Software User Guide

Analyst Software

RUO-IDV-05-13401-B

April 2025

Contents

Introduction

This guide is for operators who are new to the Analyst software. Use the procedures to learn how to use the software and the mass spectrometer.

WARNING! Personal Injury Hazard. Do not move the system. Risk of personal injury or instrument damage. If you need to move the system, contact a SCIEX FSE to assist you.

Hardware Profiles and Projects 1

Hardware Profiles

A hardware profile tells the software how the mass spectrometer and the devices are configured and connected to the computer. Multiple hardware profiles can be configured, but only one profile can be active at any time.

When a hardware profile is created in the Hardware Configuration Editor, the peripheral devices must be configured so that the software can communicate with them. These procedures are used to configure the peripheral devices:

- Make the physical connections. For information about making the physical connections to the devices, refer to the document: *Peripheral Devices Setup Guide*.
- Configure the software to communicate with the peripheral devices. For a list of the supported devices, refer to the Analyst software document: *Software Installation Guide*.

When the software is installed, the driver required for each peripheral device is also installed. After the peripheral devices are physically connected to the computer, configure the appropriate configuration information.

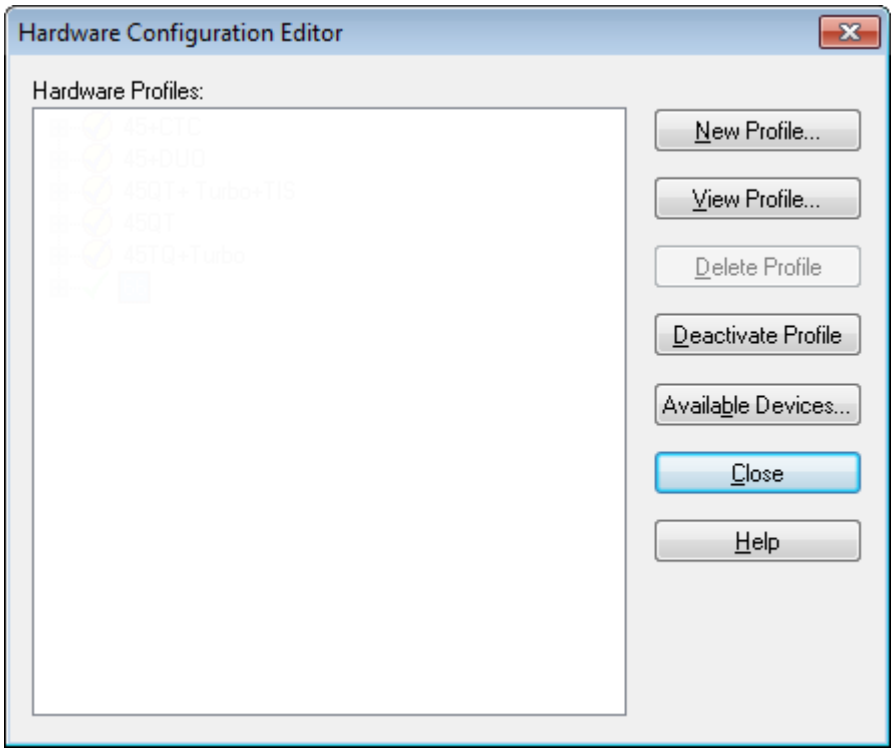
Each hardware profile must include a mass spectrometer. Before an acquisition method, is created make sure that all devices to be used in the method are included in the hardware profile. The devices configured in the active hardware profile and selected in the Add/Remove Device Method dialog are shown as icons in the Acquisition method pane. Only peripheral devices included in the active hardware profile can be used to create acquisition methods.

Create a Hardware Profile

The user can create multiple hardware profiles, but only one profile can be active at any time.

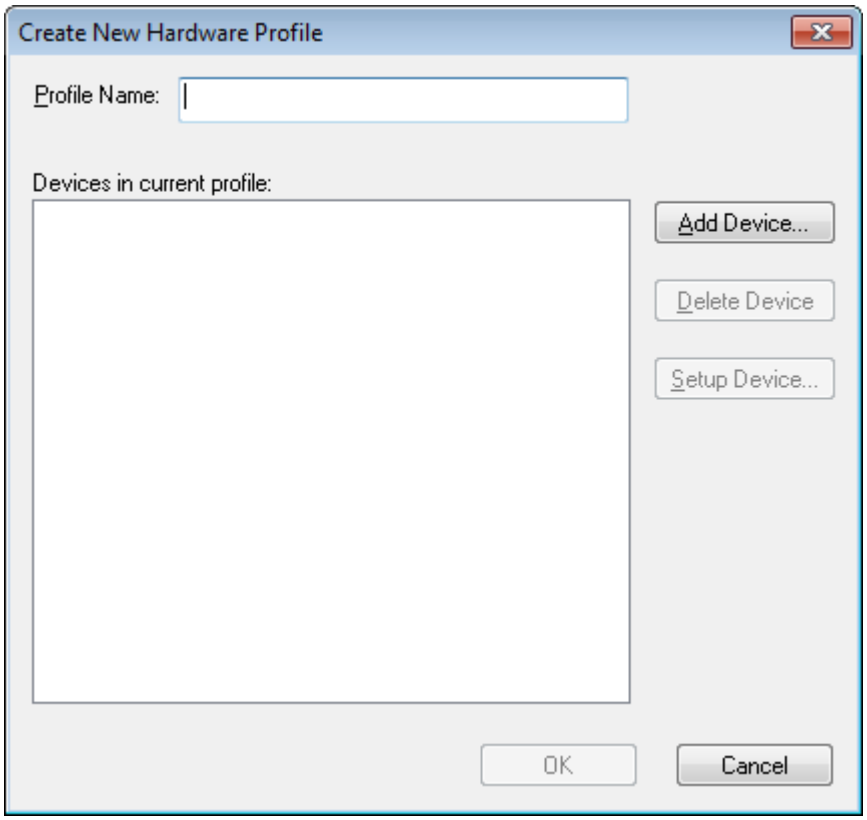
1. On the Navigation bar, under **Configure**, double-click **Hardware Configuration**.

Figure 1-1 Hardware Configuration Editor Dialog



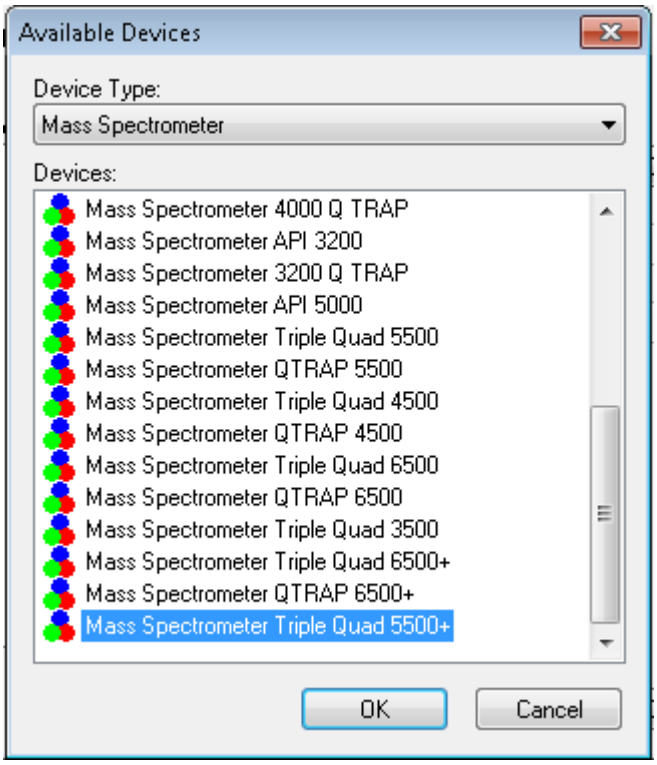
2. Click **New Profile**.

Figure 1-2 Create New Hardware Profile Dialog



3. Type a name in the **Profile Name** field.
4. Click **Add Device**.

Figure 1-3 Available Devices Dialog



In the Available Devices dialog, **Mass Spectrometer** is the preset value for the **Device Type** field.

5. In the **Devices** list, select the appropriate mass spectrometer and then click **OK**.
6. On the Create New Hardware Profile dialog, click **Setup Device**.
   For SCIEX 5500+ systems, the QTRAP License information is shown at the bottom of the dialog. If a QTRAP license was purchased, then the Linear Ion Trap features are enabled.

Figure 1-4 Linear Ion Trap Features Enabled

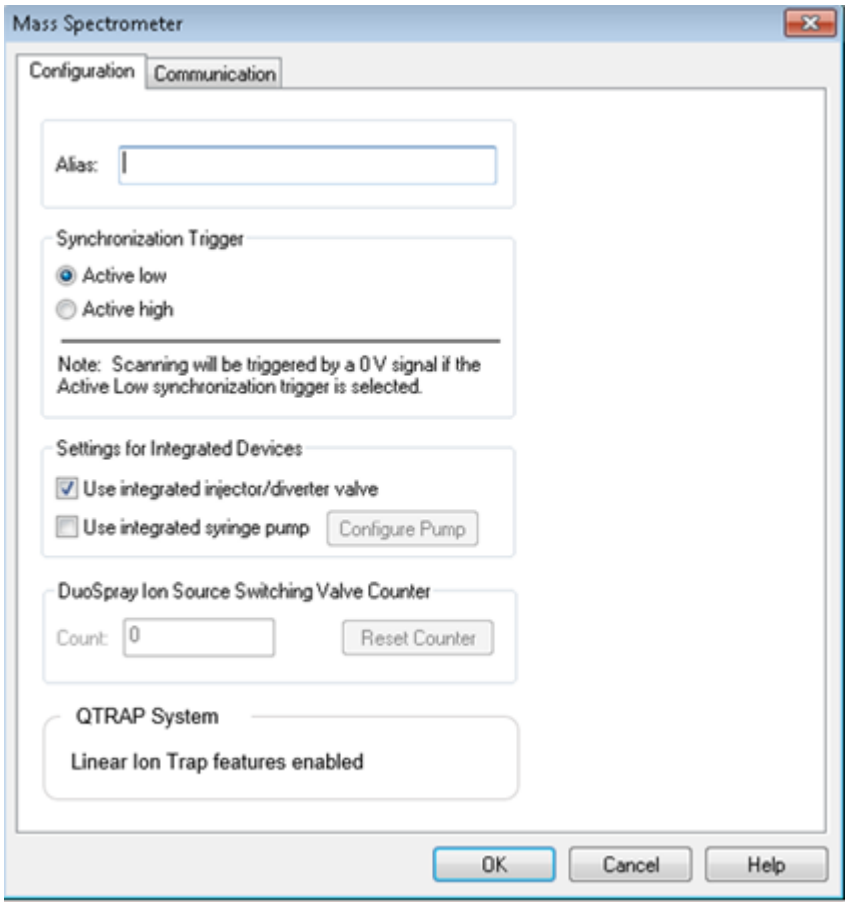
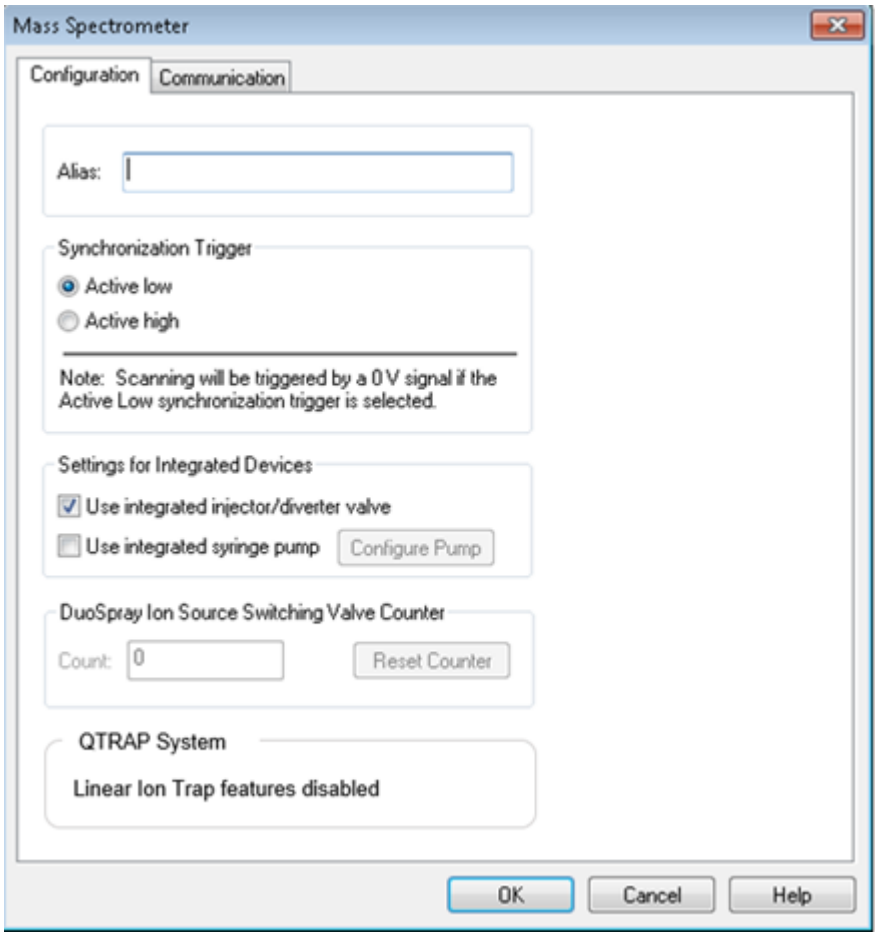


Figure 1-5 Linear Ion Trap Features Disabled



7. (Only available for the SCIEX 6500 systems and SCIEX 6500+ systems) On the Configuration tab, in the Dual Mass Mode section, select one of the following options:

   - **Low Mass:** To operate in limited mass range, high sensitivity operating mode, select this option. The mass range is 50 Da to 1000 Da for LIT scans and 5 Da to 1250 Da for quadrupole scans.
   - **High Mass:** To operate in extended mass range operating mode, select this option. The mass range is 50 Da to 2000 Da for LIT scans and 5 Da to 2000 Da for quadrupole scans.

   Select one of the following two options for triple quadrupole systems:

   - **Low Mass**: To operate in limited mass range, high sensitivity operating mode, select this option. The mass range is 5 Da to 1250 Da.
   - **High Mass**: To operate in extended mass range operating mode, select this option. The mass range is 5 Da to 2000 Da.

8. (Optional) To configure mass spectrometers that use the integrated syringe pump, on the Configuration tab, select the **Use integrated syringe pump** check box.
9. (Optional) To configure the mass spectrometer for the diverter valve, on the Configuration tab, select **Use integrated injector/diverter valve**.
10. (Optional) Select additional features on the Configuration and Communication tabs as required.
11. Click **OK**.
12. On the Create New Hardware Profile dialog, click **Add Device** and then add and set up each device that is used with the mass spectrometer. Refer to the section: Add Devices to a Hardware Profile.
13. Click **OK** in the Create New Hardware Profile dialog.
14. Click the hardware profile to be activated in the Hardware Configuration Editor.
15. Click **Activate Profile**.
    The check mark turns green. If a red × is shown, then there is an issue with the hardware profile activation.

