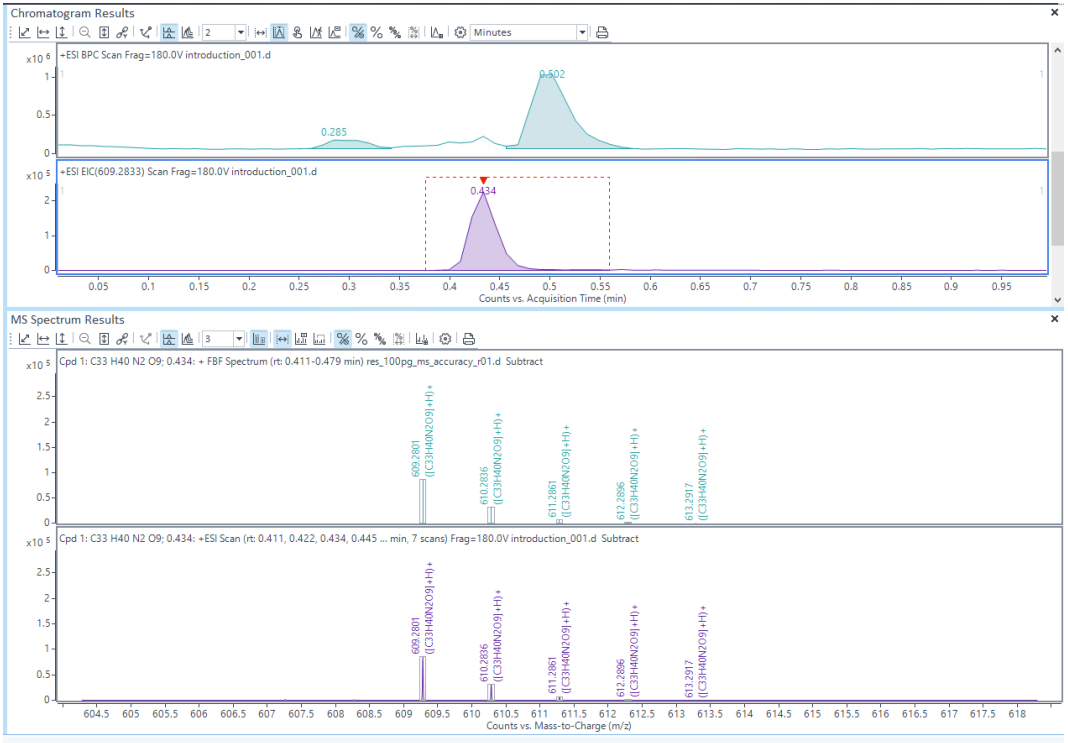


4 In the Extract Chromatograms dialog box, click **Type**: and select **EIC**.

5 Enter the m/z value: *609.2833*, then click **OK**.



6 Review the results.



Review the Results.

1 What is the retention time for Reserpine?

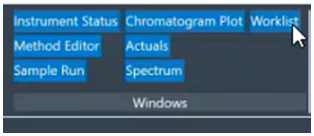
2 What is the m/z observed for Reserpine in the mass spectrum?

6 Run a Worklist

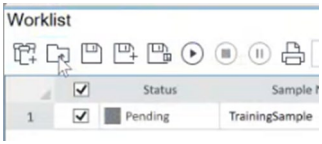
Introduction

Create and edit a worklist

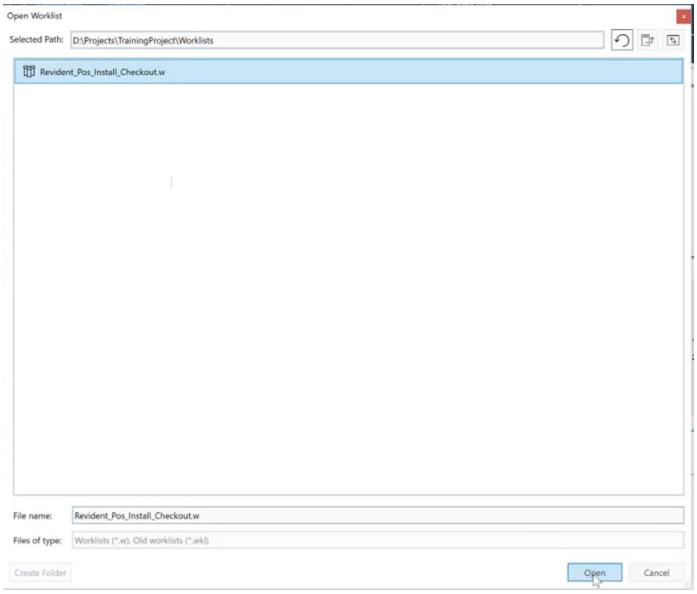
1 Click **Worklist** to show the Worklist window.



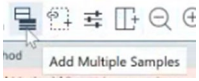
2 In the worklist window, click **Open Worklist**



3 Select the Revident_Pos_Install_Checkout.w worklist and click **Open**.



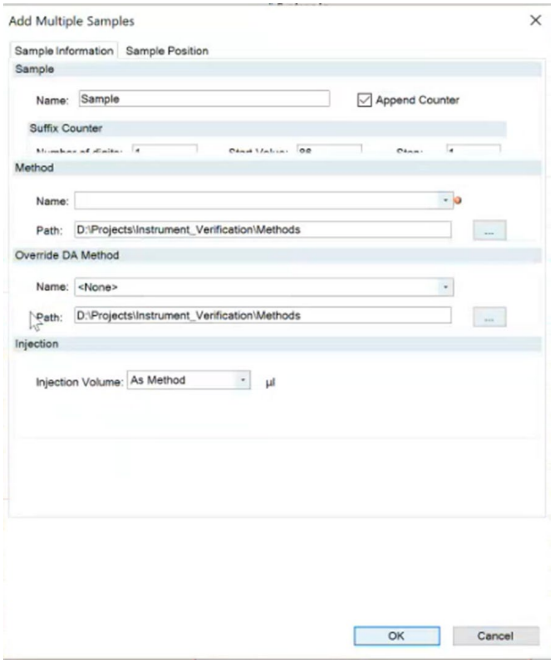
4 Click **Add Multiple Samples** . The Add Multiple Samples dialog box opens.



NOTE Samples are also be added one-by-one (user only needs to run a few samples, or several replicates of the same sample).

Add Multiple Samples

1 On the Sample Position tab, specify the sample vial locations (make sure the specific sample tray type has been configured by right clicking the autosampler device image).



2 Specify the locations and click **OK**.

3 To set up the worklist run, click **Worklist Run Parameters** .

4 On the Run Parameters tab, type the paths for the method.

5 On the Data File Settings tab, enter or select the folders for the data files. Select the File Naming options.

6 For information on the iReflex tab, refer to the online Help.

.

7 To start the worklist, click Run Worklist.

7 Set Up and Quantitate a Batch of Acquired Q-TOF Data Files

Overview

In this exercise, set up a quantitation method for a batch of acquired Q-TOF data files. Conduct the exercise with the LC-QTOF Pesticide data files and learn how to perform the following tasks:

- Set up a Batch Table containing sample and calibration data files for the solvent.
- Set up a new quantitation method based on the calibration standard of the highest concentration.
- Set up a target compound.
    - View the product ion and chromatographic parameters for the solvent compound in the data file.
- Set up quantitation for the method.
    - Create levels from calibration samples.
    - Set up qualifier ions and the calibration curve.
- Quantitate the batch and save the results.

Before You Begin These Exercises

- Make sure that you have copied the **LC-QTOF Pesticide** folder from the **Supplemental/Data/Quant Examples/Q-TOF** folder of the installation media to a folder on your system.
- If the default MassHunter Quantitative Analysis Software Supplemental installation was completed, the data files needed for these exercises should be present in MassHunter/Data/QuantExamples.
- If the default MassHunter Quantitative Analysis Software Supplemental installation was not completed, copy the data from the installation media (Supplemental/MassHunter/Data/QuantExamples) to the Data folder within the Training Project created in the prior exercise.

Set up a New Batch

Set up a Batch Table containing data files for three unknown samples and several calibration samples of drugs of abuse: amphetamine, cocaine, methamphetamine, and MDMA.

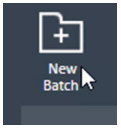
Create a batch to hold samples

1 To start the Quantitative Analysis program, double-click the **Quantitative Analysis (TOF) icon** on your desktop.

2 Select a Project and click **OK**.

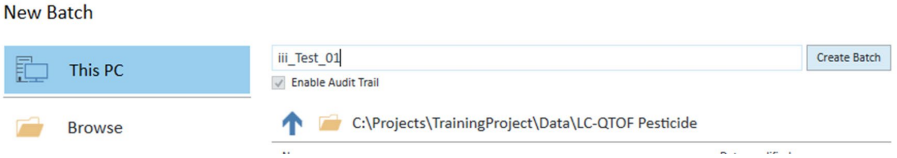
Quantitative Analysis (for Q-TOF) opens.

3 Click **New Batch.** The system opens the New Batch dialog box.



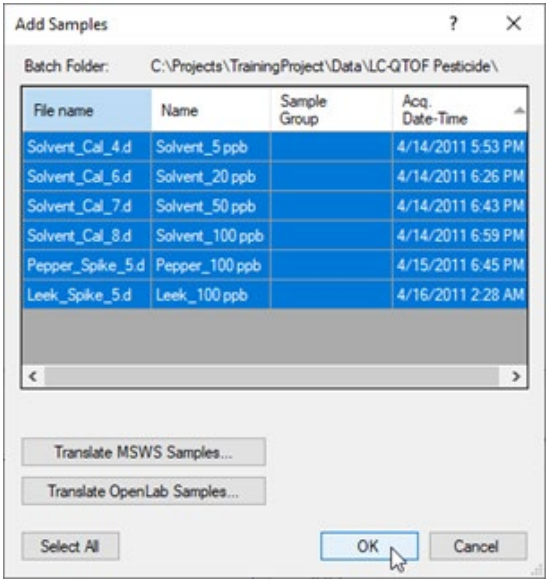
4 Navigate to the folder \Your Directory\LC-QTOF Pesticide.