    Tip! A hardware profile need not be deactivated before another is activated. Click a hardware profile and then click **Activate Profile**. The active profile is deactivated automatically.
16. Click **Close**.

    Note: SCIEX 6500 systems and SCIEX 6500+ systems: The current operating mode of the active hardware profile can be viewed in the Detailed Status dialog for the instrument by double-clicking the Mass Spec icon on the lower-right section in the Analyst software window.

Add Devices to a Hardware Profile

Devices must be configured to enable the software to communicate with them. When the software is installed, the driver required for each device is also installed. Before devices can be configured, they must be physically connected to the computer. For more information, refer to the document: *Peripheral Devices Setup Guide*.

Only the devices configured in the active hardware profile and selected in the Add/Remove Device Method dialog are shown as icons in the Acquisition Method Browser pane.

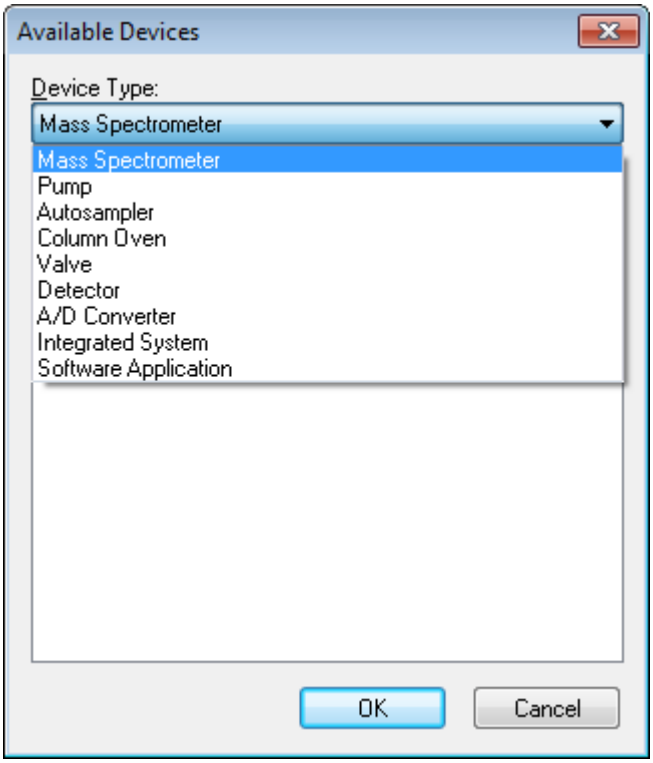
1. Open the Hardware Configuration Editor.
2. In the **Hardware Profiles** list, deactivate the hardware profile.
3. Click **Edit Profile**.
4. Click **Add Device**.

Note: Remember to add a mass spectrometer. For more information, refer to the section: Create a Hardware Profile.

The Available Devices dialog opens.

5. In the **Device Type** list, select the device and then click **OK**.

Figure 1-6 Available Devices Dialog



6. Click **OK**.
7. Select the device from the **Devices** list and then click **OK**.
8. Click **Setup Device**.
   A dialog containing configuration values for the device opens.
9. (Optional) On the Communication tab, in the **Alias** field, type a name or other identifier for the device.

Note: For devices using serial communication, make sure that the serial port selected matches the serial port to which the device is physically connected. When the serial expansion cable is used, the number selected in the profile is the number on the cable plus two.

Note: The **Alias** field might also be referred to as the **Name** box and might be found on another tab under **Alias**.

- If the device uses a **Serial Port** as a communication interface, then in the **COM Port Number** list, select the COM port to which the device is connected.
- If the device uses **Ethernet** as a communication interface, then type the **IP Address** assigned to the device by the administrator or use the corresponding **Host Name** for the address.
- If the device uses **GPIB Board** as a communication interface, then do not change the settings for the GPIB board.

The rest of the preset values for the device are probably appropriate. Do not change them.

10. To restore the device preset values, on the Communication tab, click **Set Defaults**.
11. To save the configuration, click **OK**.
12. Repeat step 4 to step 11 for each device.
13. Click **OK** in the Create New Hardware Profile dialog.
14. To activate the hardware profile, do this:
    a. In the Hardware Configuration Editor, click the hardware profile.
    b. Click **Activate Profile**.

    The check mark turns green. If a red × is shown, then there is an issue with the hardware profile activation. For more information, refer to the section: Troubleshoot Hardware Profile Activation.

    Tip! An active hardware profile does not have to be deactivated before another one is activated. Click an inactive hardware profile and then click **Activate Profile**. The other profile is deactivated automatically.
15. Click **Close**.

Troubleshoot Hardware Profile Activation

If a hardware profile fails to become active, then a dialog opens indicating which device in the profile failed to activate. A device might fail to activate because of communications errors.

1. Read the error message generated. Depending on the message, there might be an issue with a device or how the communication is set up.
2. Make sure that the device is connected to the mains supply and is turned on.
3. Make sure that the COM port or IP address assigned to the device is correct.

Tip! On computers with two built-in serial ports, the first port on the serial port expansion card is usually COM3, even though the cable indicates P1.

4. Make sure that the communication settings for the device, for example, the dual inline package (DIP) switch settings, are set correctly and match the settings on the Communication tab.
5. Turn off the device.
6. Wait 10 seconds.
7. Turn on the device.
   Wait until all of the device power-up activities are complete before trying to activate the hardware profile again. Some devices might require 30 seconds or more to complete the power-up activities.
8. Activate the hardware profile.
9. If the issue persists, then delete the failing profile and create a new one.
10. If the issue still persists, then go to sciex.com/request-support.

Projects and Subprojects

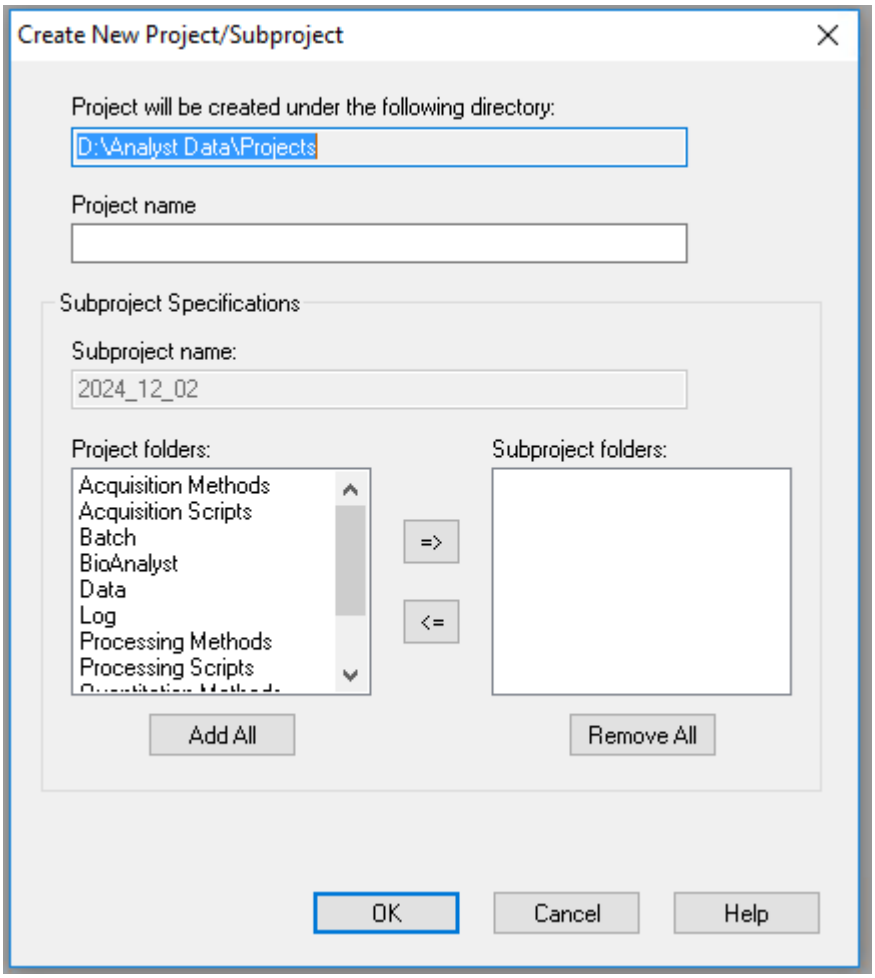
Before beginning an experiment, decide where to store the files related to the experiment. Use projects and subprojects for each experiment to better manage data and compare results. For example, use subprojects to store the results for specific dates.

Create Projects and Subprojects

To use a subproject structure within a project, create the subproject structure when the project is created.

1. Click **Tools** > **Project** > **Create Project.**

Figure 1-7 Create New Project/Subproject Dialog



Note: A new subproject cannot be created for a project that was not originally created with a subproject.

2. Type a project name in the **Project name** field.
3. (Optional) To use subprojects, do this:
   a. Select the required folders and then use the arrow buttons to move them to the **Subproject folders** list.
   b. In the **Subproject name** field, type a name for the first subproject or use the existing date.
4. Click **OK**.

Create Subprojects

Subprojects can only be created in a project that has an existing subproject structure.

1. On the **Project** tool bar, from the **Project** list, select the project.
2. Click **Tools** > **Project** > **Create Subproject.**
3. In the **Subproject name** box, type a name for the subproject or use the existing date.
4. Click **OK**.

Copy Subprojects

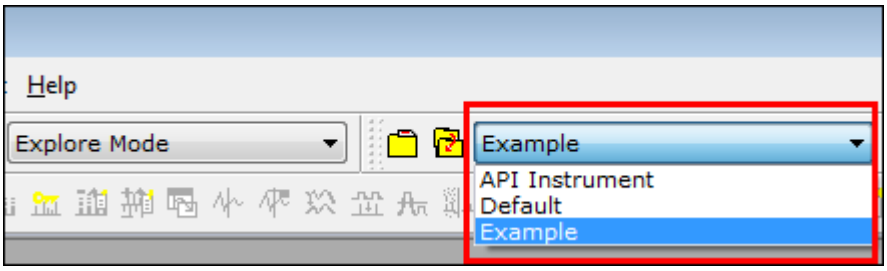
A subproject can be copied from another project that has existing subprojects. If the copied subprojects contain folders that also exist in the destination project folder, then the software uses the project level folders.

1. Click **Tools** > **Project > Copy Subproject.**
   The Copy Subproject dialog opens.
2. Click **Browse** to browse to the subproject source.
3. Click **OK**.
4. Select the subproject from the **Source Subproject** list.
5. Click **Browse** to browse to the subproject destination.
6. Type the name in the **Target Subproject** field.
7. Click **OK**.
8. Do one of the following:
   - To copy all folders and files from the **Subproject Source** into the **Subproject Destination**, select the **Copy Contents** check box.
   - To copy only the folders in the same structure into the **Subproject Destination**, make sure that the **Copy Contents** check box is cleared.
9. Click **Copy**.

Change Between Projects and Subprojects

- On the software tool bar, from the project list, click the required project or subproject.

Figure 1-8 Project List



The project list in this figure shows the **API Instrument**, **Default**, and **Example** folders.

Installed Project Folders

Three project folders are installed with the software: **`API Instrument`**, **`Default`**, and **`Example`**.

API Instrument Folder

The API Instrument folder is unique and very important to the correct functioning of the mass spectrometer. The API Instrument folder contains the information required for tuning and calibrating the mass spectrometer. This information includes:

- Parameter settings files
- Reference files
- Instrument data files that contain calibration and resolution information
- Acquisition methods used during automatic tuning

The API Instrument folder also contains data files for manual tuning runs that were performed using the **Start** button rather than the **Acquire** button. These data files are saved automatically in the `API Instrument\Tuning Cache` folder and named with the date and time that they were created. The Tuning Cache folder is automatically cleared periodically.

Default Folder

The Default folder contains folders that are present in new projects and serves as a template for new projects.

Example Folder

The Example folder contains sample methods and data files. Users can practice working with the Explore or Quantitate modes using the example data files. The example files are sorted into subfolders by mass spectrometer type and application area.

Back Up the API Instrument Folder

Back up the `API Instrument` folder regularly and after routine maintenance has been performed.

- Copy the `API Instrument` folder, paste it to a different location, preferably on another computer, and then rename the folder. Use the date and a mass spectrometer reference when naming the folder, if there is more than one mass spectrometer. For example, API Instrument_QT6500plus3_010121.

Recover the API Instrument Folder

Back up the `API Instrument` folder regularly and after routine maintenance has been performed.

1. Rename the current `API Instrument` folder.
2. Copy the backup folder into the `Projects` folder.
3. Change the name of the backup folder to `API Instrument`.

Tune and Calibrate 2

Run the **Verify instrument performance** option weekly or after the mass spectrometer is cleaned to confirm that the system is working properly. For triple quadrupole systems, calibration and resolution is usually maintained for three to six months unless the system loses vacuum. For QTRAP systems, the resolution should also be maintained for three to six months, but the system should be calibrated approximately monthly. If the system loses vacuum, then verify the calibration and resolution before using the system. For more information about tuning and calibration, refer to the documents: *Advanced User Guide* and the *Manual Tuning Tutorial*.

Tip! Perform maintenance tasks regularly to make sure that the mass spectrometer is performing optimally.

Prerequisites
• The spray is stable and the correct tuning solution is being used. • A printer is configured.

Required Materials
• Tuning solutions that are supplied in the Standards Chemical Kit shipped with the system. If required, a new kit can be ordered from SCIEX. • 5 mL, 1 mL, and 250 µL serial gas-tight syringes. (1 mL will be used as reference) • Red PEEK sample tubing. • (Optional) Syringe pump, if using a system without an integrated syringe pump.