5 Enter a batch file name, for this example *iii_Test_01*, where iii are your initials and click **Create Batch**.

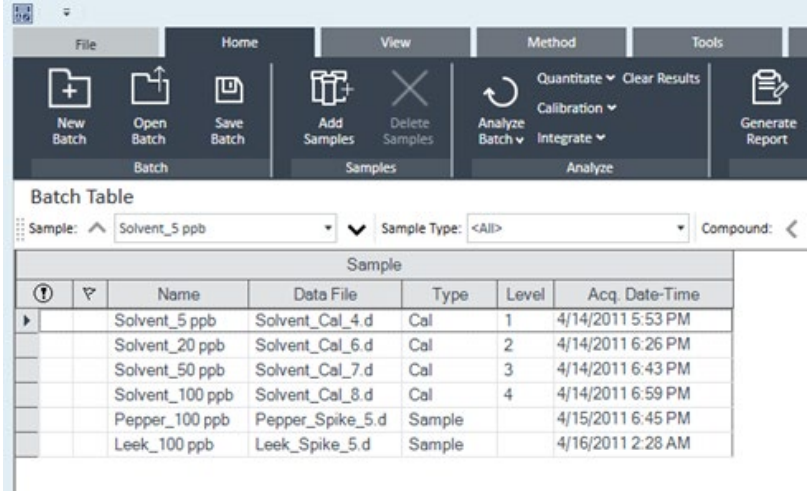


Add all the samples in the Pesticides folder to the batch

1 All Samples are selected. Click **OK** to add them to the batch.



2 The Batch Table is no longer empty. It now contains the samples.

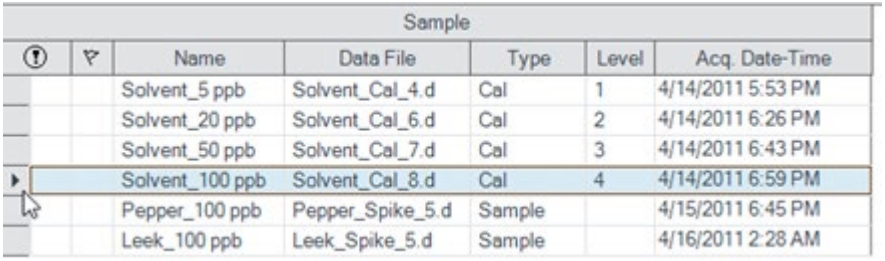


Set Up a New Method for the Batch

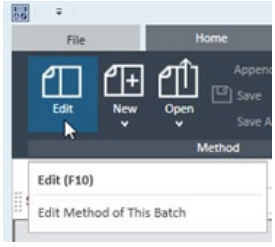
This task shows you how to set up a new quantitation method based on the calibration data file with the highest concentration of sample.

Create a method from acquired Q-TOF data.

1 Use the cursor to highlight the calibration standard that has the highest concentration level.

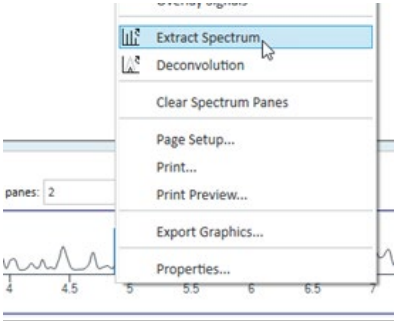


2 Click the **Method** tab, then **Edit** to switch to method editing mode.

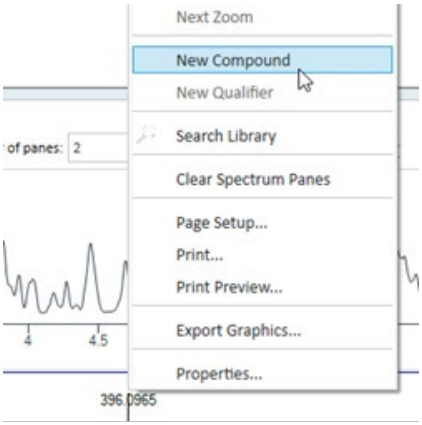


The Method Tasks appear in the column to the left of the view.

3 In the Sample Information window, click the middle of the peak at approximately 4.82 on the X-axis. Then right-click and click Extract Spectrum..



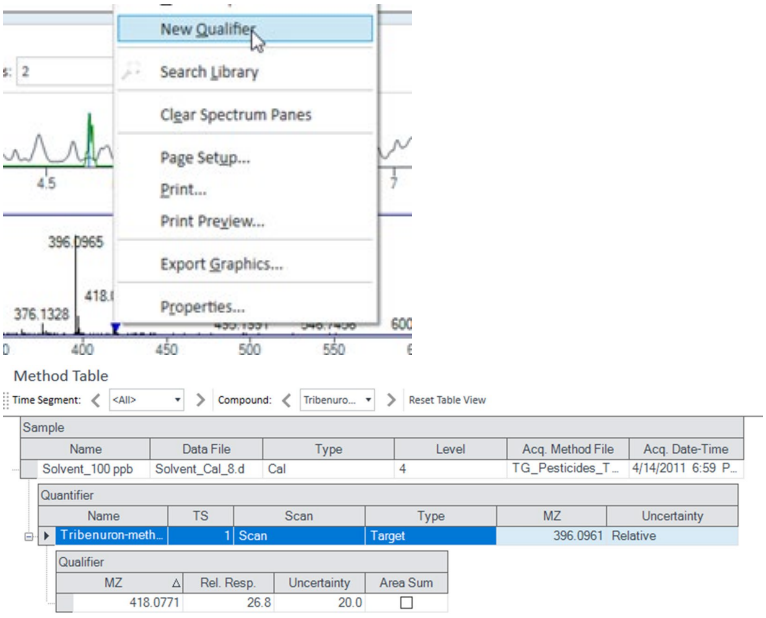
4 Click the largest ion, 396.0966. right-click that location and click New Compound.



5 Type Tribenuron-methyl as the Name in the Method Table. Keep this compound selected in the Method table while you add the qualifier in the next step.

6 To once again display the spectrum for Tribenuron-methyl, click at the peak apex to display a line running through the apex.

7 Click 418.0775 to select that ion (blue filled triangle). Right-click that location and click New Qualifier.

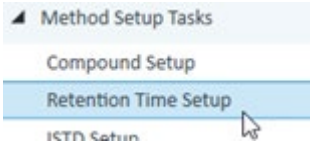


Set up Target Compounds

With this task, you learn to inspect the product ions and the RT data for the new quantitation method, which you can change for individual target compounds.

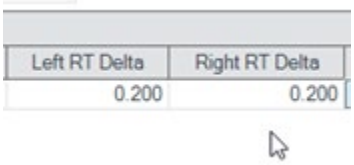
Check the new quantitation method created from the Sample Information window for the product ion.

1 To inspect the retention time set from the spectrum, click Method Setup Tasks > Retention Time Setup.



2 In the Left RT Delta column, enter 0.2.

3 In the Right RT Delta column, enter 0.2.



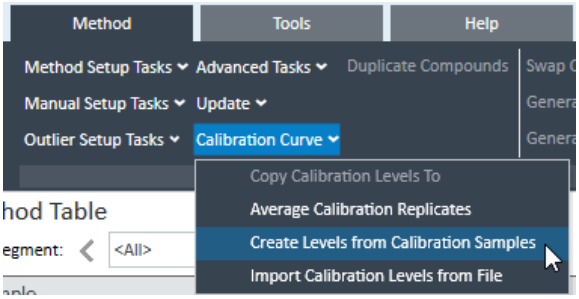
Set up Quantitation

This task presents instructions for setting up the quantitation parameters for the methods:

- Calibration levels.
- Qualifier ions.
- Calibration curve fit.

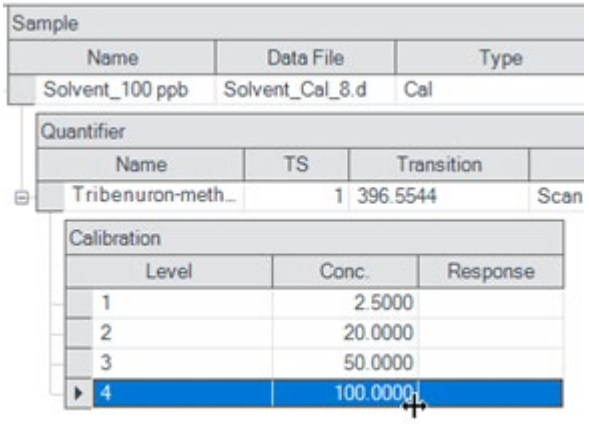
Create four calibration levels

1 From the main menu, select Calibration Curve > Create Levels from Calibration Samples.



The Calibration table opens under each Quantifier in the Method Table.

2 For one of the Quantifiers, change the default concentrations to the actual concentration for each level.



- L1–2.5000
- L2–20.0000
- L3–50.0000
- L4–100.0000

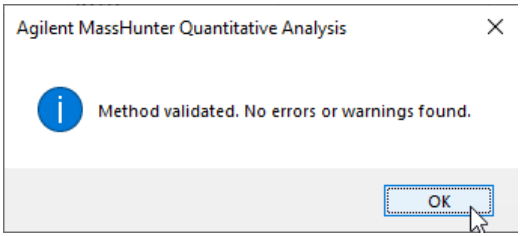
Validate the method

1 Under **Save/Exit**, click **Validate** to validate the method setup.

2 After the validation message appears, click **OK**.

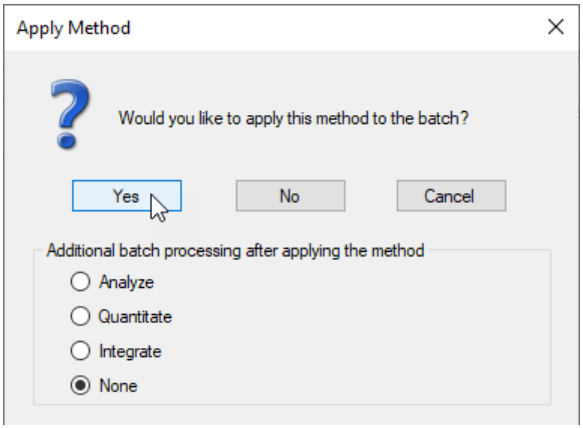
3 Under **Save/Exit**, click **Exit**, then select **None** under **Additional batch processing after applying the method**, and click **Yes** to the **Would you like to apply this method to the batch?** prompt.