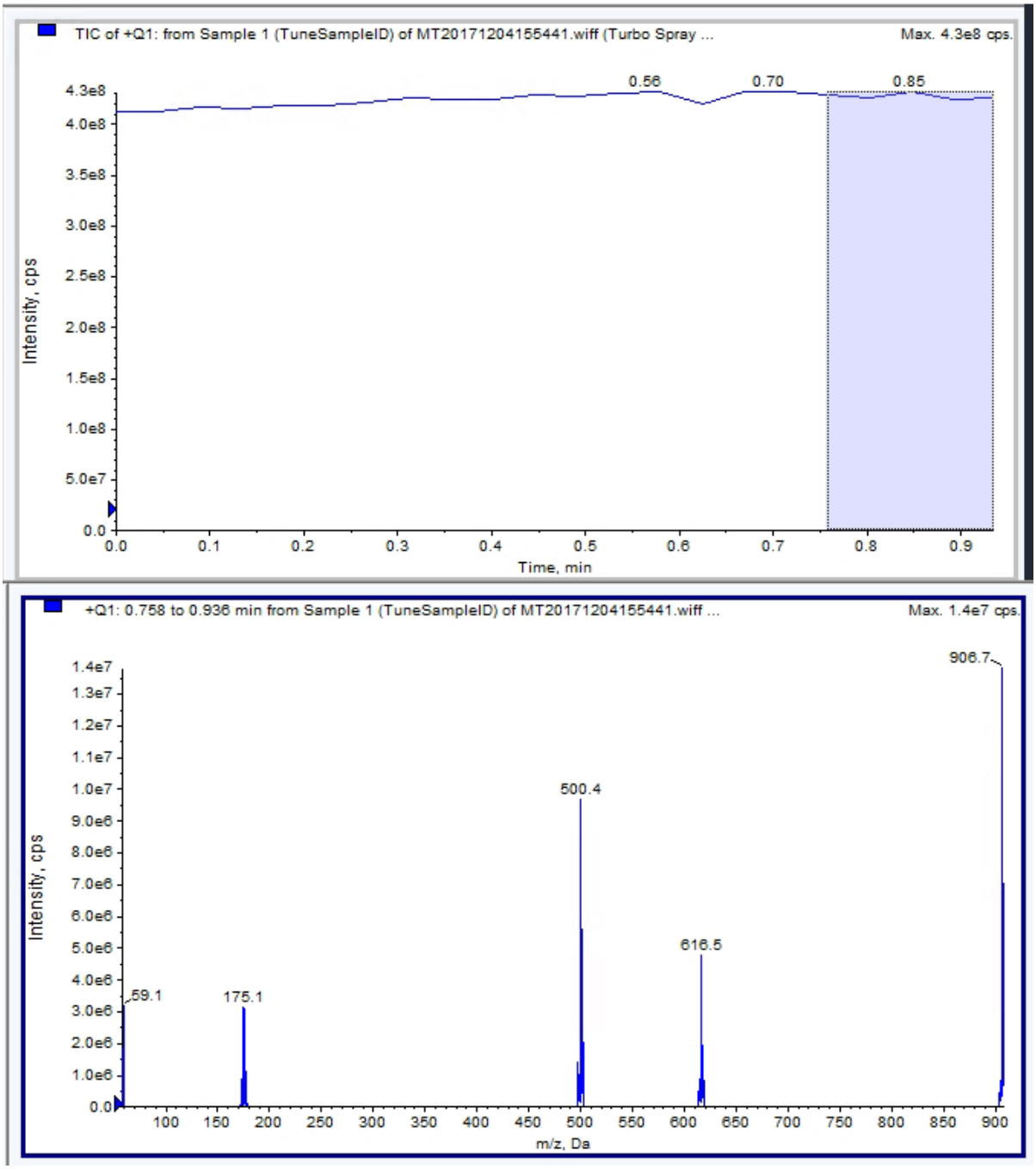
Verify Instrument Performance

Use this procedure to verify or adjust the performance of the mass spectrometer. For information about using the other instrument performance options, refer to the document: *Help*.

Prerequisites
• The syringe pump is activated in the hardware profile. If the syringe pump is not activated, then edit the hardware profile. Refer to the section: Add Devices to a Hardware Profile. • The API Instrument folder is selected.

1. On the Navigation bar, under **Tune and Calibrate**, double-click **Manual Tuning**.
2. Start the syringe pump, type **5** in the **Duration** field, and then run a calibration method. Confirm that the total ion chromatogram (TIC) is stable and that the peaks of interest are present in the spectrum.

Figure 2-1 Example of a Stable TIC and Peaks of Interest



3. On the Navigation bar, under **Tune and Calibrate**, double-click **Instrument Optimization**. The Instrument Optimization dialog opens.
4. Click **Verify instrument performance**.

5. Click **Next**.
6. Click **Approved Tuning**.
7. Click **Next**.
8. Select a **Tuning Solution** from the list.
   Depending on the solution selected, different modes are available:
   a. Click a polarity.
   b. (If available) Click **Q1** and **Q3** in the Quad section.
   c. (If available) Click the required scan speeds.
   d. (If available) Click the scan speeds in the LIT section.
   e. (If available) Click **Excitation** in the MS/MS/MS section
9. Click **Next**.
10. If the Select a mode page opens, then select **Automatic**.
11. Click **Next**.
12. Click **GO**.
    The Verifying or Adjusting Performance dialog opens. After the process has completed, the Results Summary opens. For more information, refer to the document: *Help*.
13. (If applicable, depending on the options selected) When prompted, change solutions for different scan types and polarities.

Verifying or Adjusting Performance Dialog

The top left corner shows the part of the instrument that is being tuned.

The Current Spectrum graph shows the spectrum of the current scan, the optimal scan selected by the software, or the scan at the current parameter value when the software results are viewed in interactive mode.

The Instrument Optimization Decision Plots, in the top right graph, dynamically show the intensity versus voltage curves of the parameters that are currently being optimized.

Results Summary

The Results Summary is a record of any instrument settings changes that were made by the Instrument Optimization wizard.

Figure 2-2 Results Summary: SCIEX Triple Quad 3500 System

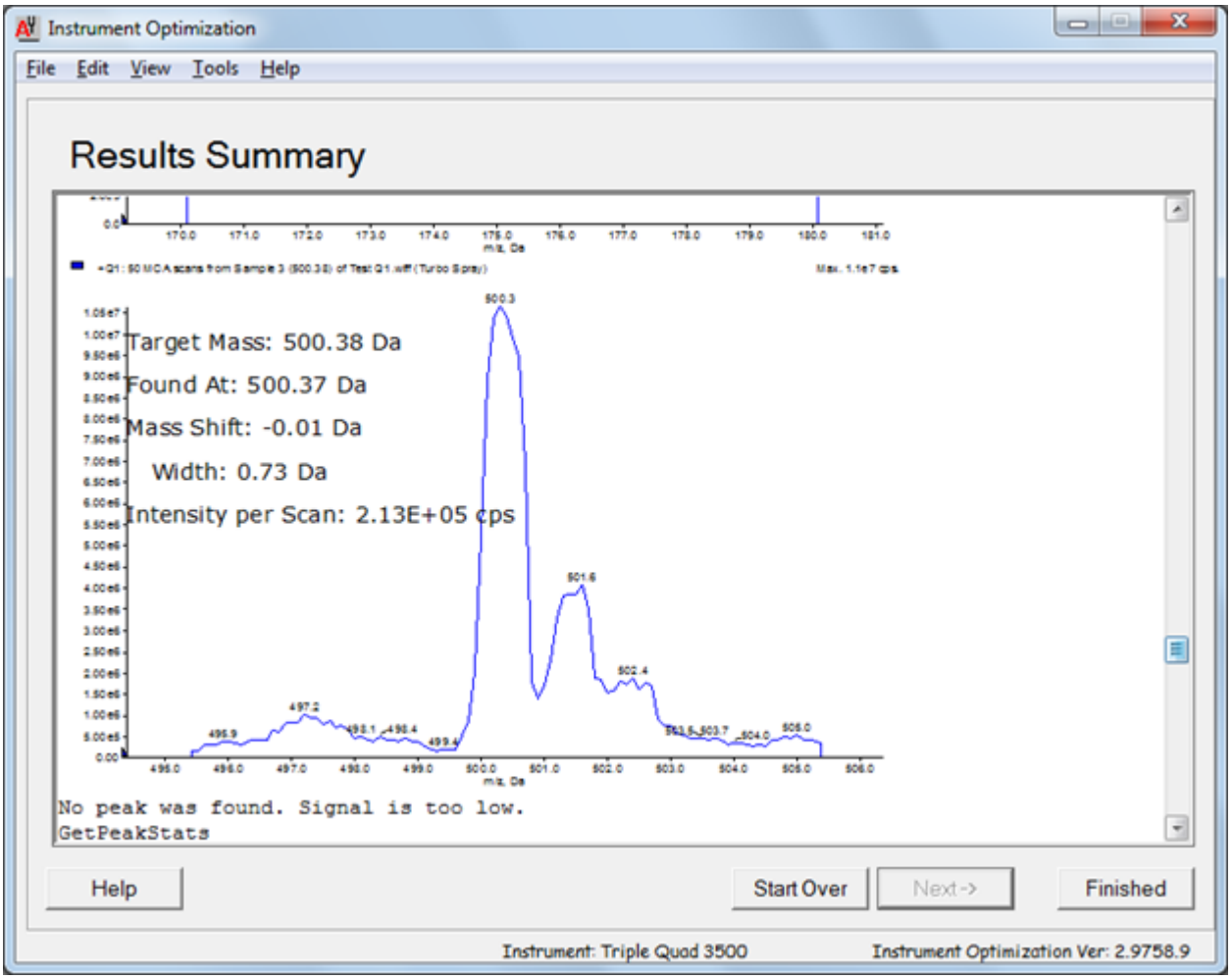


Figure 2-3 Results Summary: SCIEX Triple Quad 6500 System, High Mass

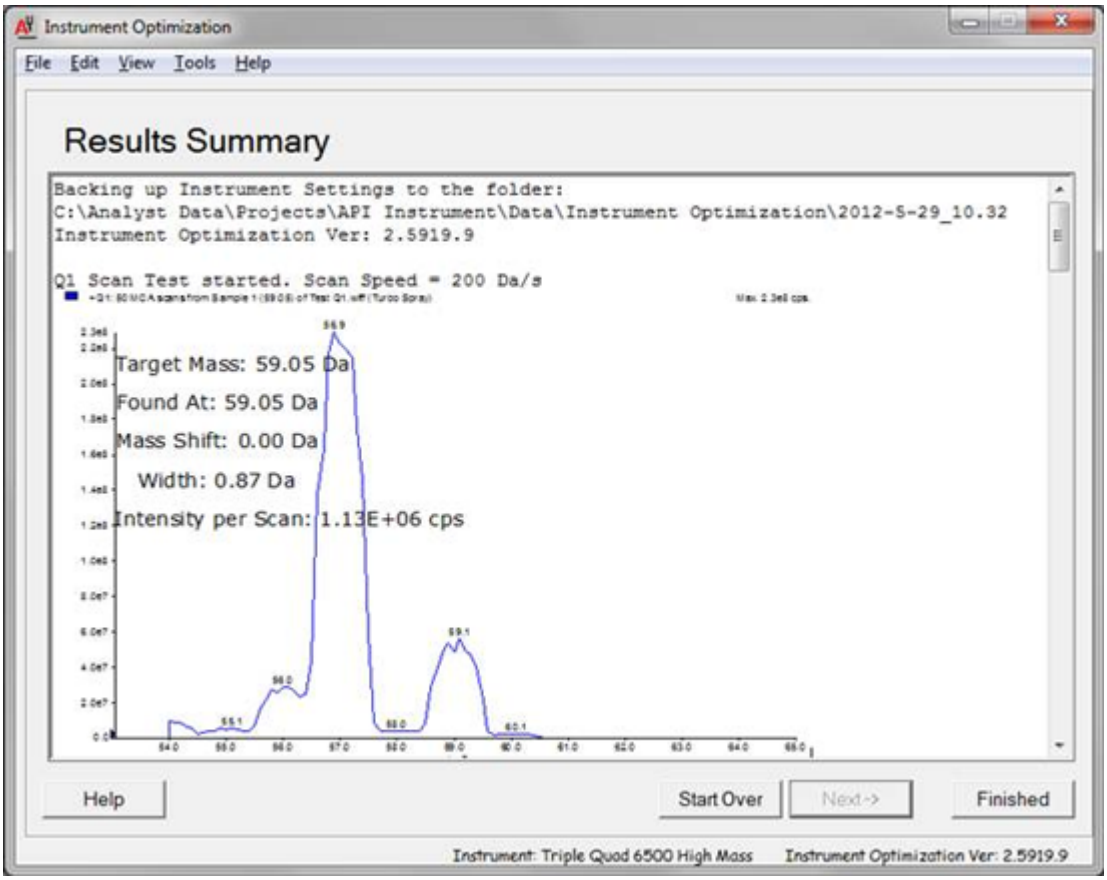
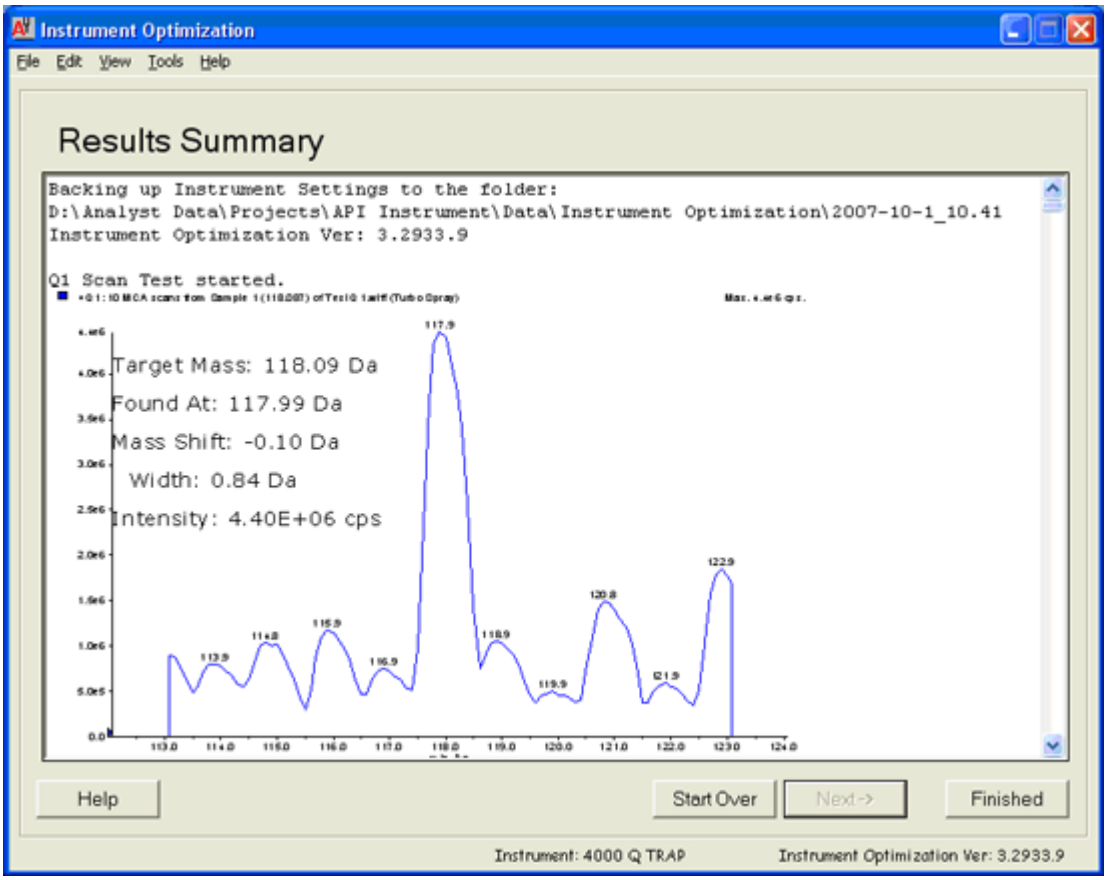


Figure 2-4 Results Summary: 4000 QTRAP System



The Results Summary includes the location of the data and instrument settings backup files, as well as a step-by-step record of the changes and results during optimization.

The Results Summary also includes a verification report. This report contains a snapshot of the mass spectrum for each relevant mass for the scan modes being verified. The spectrum is labeled with the target mass, where the mass was found, the mass shift, the peak width, and the peak intensity. The spectrum can be used as a visual record of peak shape or scan mode performance. A summary table of results follows the spectra.