4 After the validation message appears, click **OK**.



5 Click **Save/Exit** > **Exit**.

6 Select **None** under **Additional batch processing after applying the method** and click **Yes** to the **Would you like to apply this method to the batch**? prompt.

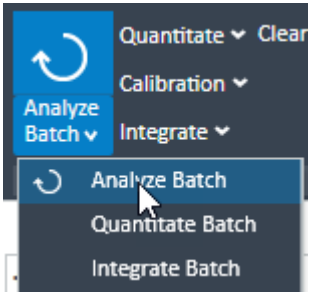


Analyze and Save the Batch

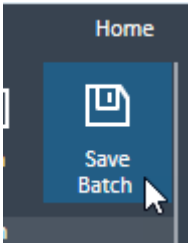
In this exercise, you automatically quantitate the batch and then save the results

Analyze the batch and inspect the results for each compound.

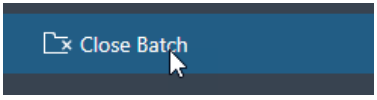
1 On the Home tab, click Analyze Batch.



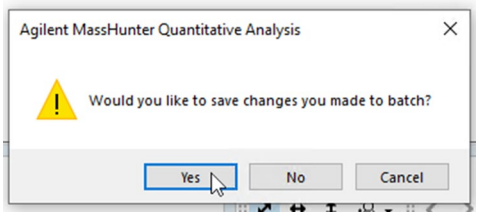
2 On the Home tab, click Save Batch.



3 Click File > Close Batch to close the batch.



4 Click Yes to the Would you like to save changes you made to batch? prompt.



Review Quantitation Results

The tasks in this exercise show you how to inspect the sample and compound data in a batch file, customize result layouts, export your data to Microsoft Excel, and preview and print the data.

Use the DrugsOfAbuse batch in this exercise.

Navigate the Batch Table Results

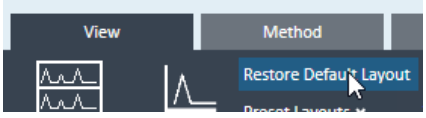
This task shows you how to scroll through your samples and compounds, while observing changes in the Batch Table and compound information data. It also shows you how to display various sample types.

Open the batch file DrugsOfAbuseDemo.batch.bin.

1 On the Home tab, click Open Batch.

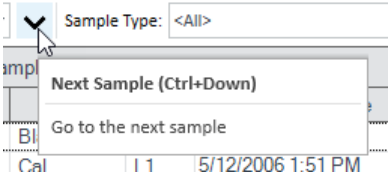
2 Navigate to \Your Directory\DrugsOfAbuse and click iii_Test_01.batch.bin

3 On the View tab, click Restore Default Layout.

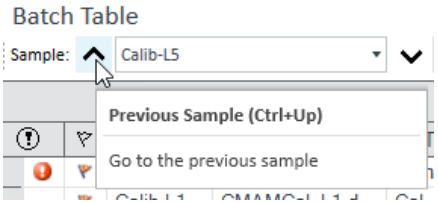


Scroll from sample to sample until you reach the end of the Batch Table, and then return to Cal-L5

1 Click the Next Sample arrow in the Batch Table Standard toolbar until the system displays the desired sample. Inspect the changes in the Compound Information window.



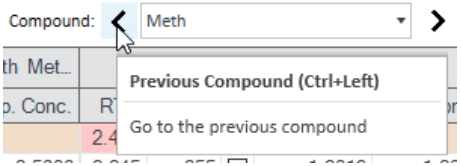
2 Return to Cal-L5, clicking the **Previous Sample icon** in the Batch Table Standard toolbar if needed.



3 Select any cell in the row for sample **Calib_L4** in the Batch Table window to view the changes.

Scroll from compound to compound through all four compounds

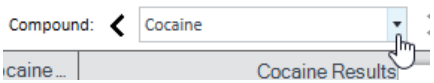
1 Click the **Next Compound** or **Previous Compound** arrow in the toolbar until the system displays the desired compound.



2 Inspect the changes in the **Batch Table**, **Compound Information**, and **Calibration Curve** windows.

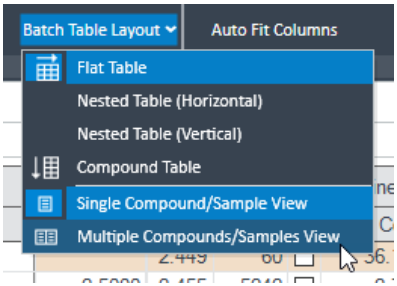
3 Click the down arrow next to the **Compound** list.

4 Click **Cocaine**.



Examine results for multiple compounds

1 On the View tab, select Batch Table Layout > Multiple Compounds/Sample View.



2 Click the Cal-L4 cell and note the difference in RT in the Compound Information window for each compound.

Sample							Amp Results			Meth Results			MDMA Results			Cocaine Results		
		Name	Data File	Type	Level	Acq. Date-Time	RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy	RT	Final Conc.	Accuracy
		Blank-1	CMAMBlk_01.d	Blank		5/12/2006 1:48 PM							2.284	1.9296		2.433	11.8235	
		Calib-L1	CMAMCal_L1.d	Cal	L1	5/12/2006 1:51 PM	2.141	3.3187	132.7	2.247	2.5936	103.7	2.276	2.2824	91.3	2.453	2.3087	92.3
		Calib-L2	CMAMCal_L2.d	Cal	L2	5/12/2006 1:54 PM	2.140	5.7493	115.0	2.248	5.1011	102.0	2.277	4.6561	93.1	2.454	4.2682	85.4
		Calib-L3	CMAMCal_L3.d	Cal	L3	5/12/2006 1:57 PM	2.134	13.6808	109.4	2.247	15.1623	121.3	2.277	11.2728	90.2	2.459	11.5607	92.5
		Calib-L4	CMAMCal_L4.d	Cal	L4	5/12/2006 2:00 PM	2.022	26.7561	107.0	2.228	27.2574	109.0	2.264	24.8702	99.5	2.449	25.2511	101.0
		Calib-L5	CMAMCal_L5.d	Cal	L5	5/12/2006 2:03 PM	2.101	124.4844	99.6	2.237	124.2764	99.4	2.271	125.1668	100.1	2.448	125.0768	100.1
		QC-L2	CMAMQC_L2.d	QC	L2	5/12/2006 2:06 PM	2.142	5.2293	104.6	2.248	5.2414	104.8	2.276	4.8567	97.1	2.453	4.2831	85.7
		QC-L4	CMAMQC_L4.d	QC	L4	5/12/2006 2:09 PM	2.135	27.8039	111.2	2.246	27.7713	111.1	2.276	23.0331	92.1	2.455	24.5377	98.2
		Sample-1	CMAMSam_01.d	Sample		5/12/2006 2:12 PM	2.080			2.286	3.2639		2.315	5.6138		2.408		
		Sample-2	CMAMSam_02.d	Sample		5/12/2006 2:15 PM	2.143	4.8977		2.250	5.8102		2.280	5.1778		2.460	4.3735	
		Sample-3	CMAMSam_03.d	Sample		5/12/2006 2:18 PM	2.105	14.2183		2.236	14.1876		2.267	10.7772		2.446	10.9299	

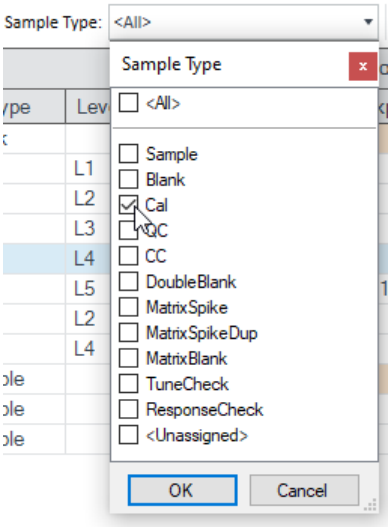
View selected sample types

1 On the View tab, select Batch Table Layout > Single Compound/Sample View.

2 If necessary, click the down arrow next to the Compound list, and click Cocaine.

3 Click the down arrow in the Sample Type drop-down list. The Sample Type dialog box is displayed.

4 Clear the **<All>** check box and mark the **Cal** check box.



5 Click **OK**. The Batch Table should contain only the Cal standards for cocaine.

6 Click the down arrow in the **Sample Type** drop-down list.

7 Click **<All>**, and then click **OK**. The system marks all the check boxes and displays all sample types.

Change Result Window Layouts

This task shows you how to customize your layout and how to recreate the default layout.

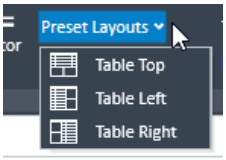
Use layout icons on the toolbar

1 Use layout options on the View Tab to position the Batch Table, Compound Information, and Calibration Curve windows.

   a On the View tab, select Preset Layouts > Table Left.

   b On the View tab, select Preset Layouts > Table Right.

   c On the View tab, select Preset Layouts > Table Top.

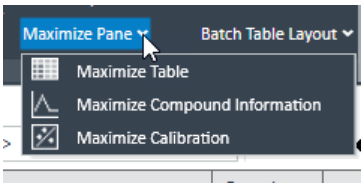


2 Use layout icons on the View Tab to maximize each individual window:

   a On the View tab, select Maximize Pane > Maximize Table.

   b On the View tab, select Maximize Pane > Maximize Compound Information.

   c On the View tab, select Maximize Pane > Maximize Calibration.