The Results Summary is automatically saved in the following path: `<drive>:\Analyst Data\Projects\API Instrument\Data\Instrument Optimization\yyyy-mm-dd\results.pdf`, where *yyyy-mm-dd* is the date on which the report was created. Users can print the Results Summary or open a previously saved Results Summary.

Create Basic Methods 3

Acquisition methods can be created for data acquisition.

About LC Methods

Creating an acquisition method using a peripheral device, such as an LC system, includes providing the operating parameters for that device. If a new acquisition method is created from an existing file, some or all of the peripheral device methods can be used in the acquisition method.

Create Mass Spectrometry Methods

Use the Acquisition Method Editor to create a mass spectrometer (MS) acquisition method. Depending on the type of mass spectrometer configured and the scan type selected, different fields and options are available. The Acquisition Method Editor validates the settings as the parameters are typed.

Create one of the following methods and then use it to acquire data. Refer to the section: Create and Submit a Batch

- Create an Acquisition Method using a Q1 MS Scan Type
- Create an Acquisition Method using a Q1 MI Scan Type
- Create an Acquisition Method using an MRM Scan Type

About Spectral Data Acquisition

For a description of the modes in which spectral data can be acquired, refer to the table: Table 3-1.

Table 3-1 Spectral Data

Mode	Description
Profile	The preset value is 0.1 Da. Profile data is the data generated by the mass spectrometer and corresponds to the intensity recorded at a series of evenly spaced discrete mass values. For example, for a mass range from 100 Da to 200 Da and a step size of 0.1 Da, the mass spectrometer scans 99.95 to 100.05 (recorded as value 100), 100.95 to 101.05 (recorded as value 101)…199.95 to 200.05 (recorded as value 200).

Table 3-1 Spectral Data (continued)

Mode	Description
Peak Hopping	The preset value is 1.0 Da. Peak hopping is a mode of operating a mass spectrometer in which large steps (approximately 1 Da) are made. It has the advantage of speed (fewer data steps are made) but with the loss of peak shape information.
Centroid	The mass spectrometer scans as in profile mode, but creates a centroid of the data, replacing found peaks with the intensity-weighted center of gravity for each peak. Centroid data has the advantage of significantly reducing file size. The disadvantage is that peak shape information is lost and if data has been collected as a centroid then it cannot be altered. We recommend the use of profile mode and centroiding of the data post-acquisition.

Required Material

Required Materials
• Reserpine solution supplied in the Standards Chemical Kit shipped with the system. If required, a new kit can be ordered from SCIEX. • 5 mL, 1 mL, and 250 µL serial gas-tight syringes • Red PEEK sample tubing • (Optional) Syringe pump, if using an instrument without an integrated syringe pump. • Required peripheral device, for example an LC.

Create an Acquisition Method using a Q1 MS Scan Type

Use the following procedure to create a method using the Q1 MS scan. The ion intensity is returned for every requested mass in the scan range.

Prerequisites
• Make sure that a hardware profile containing the mass spectrometer and syringe pump is active. • On the software toolbar, make sure that the appropriate project is selected.

1. On the Navigation bar, under **Acquire**, double-click **Build Acquisition Method**. The Acquistion Method Editor is shown with a method template based on the active hardware profile.
2. In the Acquisition Method pane, click **Acquisition Method**.

3. On the Acquisition Method Properties tab, in the **Synchronization Mode** list, make sure that **No Sync** is selected. For more information about synchronization modes, refer to the document: *Help*.
4. In the Acquisition method pane, click the **Mass Spec** icon.
5. On the MS tab, in the **Scan type** list, select **Q1 MS (Q1)**.
6. In the Polarity section, click **Positive**.
7. Clear **Center/Width** and **Parameter Range** check boxes if selected.
8. In the mass ranges table, type the values that are shown in the following table.

Figure 3-1 MS Tab Parameter Values

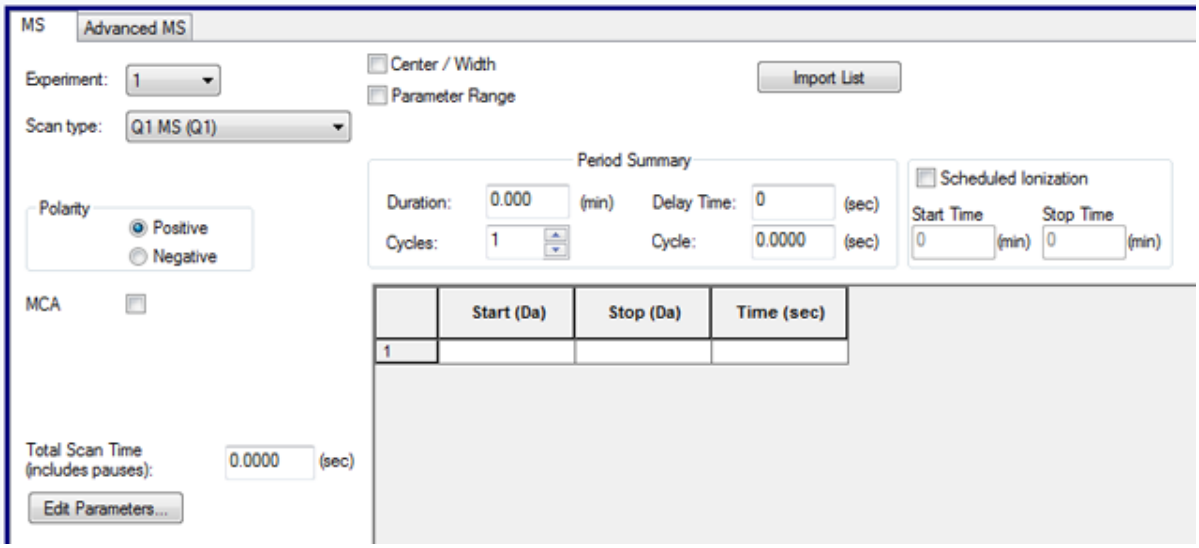
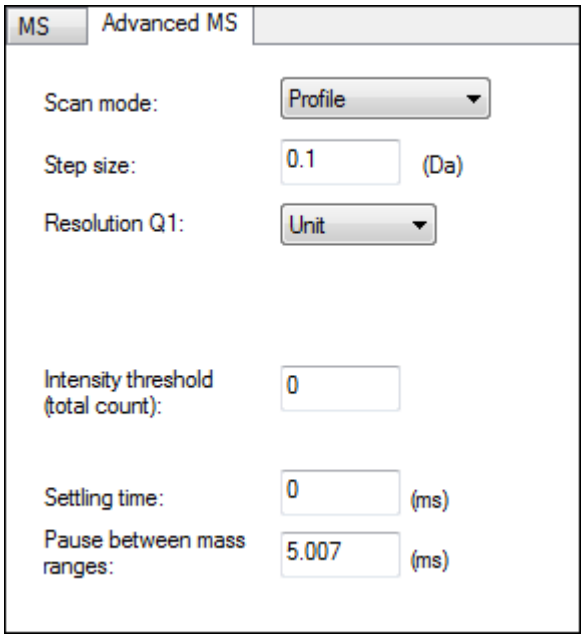


Table 3-2 MS Tab Parameter Values

Field	Example Value
Start (Da)	200
Stop (Da)	700
Time (sec)	2.5
Scan rate (Da/s)	200
Duration (min)	3

9. On the Advanced MS tab, note that the **Scan mode** is set to **Profile** and the **Step size** is 0.1.

Figure 3-2 Advanced MS tab



In this example, the quadrupole (Q1) is scanning a 500 Da range in 0.1 Da steps. Therefore, there are 5000 steps across the mass range. If the scan takes 2.5 seconds, then the dwell time is 0.5 ms per step. This is usually the fastest that Q1 or Q3 should be scanned in a standard calibration procedure. Proper consideration for mass calibration should be taken if Q1 or Q3 are to be scanned faster.

Note: The step size and the time of the scan control the dwell time per step for the scan. The dwell time is the length of time spent acquiring signal at each step in a scan.

10. On the MS tab, click **Edit Parameters**.
    The Parameter Table dialog opens.
11. On the Source/Gas tab, type the following values:

Table 3-3 Source/Gas Tab Parameters

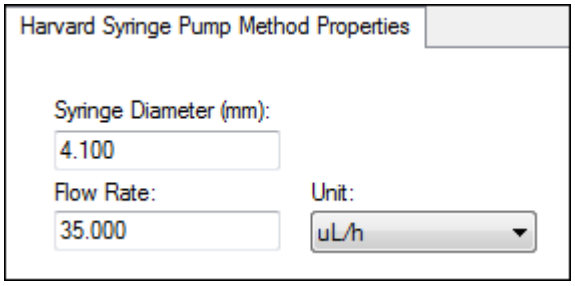
Source/Gas parameters	Typical value
Curtain Gas (CUR)	SCIEX 3200 systems, SCIEX 4000 systems, SCIEX 5000 systems: 10 Other systems: 35
IonSpray Voltage (IS)	5000
Temperature (TEM)	0
Ion Source Gas 1 (GS1)	20

Table 3-3 Source/Gas Tab Parameters (continued)

Source/Gas parameters	Typical value
Ion Source Gas 2 (GS2)	0

12. Click the Compound tab and then set the **Declustering Potential (DP)** to 90 and leave the **Entrance Potential (EP)** at 10.
    A value of 90 might not be optimal for the mass spectrometer but it is a good DP to start with.
13. Click **OK**.
14. In the Acquisition method pane, click the **Harvard Syringe Pump** or **Integrated Syringe Pump** icon.

Figure 3-3 Harvard Syringe Pump Method Properties Tab



15. Edit the syringe pump method to include **Syringe Diameter**, **Flow Rate**, and **Unit**.
16. Save the acquisition method.
    Next steps: Use the acquisition method to acquire data for preliminary analysis. To create and submit batches, refer to the section: Create and Submit a Batch.

Create an Acquisition Method using a Q1 MI Scan Type

Use the following procedure to create a method using the Q1 MI scan. The ion intensity is returned for only the specified masses.

Prerequisites
• Make sure that a hardware profile containing the mass spectrometer and syringe pump is active. • On the software toolbar, make sure that the appropriate project is selected.

1. On the Navigation bar, under **Acquire**, double-click **Build Acquisition Method**.
   The Method Editor is shown with a method template based on the active hardware profile.

2. In the Acquisition method pane, click **Acquisition Method**.
3. On the Acquisition Method Properties tab, in the **Synchronization Mode** list, make sure that **No Sync** is selected. For more information about synchronization modes, refer to the document: *Help*.
4. In the Acquisition method pane, click the **Mass Spec** icon.
5. On the MS tab, in the **Scan type** list, select **Q1 Multiple Ions (Q1 MI)**.
6. In the Polarity section, click **Positive**.
7. In the mass ranges table, type the values that are shown in the following table.

Figure 3-4 MS Tab Parameter Values

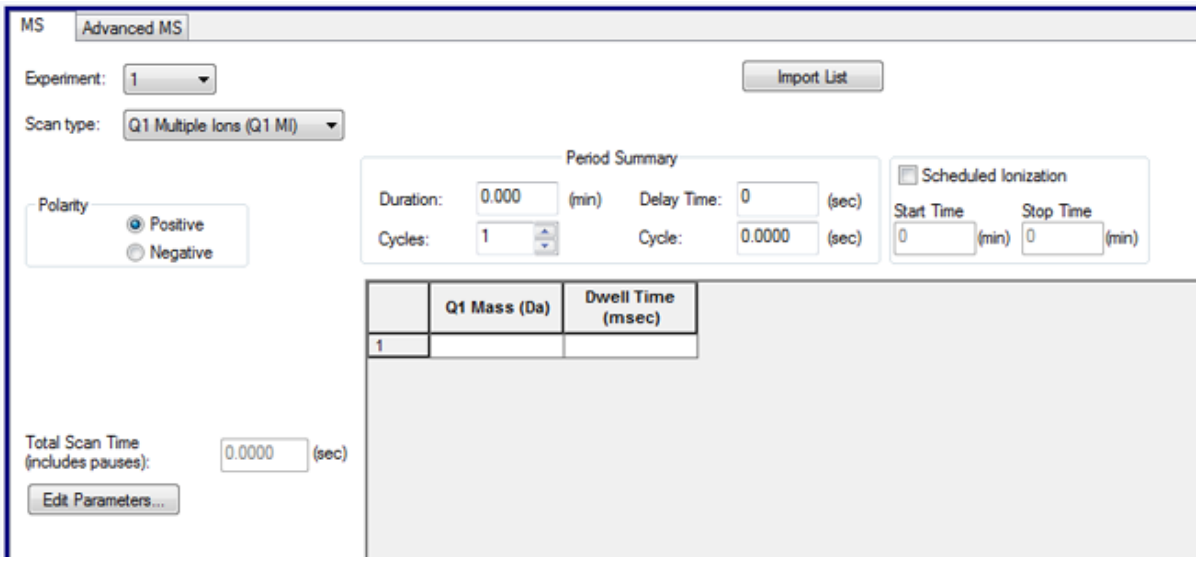


Table 3-4 MS Tab Parameter Values

Field	Value
Q1 Mass (Da)	609
Time (msec)	100

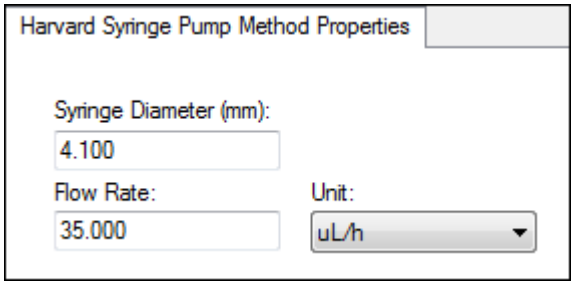
8. Click **Edit Parameters**.
   The Parameter table dialog opens.
9. On the Source/Gas tab, type the following values:

Table 3-5 Source/Gas Tab Parameters

Source/Gas parameters	Typical value
Curtain Gas (CUR)	SCIEX 3200 systems, SCIEX 4000 systems, SCIEX 5000 systems: 10 Other systems: 35
IonSpray Voltage (IS)	5000
Temperature (TEM)	0
Ion Source Gas 1 (GS1)	20
Ion Source Gas 2 (GS2)	0

10. Click the Compound tab and then set the **Declustering Potential (DP)** to 90 and leave the **Entrance Potential (EP)** at 10.
    A value of 90 might not be optimal for the mass spectrometer but it is a good DP to start with.
11. Click **OK**.
12. In the Acquisition method pane, click the **Harvard Syringe Pump** or **Integrated Syringe Pump** icon.

Figure 3-5 Harvard Syringe Pump Method Properties Tab



13. Edit the syringe pump method to include **Syringe Diameter**, **Flow Rate**, and **Unit**.
14. **Save** the acquisition method.
    Next steps: Create and submit a batch containing this acquisition method. To create and submit batches, refer to the section: Create and Submit a Batch.

Create an Acquisition Method using an MRM Scan Type

Use the following procedure to create a method using the MRM scan. This scan type is used in quantitative applications. An MRM scan can be used to determine how much of a compound

is in a sample. It is used in pharmacokinetic analysis and increasingly in applied markets and screening applications.

Prerequisites
• Make sure that a hardware profile containing the mass spectrometer and syringe pump is active. • On the software toolbar, make sure that the appropriate project is selected.

1. On the Navigation bar, under **Acquire**, double-click **Build Acquisition Method**. The Acquistion Method Editor is shown with a method template based on the active hardware profile.
2. In the Acquisition Method pane, click **Acquisition Method**.
3. On the Acquisition Method Properties tab, in the **Synchronization Mode** list, make sure that **No Sync** is selected. For more information about synchronization modes, refer to the document: *Help*.
4. In the Acquisition method pane, click the **Mass Spec** icon.
5. On the MS tab, in the **Scan type** list, select **MRM (MRM)**.
6. In the Polarity section, click **Positive**.
7. In the mass ranges table, type the values that are shown in the following table.

Figure 3-6 MRM Scan Type

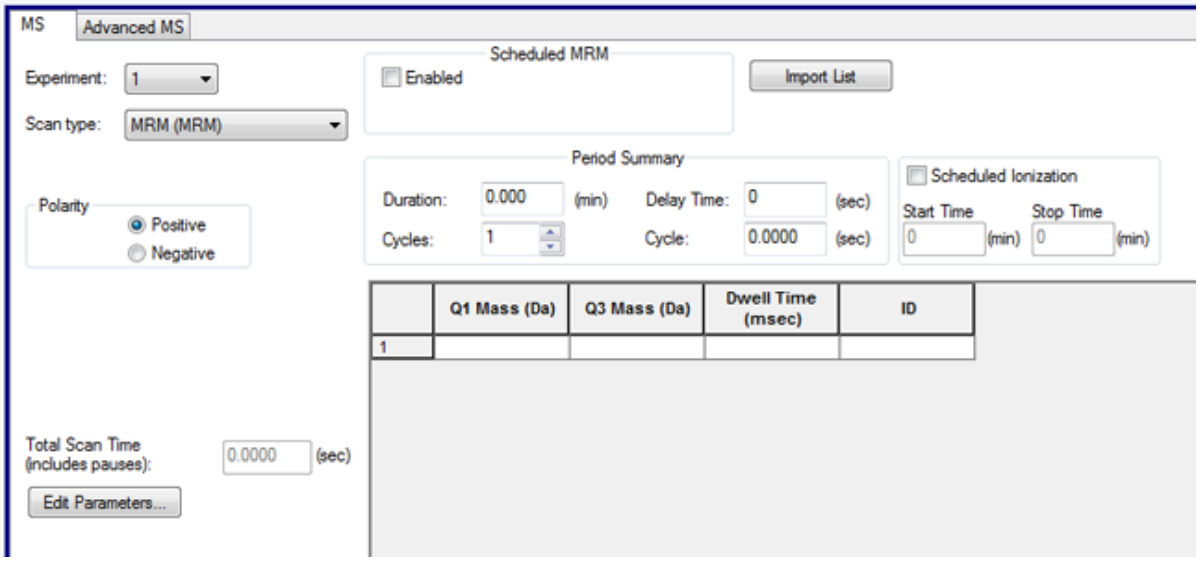


Table 3-6 Mass Range and Dwell Time

Q1 Mass (Da)	Q3 Mass (Da)	Time (msec)
609	397.2	100

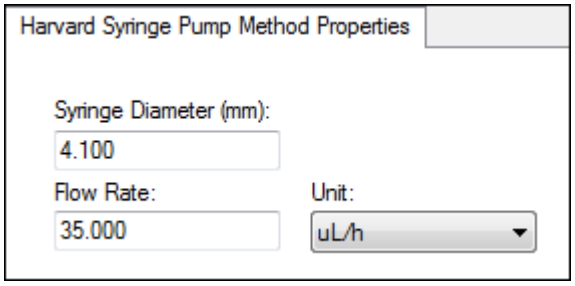
8. On the MS tab, click **Edit Parameters**.
   The Parameter Table dialog opens.
9. On the Source/Gas tab, type the following values:

Table 3-7 Source/Gas Tab Parameters

Source/Gas parameters	Typical value
Curtain Gas (CUR)	SCIEX 3200 systems, SCIEX 4000 systems, SCIEX 5000 systems: 10 Other systems: 35
IonSpray Voltage (IS)	5000
Temperature (TEM)	0
Ion Source Gas 1 (GS1)	20
Ion Source Gas 2 (GS2)	0

10. On the Compound tab, set the **Declustering Potential (DP)** to 90 and leave the **Entrance Potential (EP)** at 45.
11. Click **OK**.
12. In the Acquisition method pane, click the **Harvard Syringe Pump** icon.

Figure 3-7 Harvard Syringe Pump Method Properties Tab



13. On the Syringe Pump tab, edit the syringe pump method to include **Syringe Diameter**, **Flow Rate**, and **Unit**.
14. **Save** the acquisition method.

Next steps: Create and submit a batch containing this acquisition method. To create and submit batches, refer to the section: Create and Submit a Batch.

Add or Remove Devices From Acquisition Methods

Use the Acquisition Method Editor to customize the acquisition method by adding or removing LC peripheral device methods. If the required device icon is not in the Acquisition Method Browser pane, then add the peripheral device only if it is included in the active hardware profile. For more information, refer to the document: *Advanced User Guide*.

Note: The available parameters for the LC devices vary depending on the manufacturer.

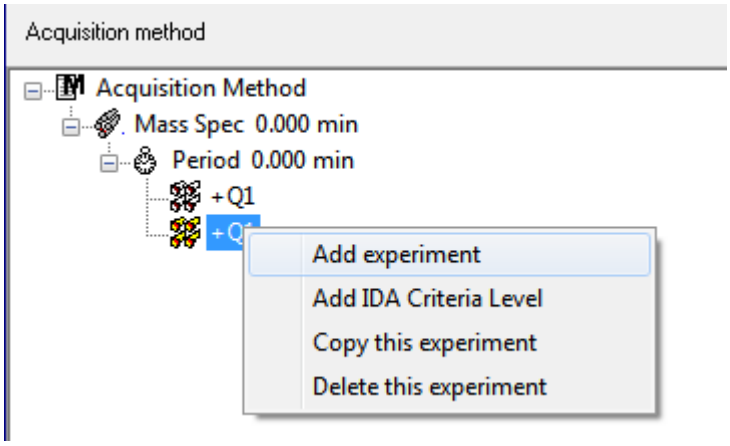
Change Acquisition Methods

In Acquire mode, users can add or delete periods and experiments to existing acquisition methods.

Add an Experiment

1. In the Acquisition method pane, on the period where the experiment is to be added, right-click and then click **Add experiment**.

Figure 3-8 Add Experiment



An experiment is added below the last experiment in the period.

Note: An experiment cannot be inserted between experiments, IDA criteria, or periods. Users can only add an experiment at the end of the period.

2. On the MS tab, select the appropriate parameters.

Copy an Experiment into a Period

1. Open a multi-period method.
2. In the Acquisition method pane, press **Ctrl**, and then drag the experiment to the period. The experiment is copied below the last experiment in the period.

Copy an Experiment within a Period

Use this procedure to add the same or similar experiments to a period if most or all of the parameters are the same.

- Right-click the experiment and then click **Copy this experiment**.

  A copy of the experiment is added below the last experiment created.

Add a Period

- In the Acquisition method pane, right-click the **Mass Spec** icon, and then click **Add period**. A period is added below the last period created.

  Note: Users cannot use multiple periods in an IDA experiment.

Batches 4

CAUTION: Potential System Damage. If the LC system connected to the mass spectrometer is not controlled by the software, then do not leave the mass spectrometer unattended while in operation. The liquid stream from the LC system can flood the ion source when the mass spectrometer goes in Standby state.

A batch is a collection of information about the samples to be analyzed. Samples are usually grouped into sets to simplify submission. Grouping the samples into a set also reduces the amount of data that must be typed manually. A set can consist of a single sample or multiple samples. All of the sets in a batch use the same hardware profile. However, samples in a set can have different acquisition methods. A batch can be submitted only from an acquisition station.

Batches include the following information:

- Sample information, such as name, ID, and comment
- Autosampler location (rack information)
- Acquisition methods
- Processing method or script(optional)
- Quantitation information (optional)
- Custom sample data (optional)
- Set information.

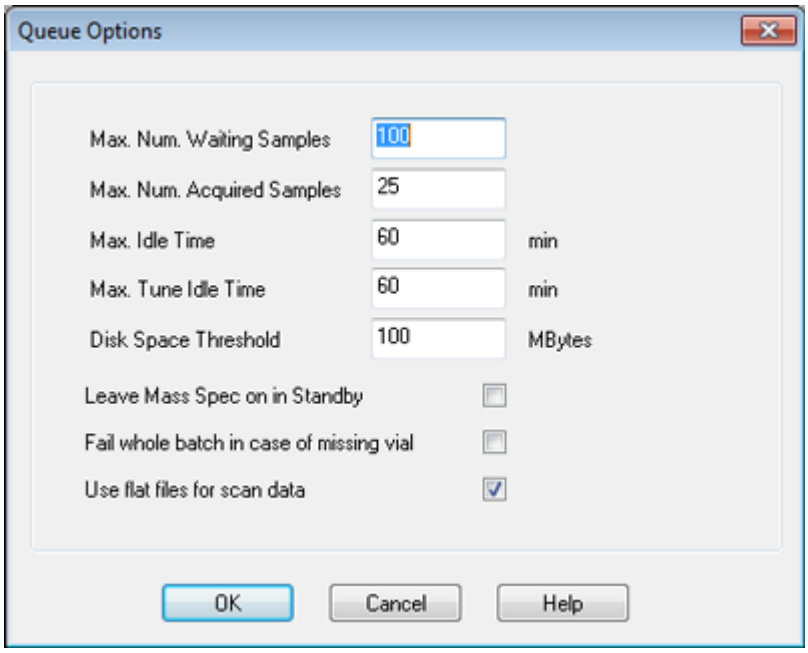
Set Queue Options

The software goes one-by-one through the list of samples in the queue, acquiring each sample with the selected acquisition method. After all of the samples have been acquired, the acquisition stops and the mass spectrometer goes into Standby state after the **Max. Idle Time** set in the Queue Options has elapsed. In the Standby state, the LC pumps stop and some instrument voltages are turned off.

The user can change the amount of time between acquisition of the last sample and the change to Standby state.

1. On the Navigation bar, click **Configure**.
2. Click **Tools** > **Settings** > **Queue Options.**

Figure 4-1 Queue Options Dialog



3. In the **Max. Num. Waiting Samples** field, set the maximum number of samples to a value that is greater than the number of samples that will be submitted to the queue.
4. In the **Max. Idle Time** field, type the amount of time the software will wait after acquisition is completed before going to Standby state. The preset value is 60 minutes.

   If gas cylinders are used, then adjust this time to make sure that the gas in the cylinders is not depleted.

   If an LC method is used, then before the run is started, make sure that there is enough solvent in the reservoirs for all of the sample runs at the primary flow rate and the maximum idle time.
5. Select the **Leave Mass Spec on in Standby** check box to keep the mass spectrometer running after analysis has been completed.

   This feature allows the heaters and gases to continue running, even after devices have entered Idle state, so that the ion source and entrance to the mass spectrometer are kept free of contaminants.
6. Select the **Fail Whole Batch in Case of Missing Vial** check box to make the entire batch fail when a missing vial is encountered.

   If this option is not selected, then only the current sample will fail and the software will continue to the next sample.

Create and Submit a Batch

Use this workflow to create a batch.

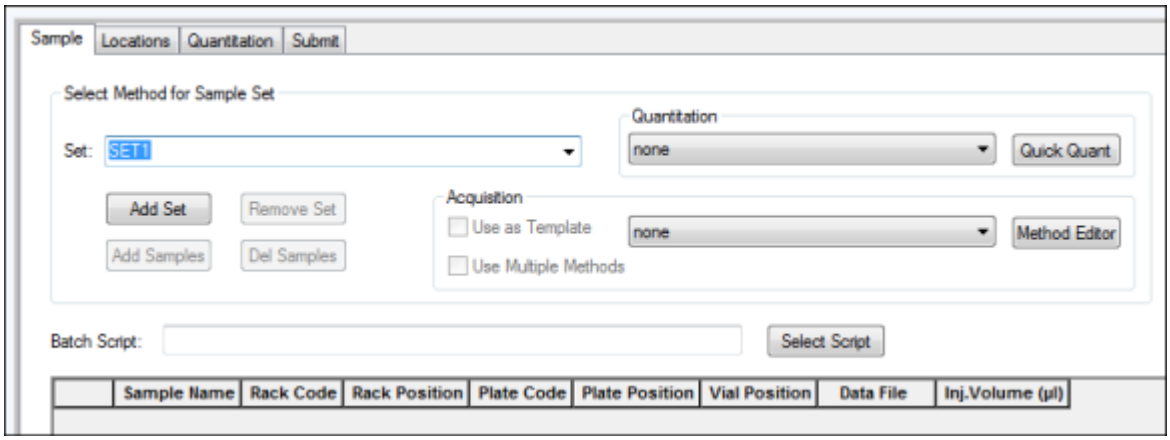
Add Sets and Samples to a Batch

A set can consist of a single sample or multiple samples.

Note: For more information about adding quantitation information to a batch, refer to the document: *Advanced User Guide*.

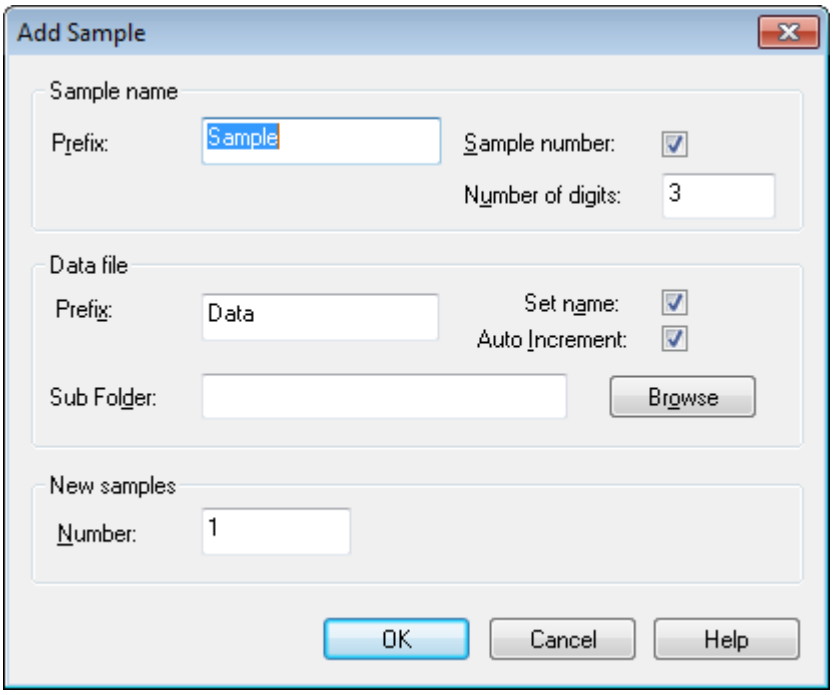
1. On the Navigation bar, under **Acquire**, double-click **Build Acquisition Batch**.

Figure 4-2 Batch Editor Dialog



2. On the Sample tab, in the **Set** list, type a name.
3. Click **Add Set**.
4. Click **Add Samples** to add samples to the new set.