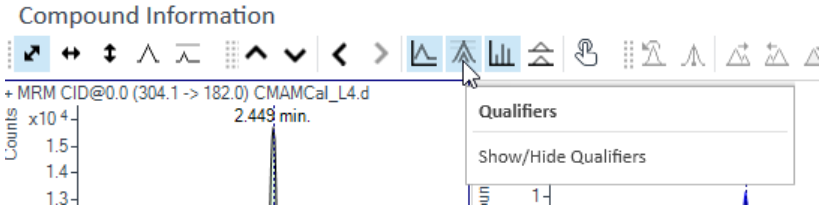


3 On the View tab, click Restore Default Layout.

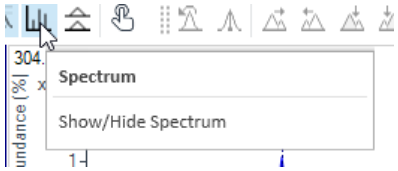
Change the panes in the Compound Information window for Cal-L4

1 In the Batch Table, select the Cal-L4 row.

2 In the Compound Information toolbar, click the Show/Hide Qualifiers icon.



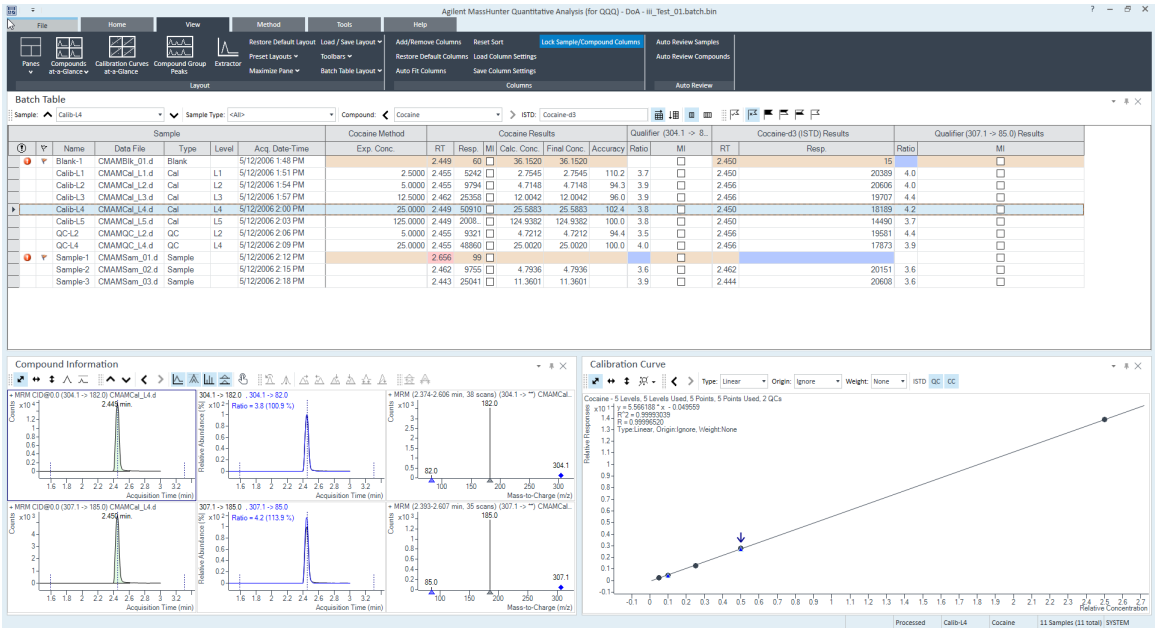
3 Click the Show/Hide Spectrum icon.



4 Click the Show/Hide ISTD icon.

5 The layout and results look like those in the following figure.

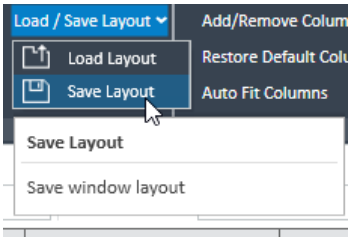
Set Up and Quantitate a Batch of Acquired Q-TOF Data Files



Save the default layout without the calibration curve

1 Close the Calibration Curve window.

2 On the View tab, select Load/Save Layout > Save Layout. The system displays the Save Layout File dialog box.



3 Name the layout file Batch Table plus Compound Information and click Save.

Load the newly created layout

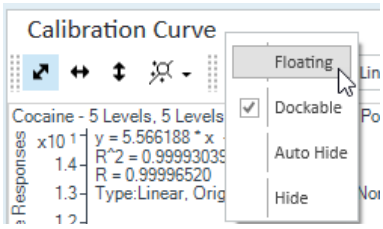
1 On the View tab, click Restore Default Layout.

2 On the View tab, select Load/Save Layout > Load Layout. The system displays the Load Layout dialog box.

3 Click Batch Table plus Compound Information and click Open.

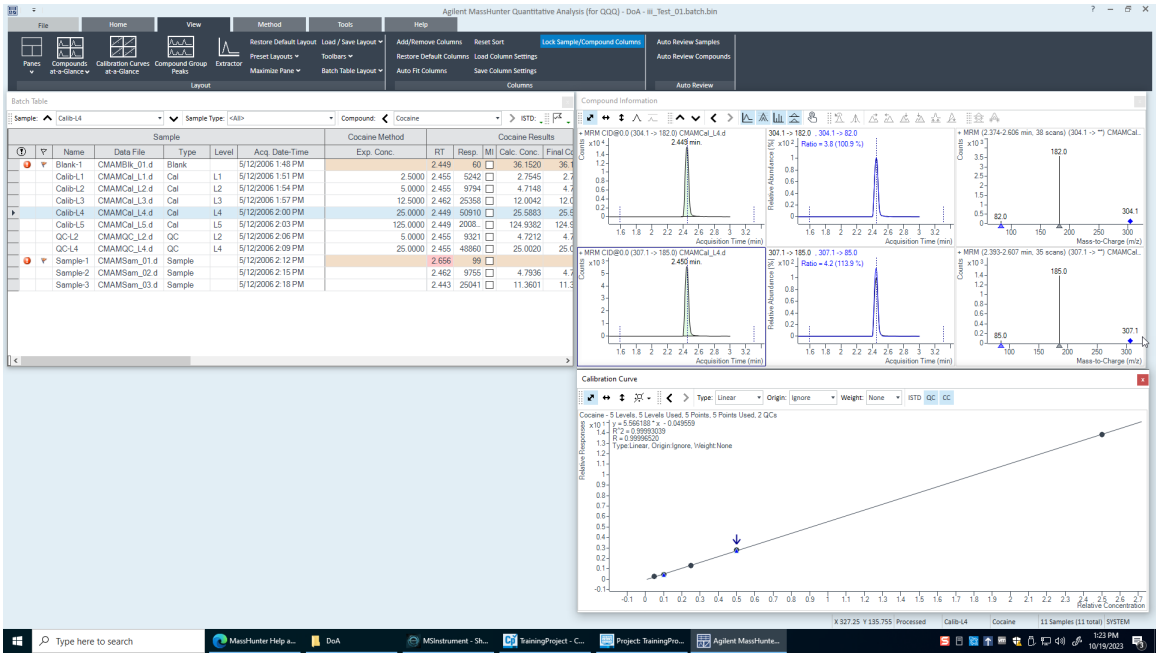
4 On the View tab, click Restore Default Layout.

5 Right-click inside the title bar of the Calibration Curve window, and then mark the Floating check box.



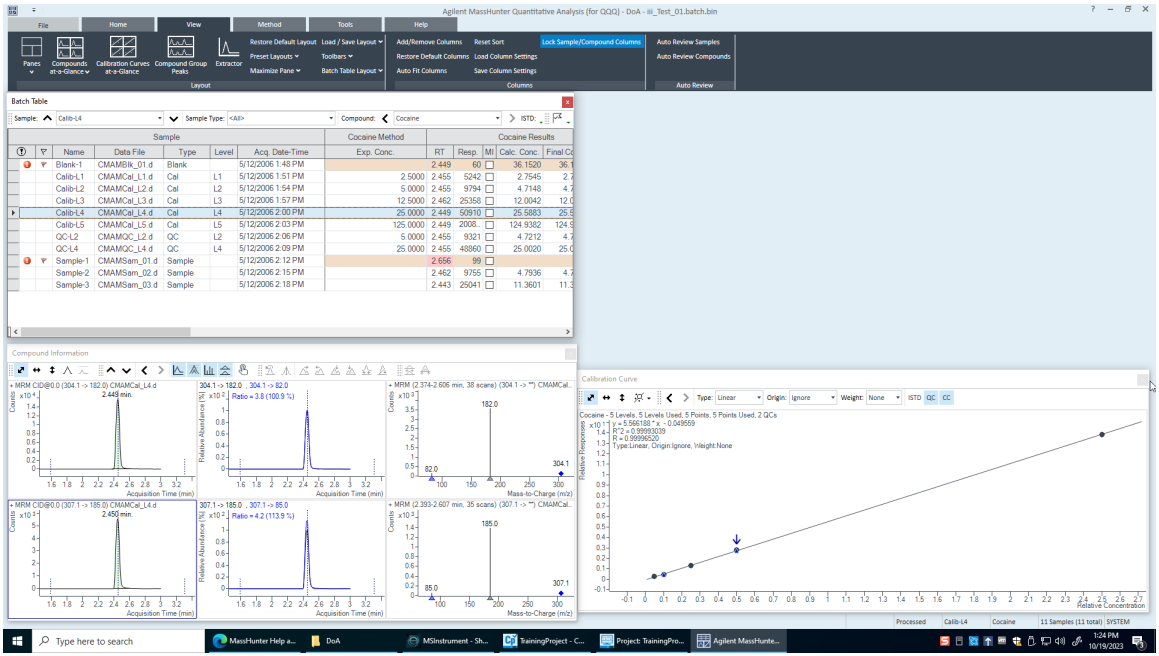
6 Right-click the title bar of the Compound Information window, and then mark the Floating check box.