Figure 4-3 Add Sample Dialog



5. In the Sample name section, in the **Prefix** field, type a name for the samples in this set.
6. To add incremental numbering to the end of the sample name, select the **Sample number** check box.
7. If the **Sample number** check box is selected, then in the **Number of digits** field, type the number of digits to include in the sample name.
   For example, if 3 is typed, then the sample names would be samplename001, samplename002, and samplename003.
8. In the Data file section, in the **Prefix** field, type a name for the data file that will store the sample information.
9. Select the **Set name** check box to use the set name as part of the data file name.
10. Select the **Auto Increment** check box to increment the data file names automatically.

Note: The data for each sample can be stored in the same or a separate data file. The names of the data file will have numerical suffixes starting from 1.

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11. Type a name in the **Sub Folder** field.
    The folder is stored in the `Data` folder for the current project. If the **Sub Folder** field is left blank, then the data file is stored in the `Data` folder and a subfolder is not created.
12. In the New samples section, in the **Number** field, type the number of new samples to add.
13. Click **OK**.

The sample table fills with the sample names and data file names.

Tip! Fill Down and **Auto Increment** options are available in the right-click menu after a single column heading or several rows in a column are selected.

14. On the Sample tab, in the Acquisition section, select a method from the list.
    Depending on how the system is set up, specific information for the autosampler must be entered. Even if the injection volume is set in the method, the user can change the injection volume for one or more samples by changing the value in the injection volume column.

    Note: To use different methods for some of the samples in this set, select the **Use Multiple Methods** check box. The **Acquisition Method** column is shown in the Sample table. Select the acquisition method for each sample in this column.

15. To change the injection volumes from the volumes listed in the method, in the **Inj. Volume (µL)** column, type the injection volume for each sample.
16. To set sample locations, do one of the following:
    - Set Sample Locations in the Batch Editor
    - Select Vial Positions Using the Locations Tab (Optional)
17. (Optional) To define quantitation details prior to submitting the batch, refer to the section: Set Quantitation Details in the Batch Editor (Optional).
18. Open the Submit tab.

    Note: The order of samples can be edited before the samples are submitted to the queue. To change the order of samples, on the Submit tab, double-click any of the numbers at the far left of the table (a very faint square box is shown), and then drag them to the new location.

19. If the Submit Status section contains a message about the status of the batch, then do one of the following:
    - If the message indicates that the batch is ready for submission, then go to step 20.
    - If the message indicates that the batch is not ready for submission, then make the changes as indicated by the message.
20. After confirming that all of the batch information is correct, click **Submit**.
    The batch is submitted to the queue and can be viewed in the Queue Manager.
21. Save the file.

Equilibrate the System

Equilibrate the system before submitting a batch. Equilibration warms up and prepares the mass spectrometer for the next sample or batch.

1. Click **Equilibrate** ().
2. Select the acquisition method used for the submitted batch.
3. Type the equilibration time in the **Time (min)** field, in minutes.
4. Click **OK**. The system starts the equilibration.
   After the equilibration is completed, the system state changes to Ready.

Tip! If the equilibration does not complete, or if the system status does not change to Ready after the equilibration completes, then make sure that the following conditions are true:

- The activated hardware profile is applicable for the acquisition method.
- The LC system is turned on.
- The LC system is in communication with the software.

Submit a Sample or Set of Samples

Note: Run the sample again if an abnormal termination occurs during sample acquisition. If the abnormal termination is caused by a power failure, then the temperature of the autosampler tray is not maintained and sample integrity might be compromised.

1. Select one sample or a set of samples.
2. Open the Submit tab in the Batch Editor.
3. If the Submit Status group contains a message about the status of the batch, then do one of the following:
   - If the message indicates that the batch is ready for submission, then go to the next step.
   - If the message indicates that the batch is not ready for submission, then make the changes as indicated by the message.
4. Click **Submit**.

Change Sample Order

The order of the samples can be changed before the samples are submitted to the **Queue**.

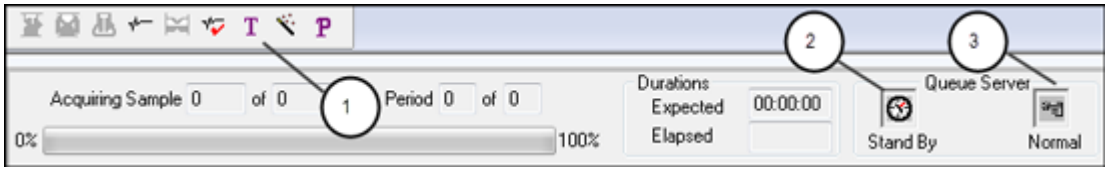
- On the Submit tab, double-click any of the numbers at the far left of the table (a very faint square box is visible), and then drag them to the new location.

Acquire Data

The software must not be in Tune and Calibrate mode when sample acquisition is started. Also, if the system has been previously run that day and has not yet been set to Standby state, then sample acquisition will start automatically.

1. Make sure that the column oven temperature is reached.
2. Make sure that the **Reserve Instrument for Tuning** (T) icon is not pressed in.
3. On the Navigation bar, click **Acquire**.
4. Click **View** > **Sample Queue.**
   The Queue Manager opens with all of the submitted samples.

Figure 4-4 Queue Manager



Item	Description
1	The **Reserve Instrument for Tuning** icon should not be pressed in.
2	Queue state must be Ready.
3	**Queue Server** state must be Normal. Refer to the section: Queue States.

5. Click **Acquire** > **Start Sample.**

Set Sample Locations in the Batch Editor

If an autosampler is used in the acquisition method, then the vial positions of the samples must be defined in the acquisition batch. Define the location in the Sample tab or in the Locations tab. For more information about creating batches, refer to Add Sets and Samples to a Batch.

1. In the Sample tab, from the **Set** list, select the set.
2. For each sample in the set, do the following if applicable:
   - In the **Rack Code** column, select the rack type.
   - In the **Rack Position** column, select the position of the rack in the autosampler.
   - In the **Plate Code** column, select the plate type.

- In the **Plate Position** column, select the position of the plate on the rack.
- In the **Vial Position** column, type the position of the vial in the plate or tray.

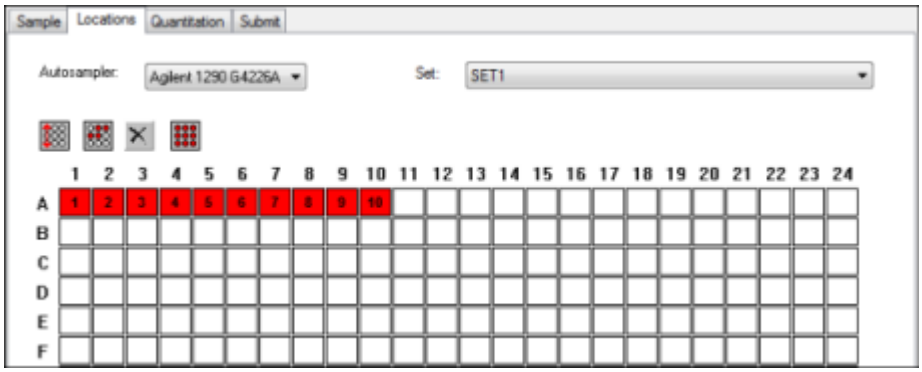
3. Save the file.

Select Vial Positions Using the Locations Tab (Optional)

1. In the Batch Editor, open the Locations tab.
2. In the **Set** list, select the set.
3. From the **Autosampler** list, select the autosampler.
4. In the space associated with the rack, right-click and then select the rack type.
   The plates or trays are shown in the rack.
5. Double-click in the white space labeled rack type. A visual sample rack layout is shown.
   The appropriate number of rack spaces for the autosampler is shown in the graphic rack view.
6. Double-click one of the rectangles.
   The circles depicting the wells or vials for the plate or tray are shown.

Tip! To see the corresponding vial number in the graphical representation, move the cursor over the sample position. Use this information to confirm that the vial positions in the software match the vial positions in the autosampler.

Figure 4-5 Locations Tab



Note: Depending on the autosampler being used, it might not be necessary to type details in additional columns.

7. To select whether samples are marked by row or column, click the **Row/Column selection** selector button.

If the button shows a red horizontal line, then the Batch Editor marks the samples by row. If the button shows a red vertical line, then the Batch Editor marks the samples by column.

8. Click the sample wells or vials in the order in which they should be analyzed.

Tip! Click a selected well or vial again to clear it.

Tip! To fill in the samples automatically, press **Shift** while clicking the first and last vial within a set. To perform multiple injections from the same vial, press **Ctrl** while clicking the vial location. The red circle changes to a green circle.

Set Quantitation Details in the Batch Editor (Optional)

If a quantitation method is used with a batch and if the user does not want to select quantitation details after acquisition, then the quantitation details (sample type, sample concentration) must be defined before the batch is submitted.

The appropriate **Internal Standard** and **Standard** columns are shown in the Quantitation tab according to the quantitation method selected in the Sample tab.

1. With a batch file open in the Batch Editor window, open the Quantitation tab.
2. Select the set containing the samples.
3. Select a **Quant Type**, **Dilution Factor**, and **Weight/Volume** for all of the samples from the list in the cell.
4. (If required) In the **Analyte** column, type the analyte concentration.
5. (If required) In the **Internal Standard** column, type the internal standard concentration.
6. Repeat this procedure for each set in the batch.

Stop Sample Acquisition

When a sample acquisition is stopped, the software completes the current scan before stopping acquisition.

1. In the Queue Manager, click the sample in the queue after the point where acquisition should stop.
2. On the Navigation bar, click **Acquire**.
3. Click **Acquire** > **Stop Sample.**
   The acquisition stops after the current scan in the selected sample is acquired. The sample status in the **Queue Manager (Local)** window changes to **Terminated**, and all other samples following in the queue are **Waiting**.

4. To continue processing the batch, click **Acquire** > **Start Sample.**

Import Batch Files

Users can import a text file containing batch information instead of creating a batch in the Batch Editor. If all of the sample details are in a spreadsheet, then rearranging and importing the data in the spreadsheet is faster than manually typing the data in the Batch Editor.

Before importing batch information from a text file, make sure that the data in the file is organized and formatted correctly. In particular, the column headings in the spreadsheet must match the Batch Editor column headings. To make sure that the text file includes the proper headings, create a batch using the Batch Editor, export it as a text file, type the appropriate values in a spreadsheet editor, and then import the file back into the Batch Editor.

For examples of correctly formatted files, refer to the Batch folder in the Example project.

The information in a batch file can also be exported for use with other applications, such as Microsoft Excel, Microsoft Access, and certain Laboratory Information Management System (LIMS) software.

Build a Batch as a Text File

Prerequisites
Make sure that the active hardware profile includes all of the devices to be used to acquire the samples.

To make sure that the text file includes the proper headings, create a batch using the Batch Editor, export it as a text file, type the appropriate values in a spreadsheet editor, and then import the file back into the Batch Editor. Users can export a batch only if it contains at least one set with at least one sample. The saved text file can be used again later as a template.

1. In the Batch Editor, create a single-set, single-sample batch.
2. Click **File** > **Export.**
   The Save As dialog opens.
3. Type a name for the text file in the **File name** field and then click **Save**.
4. Open the text file in a spreadsheet program such as Excel.
5. Type, or copy and paste, the details for the samples: one sample per row, with the details under the appropriate headings.

   Note: Do not delete any of the columns. The columns in the spreadsheet must match the columns in the Batch Editor.
6. Save the modified text file as a txt or csv file and then close the spreadsheet program.
   The text file is now ready to be imported into the Batch Editor.

Import a Batch from a Text File

1. In the Batch Editor, on the Sample tab, right-click, and then click **Import From** > **File.**
   The Open dialog opens.
2. Click the required text file and then click **Open**.
   If an autosampler is used, then the Select Autosampler dialog opens.

   Note: If the saved text file is not visible in the **Files of type** list, then select **Microsoft Text Driver (*.txt; *.csv)**. Files with the extension .txt are shown in the field.
3. In the autosampler list, select the autosampler and then click **OK**.
   The sample table fills with the details from the text file.
4. Submit the batch.

Batch and Acquisition Method Editor Tips

To Do This	Do This
To change the values in the table	(For example, to change a sample name) Click in a cell and then type the new value.
To change all the values in a column simultaneously	Click a column heading and then right-click. From the menu that is shown, select the **Auto Increment** and **Fill Down** commands to change the values in the column. This feature also works for multiple cells in the same column.
To change an existing acquisition method	From the list, select the method and then click **Method Editor**. To create a new acquisition method, from the list, select **None** and then click **Method Editor**. Only experienced users should use this feature. Do not use this feature when you are using the Use **Multiple Methods** option.
To apply a previously created quantitation method	Select the method from the **Quantitation** menu.
To select more than one well or vial at a time	Press **Shift** and click the first and last well or vial of the range you want to select.

For information on using the Batch Editor right-click menu, refer to the section: Batch Editor.

Queue States and Device Status

The Queue Manager shows queue, batch, and sample status. Detailed information about a particular sample in the queue can also be viewed.

Tip! Click **View Queue** ( ) to view the queue.

For information on using the Queue right-click menu, refer to the section: Queue.

Queue States

The current state of the queue is indicated in the Queue Server group.

Figure 4-6 Queue Server Indicator Showing Normal Mode

Figure 4-7 Queue Server Indicator Showing Tune Mode

The first icon indicates the queue state. The second icon indicates whether the queue is in Tune mode (for tuning) or Normal mode (for running samples). For descriptions of the icons and queue states, refer to the table: Table 4-1.

Table 4-1 Queue States

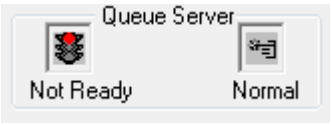
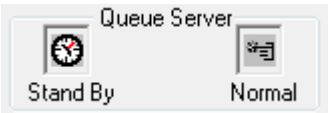
Icons	State	Definition
	**Not Ready**	The hardware profile is deactivated and the queue is not accepting any sample submissions.
	**Stand By**	The hardware profile has been activated, but all devices are idle. Pumps are not running and gases are turned off.

Table 4-1 Queue States (continued)

Icons	State	Definition
	**Warming Up**	The mass spectrometer and devices are equilibrating, columns are being conditioned, the autosampler needle is being washed, and column ovens are reaching temperature. The duration of equilibration is selected by the operator. From this state, the system can go to the **Ready** state.
	**Ready**	The system is ready to start running samples and the devices have been equilibrated and are ready to run. In this state, the queue can receive samples and will run after samples are submitted.
	**Waiting**	The system will automatically begin acquisition when the next sample is submitted.
	**PreRun**	The method is being downloaded to each device and device equilibration is occurring. This state occurs before the acquisition of each sample in a batch.
	**Acquiring**	The method is running and data acquisition is occuring.
	**Paused**	The system has been paused during acquisition.

View Instrument and Device Status Icons

Icons representing the mass spectrometer and each device in the active hardware configuration are shown on the status bar in the bottom right corner of the window. The user can view the detailed status of an LC pump to make sure the LC pump pressure is appropriate or view the detailed status of the mass spectrometer to monitor the temperature of the ion source.

Note: For each status, the background color can be red. A red background indicates that the device encountered an error while in that state.

- On the status bar, double-click the icon for the device or mass spectrometer.
  The Instrument Status dialog opens.

Table 4-2 Instrument and Device Status Icons

Status	Icon	Background Color	Description
Idle		Green or yellow	The device is not running. If the background color is yellow, then the device should be equilibrated before it is ready to run. If the background color is green, then the device is ready to run.
Equilibrating		Green or yellow	The device is equilibrating.
Waiting		Green	The device is waiting for a command from the software or another device, or for some action by the operator.
Running		Green	The device is running a batch.
Aborting		Green	The device is aborting a run.
Downloading		Green	A method is being transferred to the device.
Ready		Green	The device is not running, but is ready to run.
Error		Red	The device has encountered an error that should be investigated.

Analyze and Explore Data 5

Use the sample files installed in the Example folder to learn how to view and analyze data using the most common analysis and processing tools. For more information about the following topics, refer to the document: *Advanced User Guide*.

- Labeling graphs
- Overlaying and summing spectra or chromatograms
- Performing background subtractions
- Smoothing algorithms
- Working with smoothed data
- Working with centroid data
- Working with contour plots
- Working with the fragment interpretation tool
- Working with library databases and library records

Open Data Files

Tip! To turn off the automatic update on the mass spectrum, right-click the mass spectrum and then click **Show Last Scan**. If there is a check mark beside **Show Last Scan**, then the spectrum will update in real-time.

1. On the Navigation bar, under **Explore**, double-click **Open Data File**.
   The Select Sample dialog is shown.
2. In the **Data Files** list, navigate to the data file to open, select a sample, and then click **OK**.
   The data acquired from the sample is shown. If data is still being acquired, then the mass spectrum, DAD/UV trace, and TIC continue to update automatically.

Navigate Between Samples in a Data File

Note: If samples were saved in separate data files, then open each file individually.

For descriptions of the navigation icons used in this procedure, refer to the table: Table B-4.

- Open a data file that contains multiple samples and then do one of the following:
  - To skip to the next sample in the data file, click the **Show Next Sample** icon ().

- To skip to a non-sequential sample, click the **Go to Sample** icon ().
- In the Select Sample dialog, from the **Sample** list, select the sample to view.
- To go to the previous sample in the data file, click the **Show Previous Sample** icon ().

View Experimental Conditions

The experimental conditions used to collect data are stored in the data file with the results. The information contains the details of the acquisition method used: the MS acquisition method, that is, the number of periods, experiments, and cycles, including instrument parameters, and the LC device method, including the LC pump flow rate. In addition, it also contains the MS resolution and mass calibration tables used for the sample acquisition. For the software functionality available when the user views the file information, refer to the section: Show File Information Pane Right-click Menu.

Note: If data is acquired from more than one sample into the same wiff file, then the file information pane does not refresh automatically when the user scrolls through the samples. Close the file information pane and then open it again to view the details for the next sample in the wiff file.

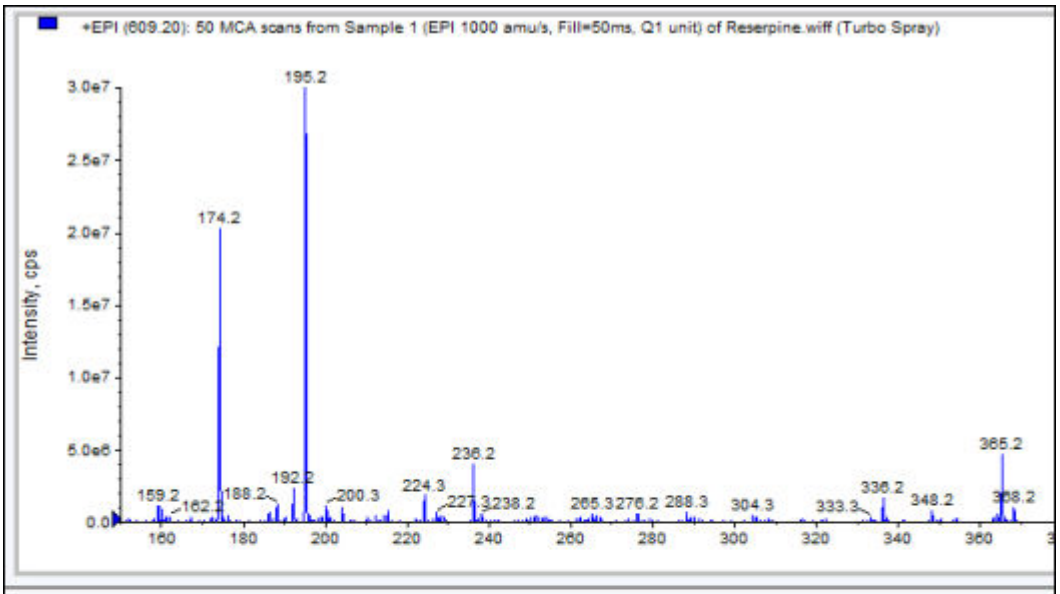
- Click **Explore** > **Show** > **Show File Information.**
  The File Information pane opens below the graph.

  Tip! To create an acquisition method from the File Information pane, right-click the File Information pane and then click **Save Acquisition Method**.

Show Data in Tables

1. Open a data file.
2. Click **Explore** > **Show** > **Show List Data.**
   The data is shown in a pane below the graph.

Figure 5-1 Peak List Tab (QTRAP systems)

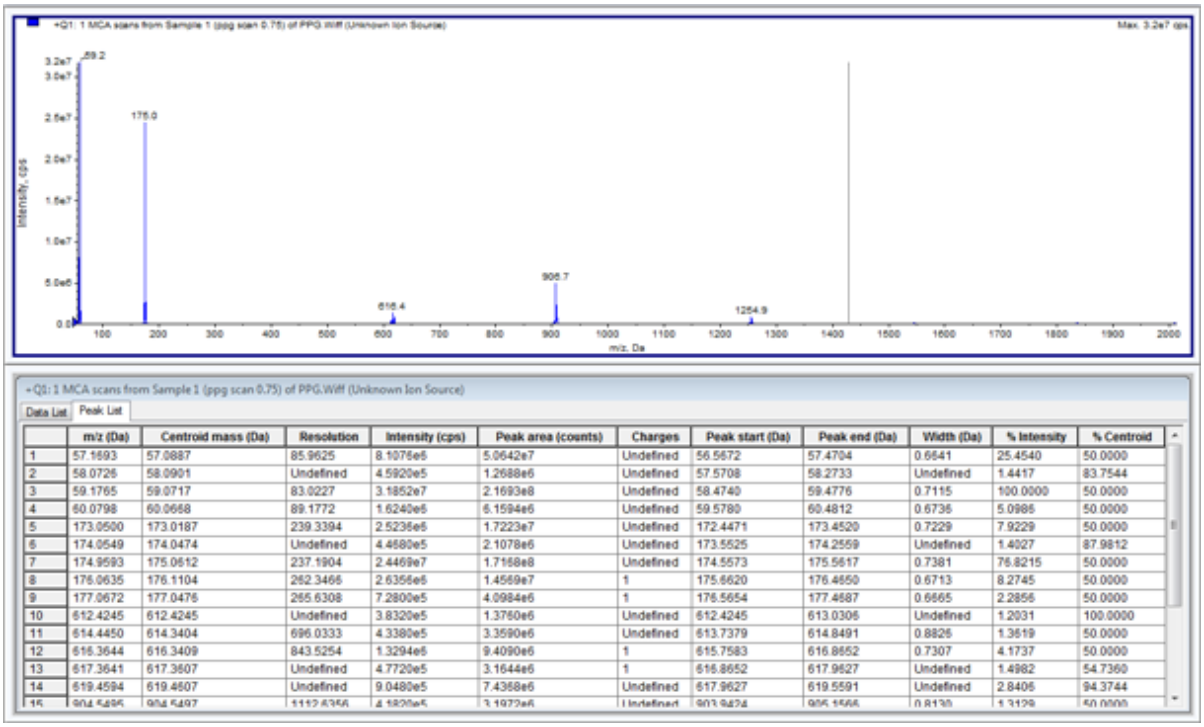


+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)

Data List | Peak List

	m/z (Da)	Centroid mass (Da)	Resolution	Intensity (cps)	Peak area (cou
1	159.1800	159.1685	654.9998	1.2000e6	5.7500e6
2	160.1400	160.1720	701.2606	9.5000e5	4.1333e6
3	161.1600	161.2024	847.5389	3.8333e5	1.3333e6
4	162.1800	162.1859	1105.7427	4.1667e5	1.4333e6
5	167.2200	167.1912	759.9557	4.0000e5	1.6667e6
6	172.2000	172.1858	1683.6625	3.5000e5	1.1500e6
7	174.1800	174.2020	696.6370	2.0250e7	9.8817e7
8	176.1600	176.2059	940.4631	4.8333e5	1.5833e6
9	186.2400	186.2193	1048.2067	6.5000e5	2.4333e6
10	188.2200	188.2062	1045.6328	1.3000e6	4.5000e6
11	190.2000	190.1959	985.6947	3.1667e5	1.1333e6
12	192.2400	192.2093	783.1276	2.3167e6	1.0567e7
13	195.1800	195.1662	832.2716	3.0050e7	1.3722e8
14	196.1400	196.1551	876.3162	5.0000e5	2.0167e6
15	199.2000	199.2103	754.5717	3.8333e5	1.5833e6

Figure 5-2 Peak List Tab (SCIEX Triple Quad 3500 system)



	m/z (Da)	Centroid mass (Da)	Resolution	Intensity (cps)	Peak area (counts)	Charges	Peak start (Da)	Peak end (Da)	Width (Da)	% Intensity	% Centroid
1	57.1693	57.0887	85.9625	8.1076e6	5.0642e7	Undefined	56.5672	57.4704	0.6641	25.4540	50.0000
2	58.0726	58.0901	Undefined	4.5920e5	1.2688e6	Undefined	57.5708	58.2733	Undefined	1.4417	83.7544
3	59.1765	59.0717	83.0227	3.1852e7	2.1693e8	Undefined	58.4740	59.4776	0.7115	100.0000	50.0000
4	60.0798	60.0668	89.1772	1.6240e6	6.1594e6	Undefined	59.5780	60.4812	0.6736	5.0986	50.0000
5	173.0500	173.0187	239.3394	2.5236e6	1.7223e7	Undefined	172.4471	173.4520	0.7229	7.9229	50.0000
6	174.0549	174.0474	Undefined	4.4680e5	2.1078e6	Undefined	173.5525	174.2559	Undefined	1.4027	87.9812
7	174.9593	175.0612	237.1904	2.4469e7	1.7168e8	Undefined	174.5573	175.5617	0.7381	76.8215	50.0000
8	176.0635	176.1104	262.3466	2.6356e6	1.4569e7	1	175.6620	176.4650	0.6713	8.2745	50.0000
9	177.0672	177.0476	265.6308	7.2800e5	4.0984e6	1	176.5654	177.4687	0.6665	2.2856	50.0000
10	612.4245	612.4245	Undefined	3.8320e5	1.3760e6	Undefined	612.4245	613.0305	Undefined	1.2031	100.0000
11	614.4450	614.3404	696.0333	4.3380e5	3.3590e6	Undefined	613.7379	614.8491	0.8826	1.3619	50.0000
12	616.3644	616.3409	843.5254	1.3294e6	9.4090e6	1	615.7583	616.8652	0.7307	4.1737	50.0000
13	617.3641	617.3607	Undefined	4.7720e5	3.1644e6	1	616.8652	617.9627	Undefined	1.4982	54.7360
14	619.4594	619.4507	Undefined	9.0480e5	7.4368e6	Undefined	617.9627	619.5591	Undefined	2.8406	94.3744
15	904.5486	904.5497	5112.6356	4.1820e5	3.1972e6	Undefined	903.9424	905.1666	0.8130	1.3129	50.0000

Table 5-1 Right-click Menu for the Spectral Peak List Tab

Menu	Function
Column Options	Opens the **Select Columns for Peak List** dialog.
Save As Text	Saves the data as a .txt file.
Delete Pane	Deletes the selected pane.

Table 5-2 Right-click Menu for the Chromatographic Peak List Tab

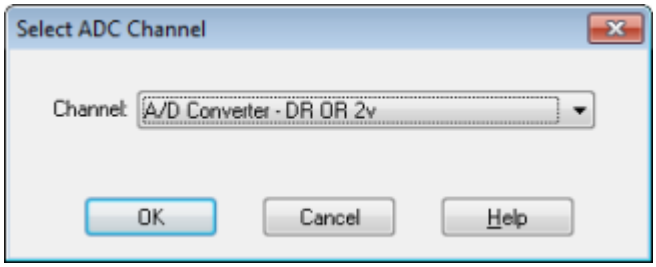
Menu	Function
Show Peaks in Graph	Show the peaks in two colors in the graph.
IntelliQuan Parameters	Opens the **Intelliquan** dialog.
Save As Text	Saves the data as a txt file.
Delete Pane	Deletes the selected pane.

Show ADC Data

Analog-to-digital converter (ADC) data is acquired from a secondary detector, for example from a UV detector through an ADC card, and is useful for comparison with mass spectrometer data. To make ADC data available, acquire the ADC data and the mass spectrometer data simultaneously. Both types of data are then saved in the same file.

1. Make sure that the project folder where the ADC data is stored is selected. For example, click the `Example` folder.
2. On the Navigation bar, under **Explore**, double-click **Open Data File**.
   The Select Sample dialog opens.
3. In the **Data Files** field, double-click the sub-data folder (if applicable), and then click the data file to be opened. For example, in the `Example` folder, double-click **Devices** and then click **Adc16chan.wiff**.
4. In the **Samples** list, select a sample, and then click **OK**.
5. Click **Explore** > **Show** > **Show ADC Data**.

Figure 5-3 Select ADC Channel Dialog

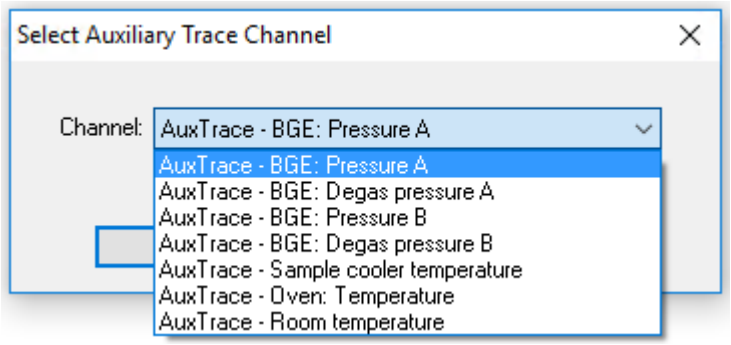


6. In the **Channel** list, select a channel, and then click **OK**.
   The ADC data is shown in a new pane beneath the active pane.

Show Auxiliary Traces

1. Make sure that the correct project folder is selected.
2. On the Navigation bar, under **Explore**, double-click **Open Data File**.
   The Select Sample dialog opens.
3. In the **Data Files** field, click the data file that was acquired after the auxiliary trace monitoring was enabled.
4. In the **Samples** list, select a sample, and then click **OK**.
5. Click **Explore** > **Show** > **Show Auxiliary Traces**.