7 Resize the windows to match the layout below.



8 Right-click inside the title bar of the Compound Information window, and then clear the **Floating** check box.

9 Resize the windows to match the layout in below.



10 Right-click inside the title bar of the **Calibration Curve** window and clear the **Floating** check box.

11 Move the **Compound Information** window so that the layout corresponds to the one pictured at the start of the task.

Recreate (don't restore) the default layout

1 Maximize the program main view.

- Anchor the **Calibration Curve** window first, and then the Compound Information window, to recreate the default layout.
- If after anchoring the two windows, the calibration curve is on the left side, right-click the title bar of the **Calibration Curve** window and drag it to the right. A gray rectangle shows where this window will be placed within the main view.
- Drag the calibration curve to the bottom-right corner of the main view.

2 On the View tab, click **Restore Default Layout**.

Use Three Tools to Evaluate Results

In this exercise, you'll use three tools to help you evaluate and obtain more accurate quantitation results:

- Curvefit Assistant, which calculates all combinations of curves and presents results with an equation and confidence band.
- Parameterless integrator, so you do not have to figure out the parameters to change to improve the integration.
- Outlier messages to help you easily detect result values that are out of the specified range.

The DrugsOfAbuse batch is used in this exercise.

Adjust the Calibration Curve Fit

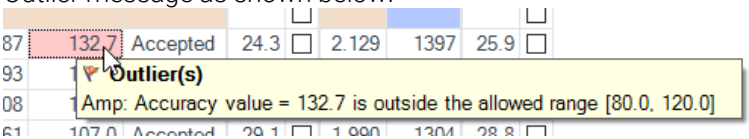
This task shows you how to find the accuracy outlier for a compound, adjust its curve fit, and reanalyze the batch.

1 If necessary, open the batch file. iii_Test_01.batch.bin. On the Home tab, click **Open Batch**.

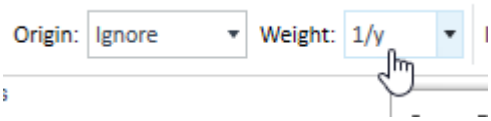
2 Navigate to **\Your Directory\ DrugsOfAbuse** and click **iii_Test_01.batch.bin**.

3 Make sure the **Batch Table** is set to single compound display mode, and the displayed target compound is **Amp**.

4 Point to the cell in the **Calib-L1** row and the **Accuracy** column to display the Outlier message as shown below.



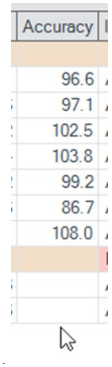
5 In the **Calibration Curve**, set **Origin** to **Ignore**, and **Weight** to **1/y**. The program displays a new window curve fit formula and R2 value.



Analyze the batch and inspect the results in the Batch Table

1 On the Home tab, click Analyze Batch.

2 Inspect the results in the Batch Table after batch analysis.



3 Click Next Compound in the Batch Table toolbar to view individual compounds, such as Cocaine, MDMA, and Meth.

4 Examine the quantitation results, especially the values in the Accuracy column.

Change the curve fit for methamphetamine and analyze the batch

1 In the Calibration Curve Fit window, set Origin to Ignore, and Weight to 1/y.

The Quantitative Analysis program displays a revised curve fit formula and R2 value.

2 On the Home tab, click Analyze Batch. The Batch Table displays the new results after batch analysis.

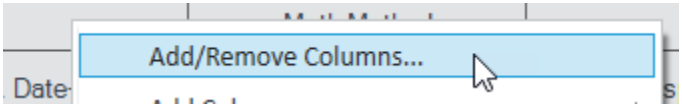
Integrate Without Parameter

This task shows you how to inspect data for proper integration. You learn how to perform the following tasks:

- Add integration columns to the Batch Table
- View default integration values
- Closely examine the chromatogram, looking for such details as:
- Outlier messages
- Baseline parameters
- Peak labels

Add integration columns to the Batch Table

3 Right-click anywhere in the **Batch Table** and click **Add/Remove Columns**.

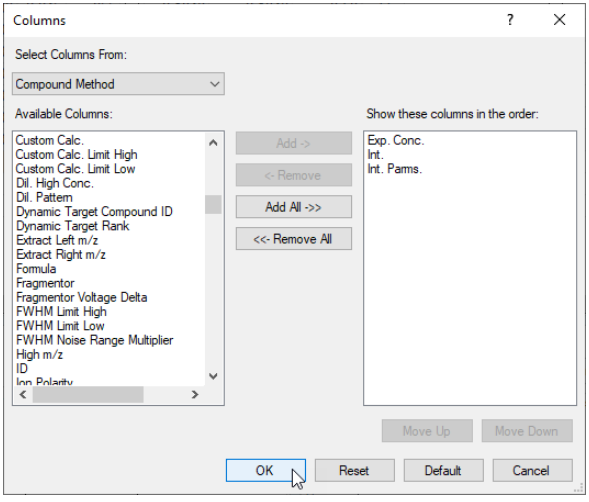


The system displays the **Columns** dialog box.

4 From the **Select Columns From** drop-down list, select **Compound Method**.

5 From the **Available Columns** list, select **Int.** (Integrator Type) and **Int. Parms.** (Integrator Parameters) and click **Add**.

6 The Quantitative Analysis program moves the selected columns to the **Show these columns in the order** list.

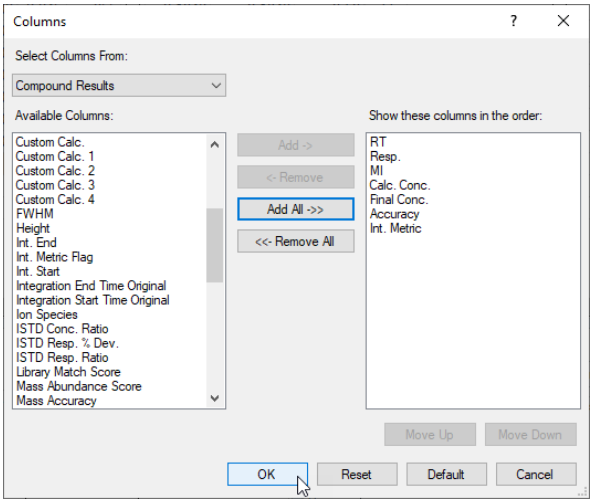


7 From the **Select Columns From** drop-down list, select **Compound Results**.

8 From the **Available Columns** list, select **Int. Metric** (Integrator Metric) and click **Add**.

9 The system moves the selected column to the **Show these columns in the order** list.

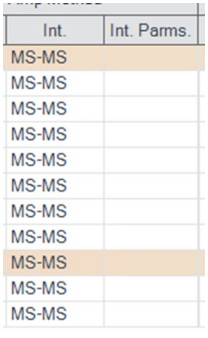
10 Click **OK**.



View the default integration values for amphetamine

1 Click **Previous Compound** in the Batch Table toolbar to view amphetamine (Amp).

2 Examine the default values in the **Int**. and **Int. Parms** columns in the **Batch Table.**



3 Examine the default values in the Int. Metric column in the Batch Table.

Amp Method			Amp Results						
Exp. Conc.	Int.	Int. Parms.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Int. Metric
	MS-MS				☐				
2.5000	MS-MS		2.141	658	☐	2.4161	2.4161	96.6	Accepted
5.0000	MS-MS		2.140	1059	☐	4.8556	4.8556	97.1	Accepted
12.5000	MS-MS		2.134	2673	☐	12.8162	12.8162	102.5	Accepted
25.0000	MS-MS		2.022	4952	☐	25.9394	25.9394	103.8	Accepted
125.0000	MS-MS		2.101	18605	☐	124.0262	124.0262	99.2	Accepted
5.0000	MS-MS		2.142	1006	☐	4.3336	4.3336	86.7	Accepted
25.0000	MS-MS		2.135	4716	☐	26.9911	26.9911	108.0	Accepted
	MS-MS		2.080	6	☐				Rejected
	MS-MS		2.143	1004	☐	4.0008	4.0008		Accepted
	MS-MS		2.105	2590	☐	13.3556	13.3556		Accepted

View integration problems for cocaine and MDMA

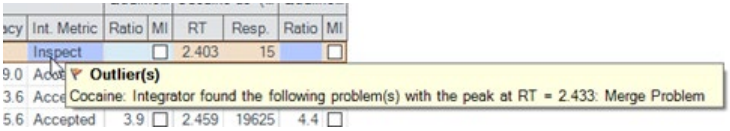
1 Close the Calibration Curve window.

2 Enlarge the chromatogram portion of the Compound Information toolbar so that only the quantifier and qualifier chromatograms appear. Click the Show/Hide Spectrum icon.

3 Also click the Show/Hide ISTD icon.

4 Click the Next Compound icon in the Batch Table toolbar until the system displays the compound b.

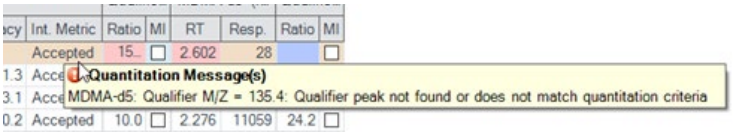
5 Select the Blank-1 row, and mouse over the word Inspect in the Int. Metric column for that row.



The system displays any outlier message for that data, as well as the integrated chromatogram for cocaine.

6 Click the Next Compound icon in the Batch Table Standard toolbar or the Previous Compound icon in the Batch Table Standard toolbar until the system displays the compound MDMA.

7 Select the Blank-1 row and point to the **Int. Metric** column.



The system displays any outlier message for that data, as well as the integrated chromatogram for MDMA.

Change the noise algorithm

1 Right-click anywhere in the **Batch Table** and click **Add/Remove Columns**.

The system displays the Columns dialog box.

2 From the **Select Columns From** drop-down list, select **Compound Method**

3 From the **Available Columns** list, select **Noise Alg**. (Noise Algorithm Type) and click **Add**.

The system moves the selected column to the Show these columns in the order list.

4 Click **OK**.

5 Click the **Previous Compound** icon in the **Batch Table** toolbar until the system displays the compound Amp.

6 Examine the values in the **Noise Alg**. and S/N (**signal-to-noise ratio)** columns.

Batch Table

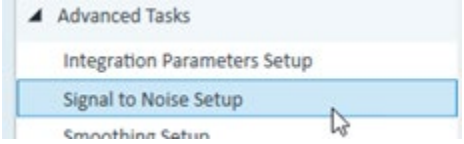
Sample: Blank-1 Sample Type: <All> Compound: Amp ISTD: Amp-d5

Sample						Amp Method				Amp Results							Qualifie...		Amp-d5 (IST...		Qualifie...	
		Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	Int.	Int. Parms.	Noise Alg.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Int. Metric	Ratio	MI	RT	Resp.	Ratio	MI
		Blank-1	CMAMBlk_01.d	Blank		5/12/2006 1:48 PM		MS-MS		RMS													
		Calib-L1	CMAMCal_L1.d	Cal	L1	5/12/2006 1:51 PM	2.5000	MS-MS		RMS	2.141	658		2.4161	2.4161	96.6	Accepted	24.3		2.129	1397	25.9	
		Calib-L2	CMAMCal_L2.d	Cal	L2	5/12/2006 1:54 PM	5.0000	MS-MS		RMS	2.140	1059		4.8556	4.8556	97.1	Accepted	33.5		2.128	1298	25.9	
		Calib-L3	CMAMCal_L3.d	Cal	L3	5/12/2006 1:57 PM	12.5000	MS-MS		RMS	2.134	2673		12.8162	12.8162	102.5	Accepted	26.7		2.121	1377	26.3	
		Calib-L4	CMAMCal_L4.d	Cal	L4	5/12/2006 2:00 PM	25.0000	MS-MS		RMS	2.022	4952		25.9394	25.9394	103.8	Accepted	29.1		1.990	1304	28.8	
		Calib-L5	CMAMCal_L5.d	Cal	L5	5/12/2006 2:03 PM	125.0000	MS-MS		RMS	2.101	18605		124.0262	124.0262	99.2	Accepted	27.0		2.076	1053	26.4	
		QC-L2	CMAMQC_L2.d	QC	L2	5/12/2006 2:06 PM	5.0000	MS-MS		RMS	2.142	1006		4.3336	4.3336	86.7	Accepted	27.7		2.131	1356	31.1	
		QC-L4	CMAMQC_L4.d	QC	L4	5/12/2006 2:09 PM	25.0000	MS-MS		RMS	2.135	4716		26.9911	26.9911	108.0	Accepted	25.6		2.121	1196	31.1	
		Sample-1	CMAMSam_01.d	Sample		5/12/2006 2:12 PM		MS-MS		RMS	2.080	6					Rejected						
		Sample-2	CMAMSam_02.d	Sample		5/12/2006 2:15 PM		MS-MS		RMS	2.143	1004		4.0008	4.0008		Accepted	30.9		2.130	1445	25.7	
		Sample-3	CMAMSam_03.d	Sample		5/12/2006 2:18 PM		MS-MS		RMS	2.105	2590		13.3556	13.3556		Accepted	25.3		2.089	1284	29.8	

Practice changing the noise algorithm from RSM to ASTM for amphetamine in the method

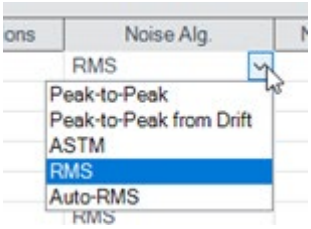
1 On the **Method** tab, click **Edit**.

2 In the **Method Tasks** column, click **Advanced Tasks** > **Signal to Noise Setup**.



The system displays the integrator parameters in the Method Table.

3 In the Method Table, click the drop-down arrow in the Noise Alg. column for Amp.



A list of available noise algorithms appears.

4 Click ASTM.

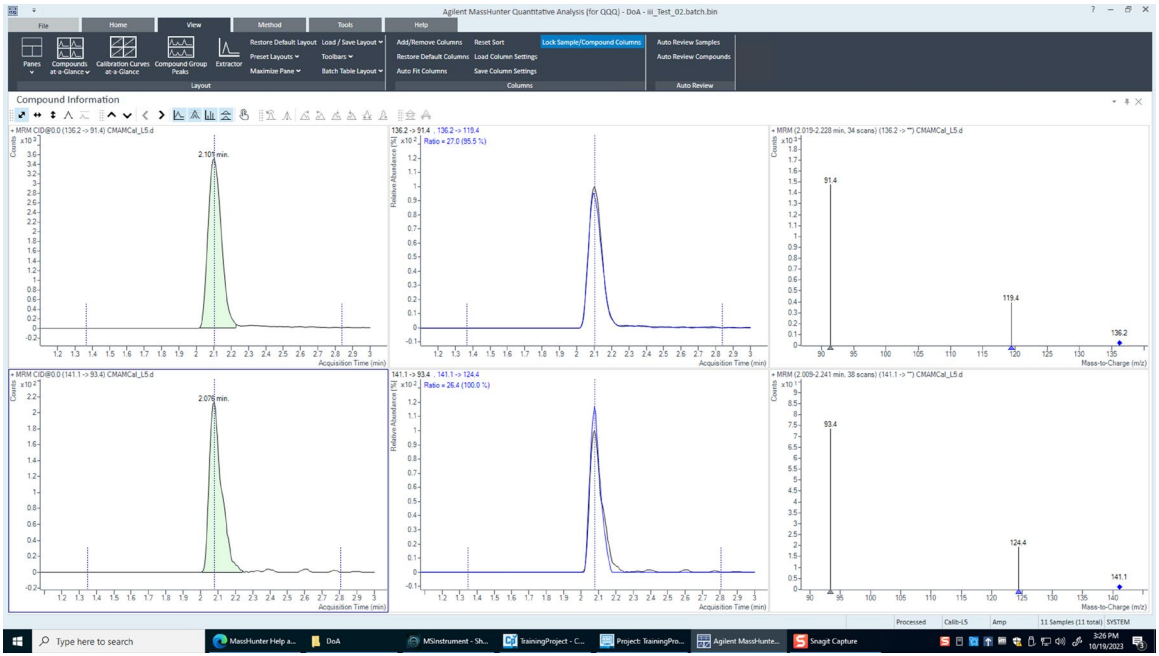
5 Under Method Tasks/Save/Exit, click Exit.

6 At the Would you like to apply this method to the batch? prompt, click No. The system displays Batch Analysis mode.

Turn off the baseline (highest concentration standard) and then back on for amphetamine

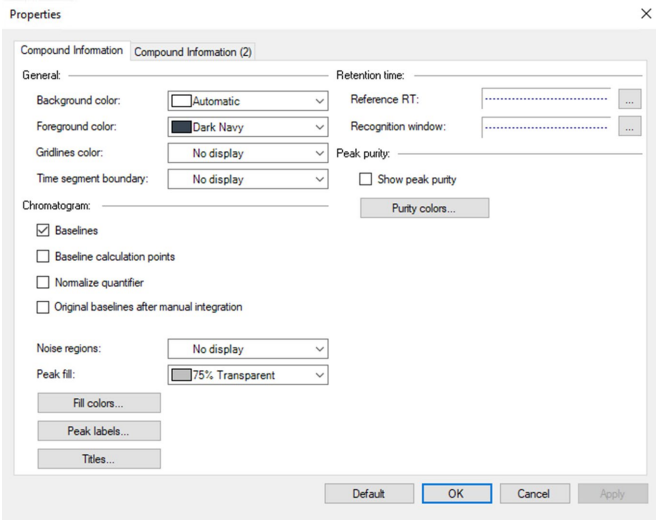
1 Select sample Calib-L5 (if it is not already selected), and on the View tab, select Maximize Pane > Maximize Compound Information.

Make sure that only the Compound Information pane is visible in the window.



2 Right-click either of the chromatograms to open the shortcut menu.

3 Click Properties at the bottom of the shortcut menu to open the Properties dialog box.



4 Clear the **Baselines** check box in the Properties dialog box.

5 Click the Apply button and observe the peak without the baseline.

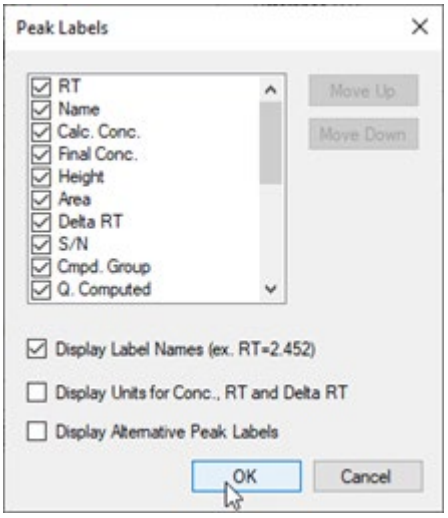
Inspect the calculation points for the baseline for amphetamine

1 Mark the Baselines check box in the Properties dialog box.
2 Click the Apply button and observe the peak with the baseline drawn.
3 Mark the Baseline Calculation Points check box in the Properties dialog box.
4 Click Apply and observe where the baseline starts and stops.
5 Clear the Baseline Calculation Points check box in the Properties dialog box.
6 Click Apply and observe the chromatograms.
7 Compare the chromatograms with and without the Baseline Calculation Points.

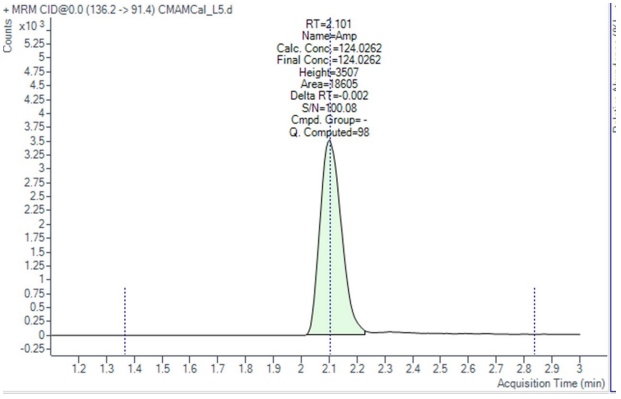
Display the peak labels for amphetamine

1 From the Properties dialog box, click Peak Labels. The system displays the Peak Label dialog box.
2 Mark all the Peak Labels check boxes, and the Display Label Names check box.

3 Click **OK**.



4 Click the **Apply** button in the Properties dialog box. The peak labels should now match those shown in the example below.



5 Click **Peak Labels** in the Properties dialog box. The system displays the Peak Labels dialog box.

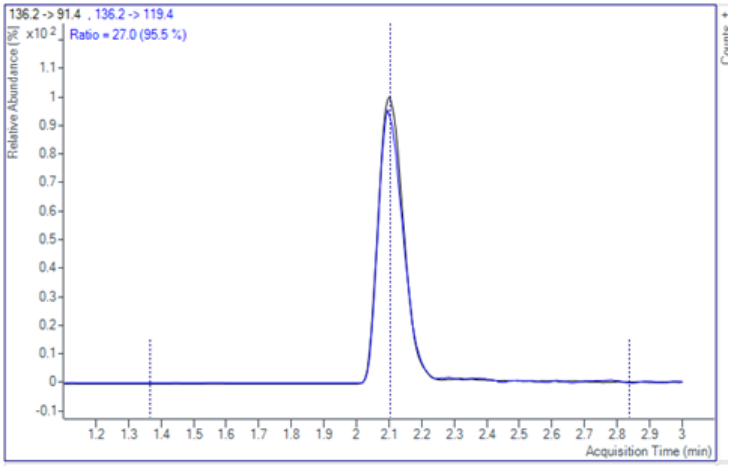
6 Clear all the **Peak Labels** check boxes except RT (retention time). Clear the **Display Label Names** check box and click **OK**.

7 Click **Apply** in the Properties dialog box and observe the change in Peak Labels.

Display the qualifier chromatogram on the right-side before and after normalization

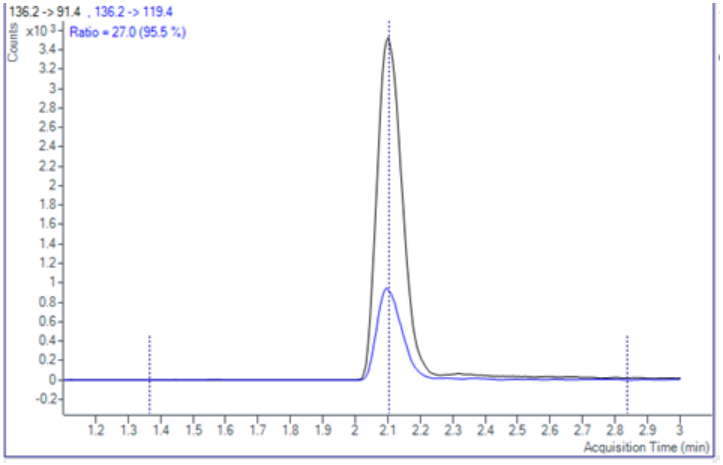
1 Click the Compound Information (2) tab. In the Qualifiers area, mark the Normalize check box.

2 Click Apply and observe that the two peaks now converge and appear as one peak.



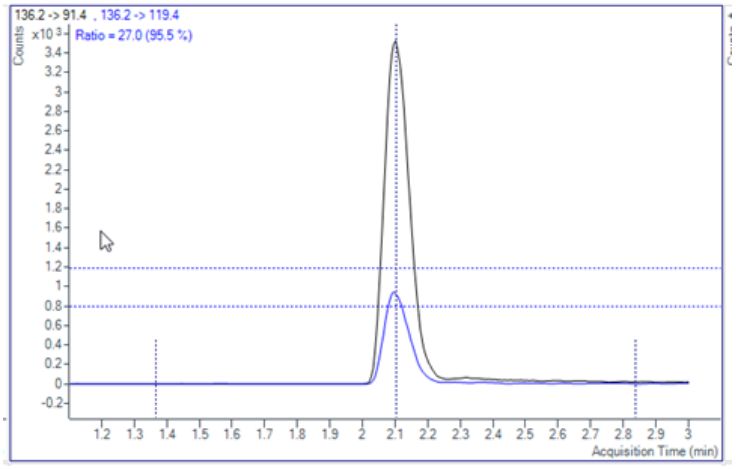
3 Clear the Normalize Qualifiers check box of the Properties dialog box.

4 Click Apply to display the qualifier second quantifier peaks again.



View the uncertainty band

1 Select the type of uncertainty band that you would like to display from the drop-down menu in the **Uncertainty Band** field of the Properties dialog box. Click Apply and the uncertainty band appears in the qualifier chromatogram.



2 Select **No** display from the **Uncertainty Band** drop-down menu of the Properties dialog box. Click **Apply** to remove the uncertainty band from the qualifier chromatogram.

3 Click **OK** to close the Properties dialog box.

4 Compare the qualifier chromatogram with and without the **Uncertainty band**.

Remove the Int. and Int. Parms columns from the Batch Table

1 On the **View** tab, click Restore Default Layout.

2 Right-click the **Compound Method** section of the Batch Table and click **Add/Remove Columns**.

3 From the right list, select **Int. and Int. Parms. (Compound Methods.)**

4 Click **Remove**, and then **OK.**

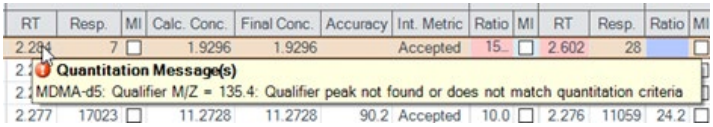
Detect Outliers

This task shows you how to fine-tune the accuracy range for a compound and hide and show results with outlier flags.

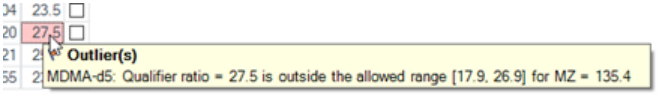
View outlier information for MDMA

1 Click **Next Compound** in the Batch Table toolbar until the system displays the compound MDMA.

2 Select the **Blank-1** row and point the cursor to the RT column.



3 Examine the outlier information in the Qualifier ... Results > Ratio column for Sample 1, as shown in the example below.



Change the accuracy range for amphetamine in the method, and reanalyze the batch

1 Click the **Previous Compound** icon in the toolbar until the system displays the compound Amp.

2 Select the **Calib-L5** row in the table.

3 On the **Method** tab, click **Edit**.

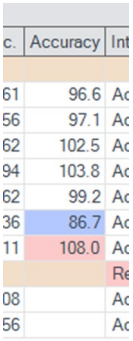
4 In the **Method Tasks** column, click **Outlier Setup Tasks > Accuracy**.

5 Set the **Accuracy Max % Dev** value to *5%* for Amp.

6 In the **Method Tasks** column, click **Save/Exit** > **Exit**, then select None under Additional batch processing after applying the method, and click **Yes** to the Would you like to apply this method to the batch? prompt.

7 Press **F5** to analyze the batch.

8 Red (high) and blue (low) outlier values now appear in the Accuracy column for Amp.



c.	Accuracy	Int
61	96.6	Ac
56	97.1	Ac
62	102.5	Ac
94	103.8	Ac
62	99.2	Ac
36	86.7	Ac
11	108.0	Ac
		Re
08		Ac
56		Ac

Using the following set of outlier flag icons

1 Click the **Display rows that have High outliers** icon on the toolbar to display only samples with high outliers.

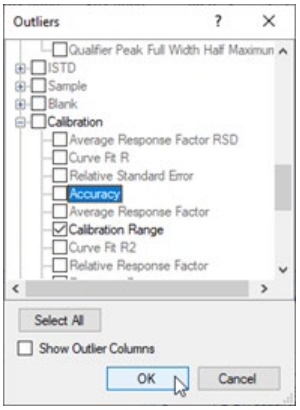
2 Click the **Turn off outlier filter** icon to display all samples.

3 Click the **Display rows that have High/Low outliers** icon on the toolbar to display only samples with low outliers.

4 Click the **Display rows that have High/Low outliers** icon again to display all the samples.

5 Click the **Select Outliers** icon to bring up the Outliers dialog box.

6 Clear the **Accuracy** and **Retention Time** check boxes and click **OK**.



7 Click the **Select Outliers** icon to bring up the Outliers dialog box.

8 Mark the **Accuracy** and **Retention Time** check boxes, and click **OK**

Generate Quantitation Reports

This exercise helps you learn how to do these tasks:

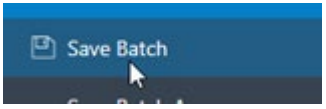
- Generate report methods using one or more report templates
- Generate a report

The DrugsOfAbuse batch is used in this exercise.

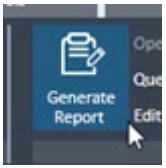
Quantitate the samples for this batch and save your results

1 On the **Home** tab, click **Analyze Batch**.

2 Click **File > Save** to save the batch.



3 On the **Home** tab, click **Generate Report**. The system displays the Generate Report dialog box.

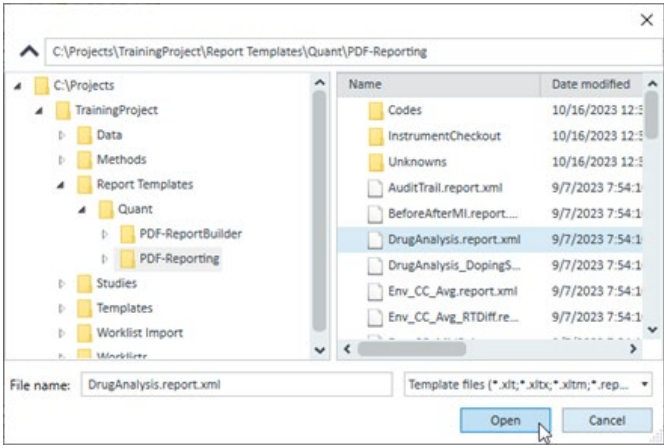


Note the Report Folder directory, which is where the report is saved.

4 Under the Report Method field, click the **New** button to create a report method.

5 Click the **Add Template button** in the Report Method Edit dialog box to open the browser.

6 Navigate to the MassHunter/Report Templates/Quant/PDF-Reporting directory, select DrugAnalysis.report.xml, then click Open.



The program adds the template to the Template field in the Report Method Edit pane.

7 Repeat steps d and e to add DrugAnalysis_DopingScreening.report.xml.

Edit the report method to create single sample and batch PDF reports

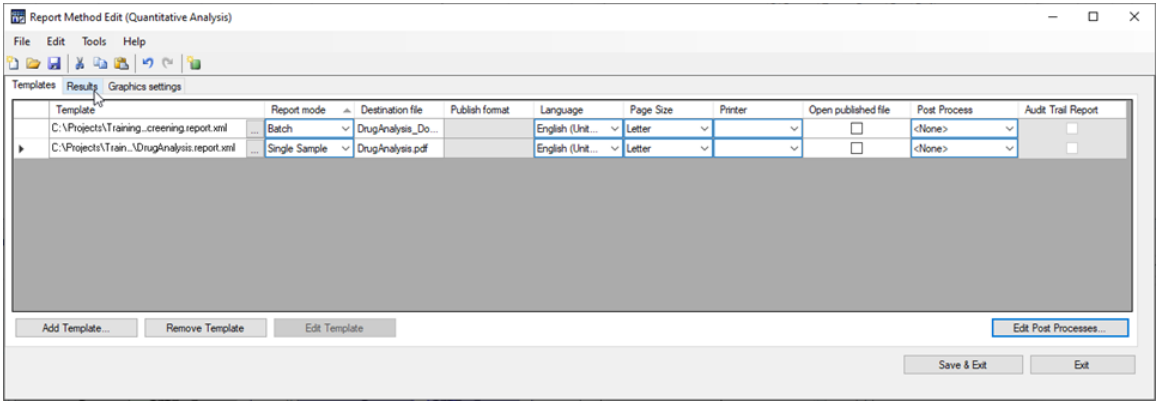
1 In the Report Method Edit dialog box, on the DrugAnalysis.report template line, Report Mode field, select Single Sample from the drop-down menu.

2 On the DrugAnalysis _Doping Screening.report template line, select Batch from the drop-down menu in the Report Mode field.

3 Select your language from the drop-down menu in the Language field.

4 Select a paper size from the drop-down menu in the Paper Size field.

5 Select the Results tab of the Report Method Edit window.

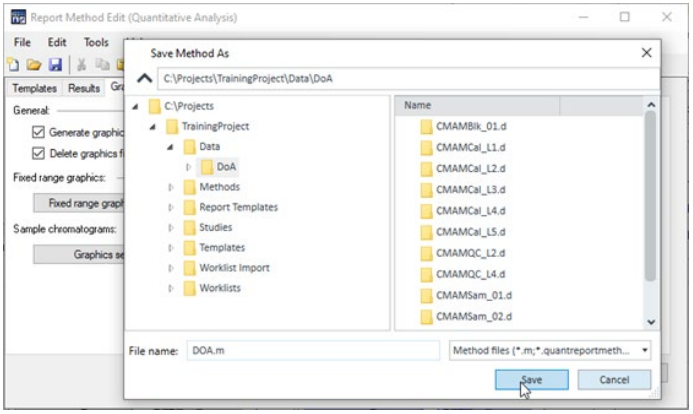


6 Leave the default settings for the rest of the graphic setting fields.

7 Click the save icon in the Report Method Edit window.

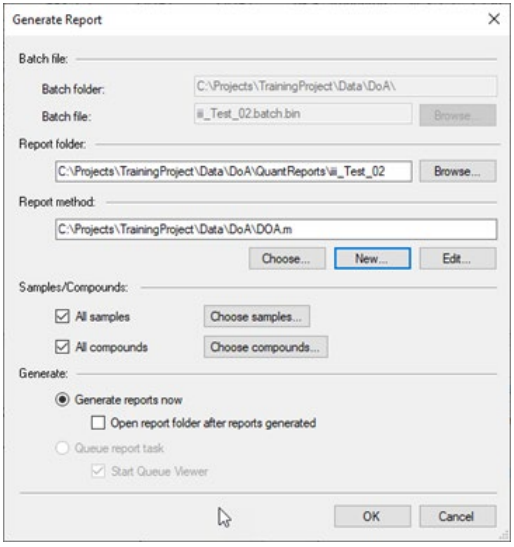
8 Name the report method DOA.m.

9 Click Save & Exit to close the Report Method Edit dialog box to return to the Generate Report window.



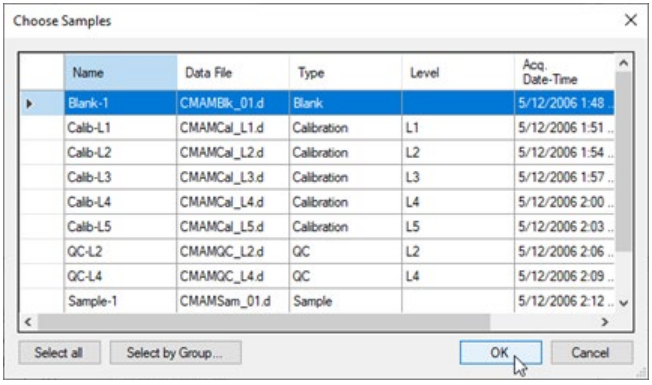
Generate a report from the method

1 Verify that the method you just created is in the **Report Method** field.

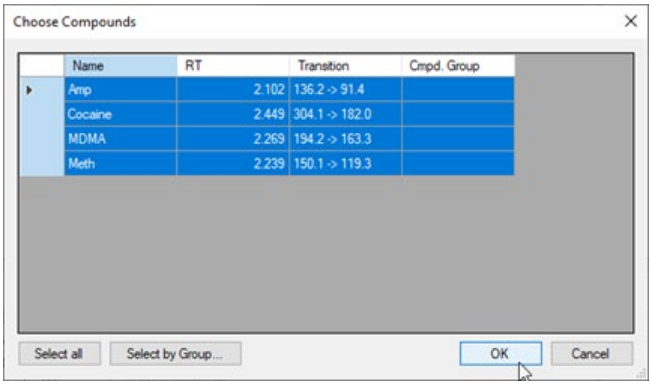


2 In the **Samples/Compounds** field, uncheck **All Samples**, to open the batch table.

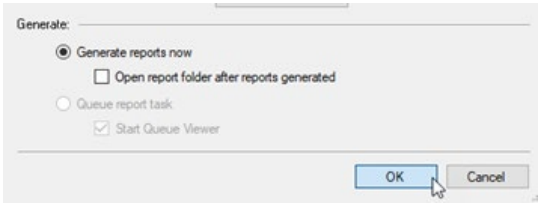
3 Highlight one of the samples in the batch table window and click **OK**.



4 Click **All Compounds** to show all the compounds in the sample you've selected.



5 Select Generate reports now and click OK to generate the report. Double-click a file to open and display the report.



6 Double-click a file to open and display the report.

8 Maintenance

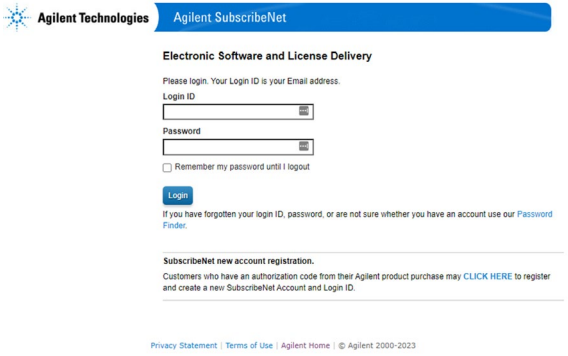
Instrument Maintenance

Register on Agilent SubscribeNet (New Account Registration)

NOTE

If you already have a SubscribeNet account set up for previously purchased Agilent products, it is not necessary to set up additional accounts.

1 Using a web browser, navigate to https://agilent.subscribenet.com/ The site loads.



2 Click the CLICK HERE link to register.

3 Enter the following required information to create the account, along with the authorization code received from the product purchase.

- **a** Authorization Code
- **b** Email
- **c** Company
- **d** Department
- **e** First Name
- **f** Last name
- **g** Phone
- **h** Address
- **i** City State/Province
- **j** Country

4 Click Submit.

You'll receive an email to start your account.

Perform Back Up and Platform Best Practices

- ☐ Safely store the software media provided for the system.
- ☐ Set up Data/Computer image backup regularly.
  - Microsoft Back up and Restore Options (https://t.ly/r2995)
- ☐ Disable power management options and automatic utilities.
  - Set power options to Put the computer to sleep = Never
  - Set Windows Update to "Check for updates but let me choose whether to download and install them."
- ☐ Turn on Windows Firewall.
  - Select the "Notify me when Windows Firewall block a new program." check box.

Locate the tune solution bottle and properly store tune solution

Locate the tune solution bottle and confirm that it is safely stored in the appropriate temperature conditions.

Perform daily cleaning of Ionization Source and Spray Chamber

Perform this maintenance daily or at the end of each shift or anytime you suspect carry over contamination from one sample or analysis to another.

After determining the Source type, find the instructions for cleaning in the user guide for the source in use.

Review routine procedures in the user guide

Perform maintenance daily or at the end of each shift or anytime you suspect carry over contamination from one sample or analysis to another.

Remove, clean, and replace the capillary

Review the steps in the user guide.

Add a new user defined EMF counter

Using the online help, set up a user defined EMF counter by entering a new threshold value for a selected EMF item.

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