Figure 5-4 Select Auxiliary Trace Channel dialog

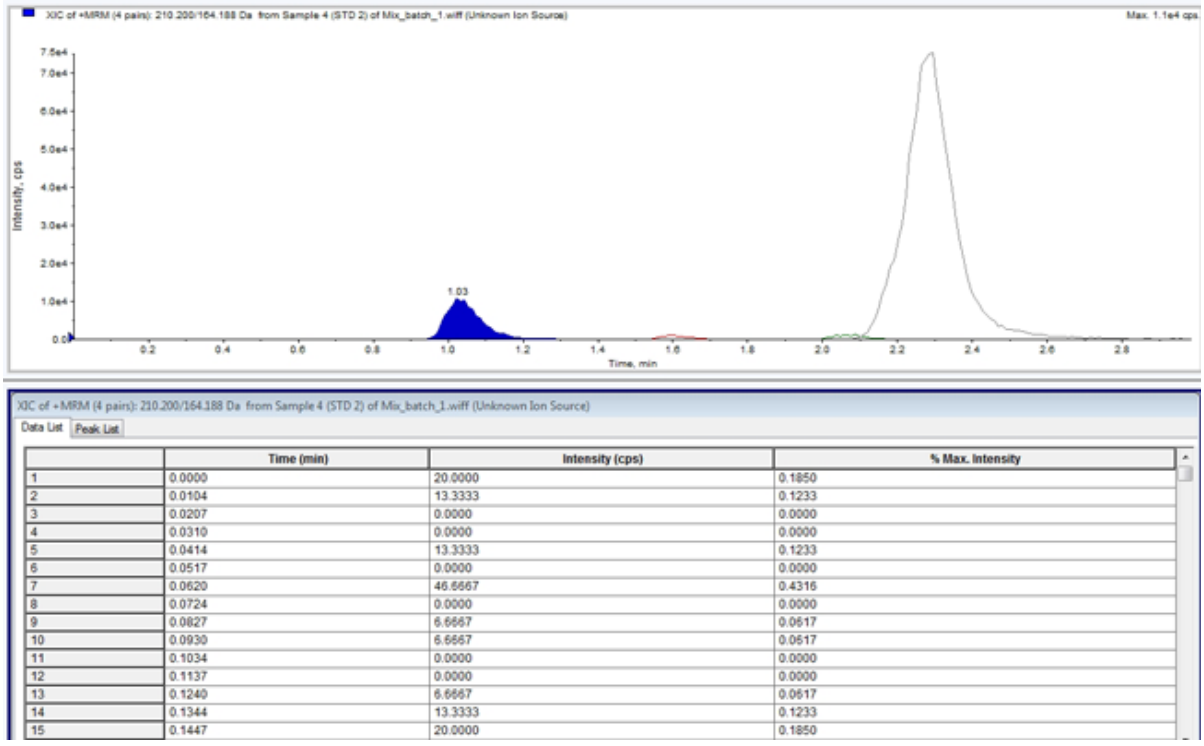


6. In the **Channel** list, select a channel, and then click **OK**.
   The selected auxiliary trace is shown in a new pane below the active pane.

Show Basic Quantitative Data

1. Open a data file.
2. Click **Explore** > **Show** > **Show List Data**.

Figure 5-5 List Data



	Time (min)	Intensity (cps)	% Max. Intensity
1	0.0000	20.0000	0.1850
2	0.0104	13.3333	0.1233
3	0.0207	0.0000	0.0000
4	0.0310	0.0000	0.0000
5	0.0414	13.3333	0.1233
6	0.0517	0.0000	0.0000
7	0.0620	46.6667	0.4316
8	0.0724	0.0000	0.0000
9	0.0827	6.6667	0.0617
10	0.0930	6.6667	0.0617
11	0.1034	0.0000	0.0000
12	0.1137	0.0000	0.0000
13	0.1240	6.6667	0.0617
14	0.1344	13.3333	0.1233
15	0.1447	20.0000	0.1850

3. On the Peak List tab, right-click and then select **Show Peaks in Graph**.
   Peaks are shown in two colors.
4. To change the peak finding algorithm settings, right-click and then select either **Analyst Classic Parameters** or **Intelliquan Parameters**, whichever is active.
5. (Optional) To remove the colored peaks, right-click in the Peak List tab and then clear **Show Peaks in Graph**.

Chromatograms

A chromatogram is a graphical view of the data obtained from the analysis of a sample. It plots the signal intensity along an axis that shows either time or scan number. For more information about software functionality available for chromatograms, and on using the Chromatogram Panes right-click menu, refer to the section: Chromatogram Panes.

The software plots intensity, in counts per second (cps), on the Y-axis against time on the X-axis. Peaks above a set threshold are labeled automatically. In the case of LC-MS, the chromatogram is often shown as a function of time. For a description of the types of chromatograms, refer to the table: Table 5-3.

For more information about using the available icons, refer to the table: Table 5-5.

Table 5-3 Types of Chromatograms

Types of Chromatograms	Purpose
Total Ion Chromatogram (TIC)	A chromatogram generated by plotting the intensity of all ions in a scan against time or scan number. When a data file is opened, it is preset to open as a TIC. If the experiment contains only one scan, then it is shown as a spectrum. If the **MCA** check box is selected during acquisition of the data file, then the data file opens to the mass spectrum. If the **MCA** check box is not selected, then the data file opens as the TIC.
Extracted Ion Chromatogram (XIC)	An chromatogram created by taking intensity values at a single, discrete mass value, or a mass range, from a series of mass spectral scans. It indicates the behavior of a given mass, or mass range, as a function of time.
Base Peak Chromatogram (BPC)	A chromatogram that shows the intensity of the most intense ion within a scan versus time or scan number.

Table 5-3 Types of Chromatograms (continued)

Types of Chromatograms	Purpose
Total Wavelength Chromatogram (TWC)	A chromatogram created by summing all of the absorbance values in the acquired wavelength range and then plotting the values against time. It consists of the summed absorbances of all ions in a scan plotted against time in a chromatographic pane.
Extracted Wavelength Chromatogram (XWC)	A subset of TWC. An XWC shows the absorbance for a single wavelength or the sum of the absorbance for a range of wavelengths.
Diode Array Detector (DAD)	A chromatogram that shows the absorption spectrum of eluting compounds at one or more wavelengths.

Show TICs from a Spectrum

To see an example data file, make sure that the `Example` project is selected.

To see an LIT spectrum, open the `LIT` folder, and then open the `Reserpine.wiff` file.

To see a triple quadrupole spectrum, open the `Triple Quad` folder, and then open the `Mix_batch_1.wiff` file.

- Click **Explore** > **Show** > **Show TIC.**
  The TIC opens in a new pane.

  Tip! Right-click inside a pane containing a spectrum and then click **Show TIC**.

For information on using the **Spectra Panes** right-click menu, refer to the section: Spectra Panes

Show a Spectrum from a TIC

A TIC is created by summing the intensity contributions of all ions from a series of mass scans. Use the TIC to view an entire data set in a single pane. It consists of the summed intensities of all of the ions in a scan plotted against time in a chromatographic pane. If the data contains results from multiple experiments, then a TIC for each experiment can be created below the TIC that represents the sum of all of the experiments.

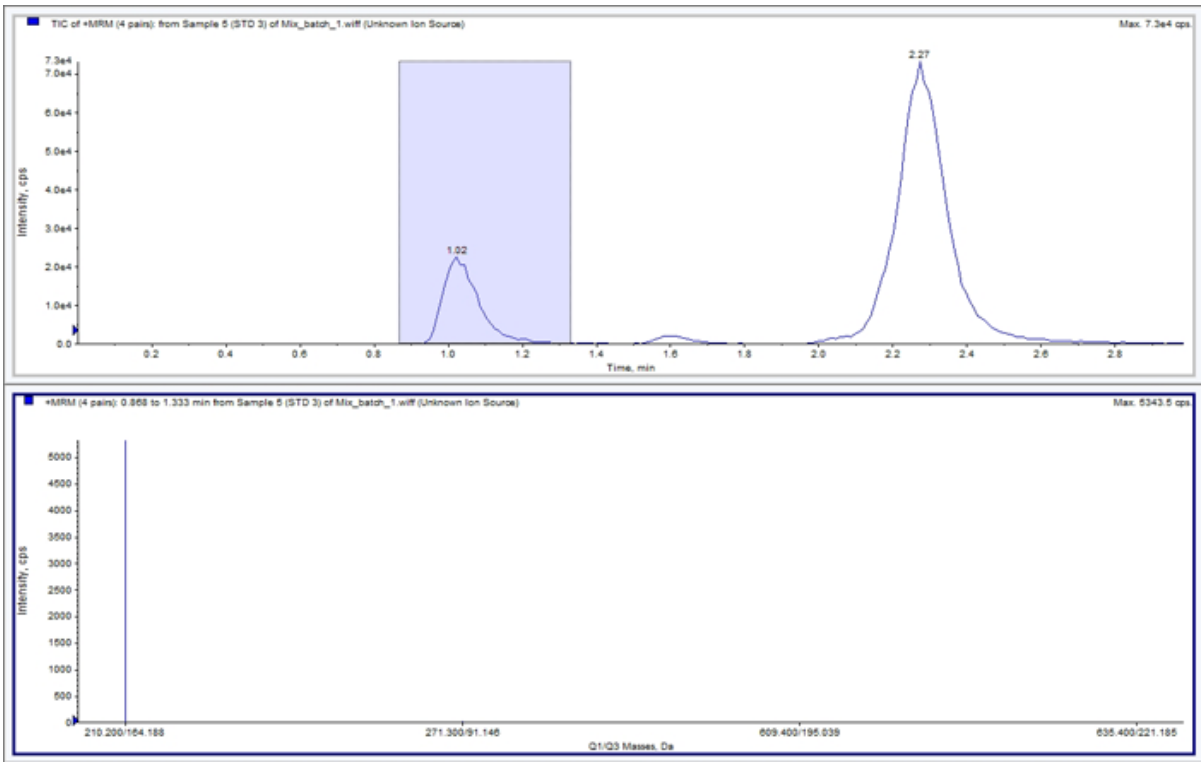
When a data file is opened, it is preset to be shown as a TIC. However, if the experiment contains only one scan, it is shown as a spectrum. If the user selects the **MCA** check box before acquiring the data file, then the data file opens to the mass spectrum. If the **MCA** check box is not selected, then the data file opens with the TIC.

For information on using the Spectra Panes right-click menu, refer to the section: Spectra Panes.

1. In a pane containing a TIC, select a range.
2. Click **Explore** > **Show** > **Show Spectrum.**
   The spectrum opens in a new pane.

Tip! Double-click in the TIC pane at a particular time to show the spectrum.

Figure 5-6 Example of a TIC



Generate XICs

XICs can be generated only from single-period, single-experiment chromatograms or spectra. To obtain an XIC from multi-period or multi-experiment data, split the data into separate panes by clicking the triangle under the X-axis. For more information about using the available icons, refer to the table: Table 5-5.

Several methods are available for extracting ions to generate an XIC, depending on whether chromatographic or spectral data is used. For a summary of methods that can be used with chromatograms and spectra, refer to the following table.

Table 5-4 Summary of XIC Generation Methods

Method	Use with Chromatogram	Use with Spectrum	Extraction
Selected range	No	Yes	Extracts ions from a selected area in a spectrum.
Maximum	No	Yes	Extracts ions from a selected area in a spectrum using the most intense peak in the selected area. This option creates an XIC using the maximum mass from the selected spectral range.
Base peak masses	Yes	Yes	Can be used only with Base Peak Chromatograms (BPCs). Use the **Use Base Peak Masses** command to extract ion results in an XIC with a different colored trace for each mass. If the selection includes multiple peaks, then the resulting XIC will have an equal number of colored traces, one for each mass.
Specified masses	Yes	Yes	Extracts ions from any type of spectrum or chromatogram. Select up to ten start and stop masses for which to generate XICs.

Generate an XIC Using a Selected Range

1. Open a data file containing spectra.
2. Select a range by pressing the left mouse button at the start of the range, dragging the cursor to the end of the range, and then releasing the left mouse button.
   The selection is shown in blue.
3. Click **Explore** > **Extract Ions** > **Use Range.**
   An XIC of the selection opens in a pane below the spectrum pane. The experiment information at the top of the pane contains the mass range and the maximum intensity in counts per second.

Generate an XIC Using the Maximum Peak

1. Open a data file containing spectra.

2. Select a range in a spectrum.
   The selection is shown in blue.
3. Click **Explore** > **Extract Ions** > **Use Maximum.**
   An XIC of the maximum peak specified selection opens below the spectrum pane. The experiment information at the top of the pane contains the mass range and the maximum intensity in counts per second.

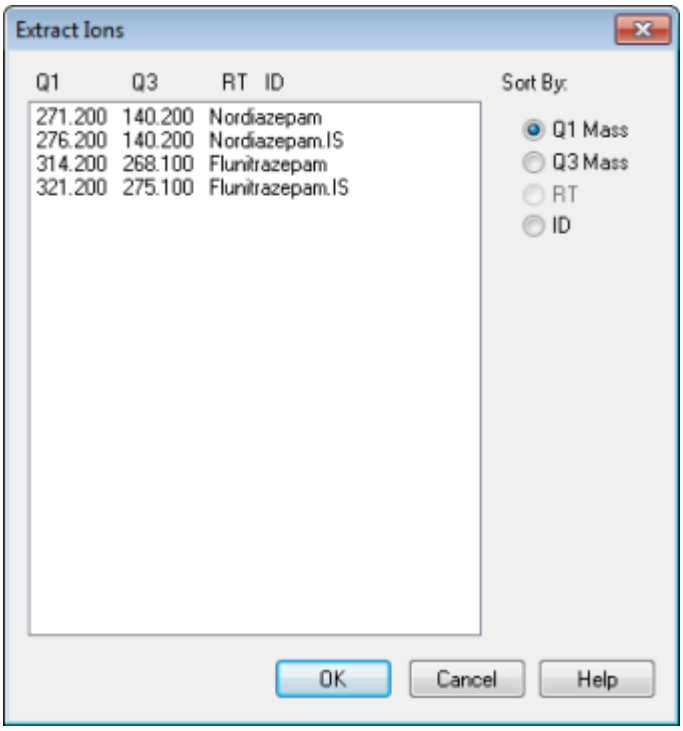
Generate an XIC Using Base Peak Masses

1. Open a data file containing spectra.
2. In a BPC, select the peak from which to extract ions.
   The selection is shown in blue.
3. Click **Explore** > **Extract Ions** > **Use Base Peak Masses.**
   An XIC of the specified selection opens below the spectrum pane. The experiment information at the top of the pane shows the mass range and the maximum intensity in counts per second.

Extract Ion by Selecting Masses

1. Open a spectrum or chromatogram.
2. Click **Explore** > **Extract Ions** > **Use Dialog.**

Figure 5-7 Extract Ions Dialog



3. Type the values for each XIC to be created.
   - In the **Start** field, type the start value (lower value) for the mass range.
   - In the **Stop** field, type the stop value (higher value) for the mass range.

   Note: If a stop value is not typed, then the range is defined by the start value.

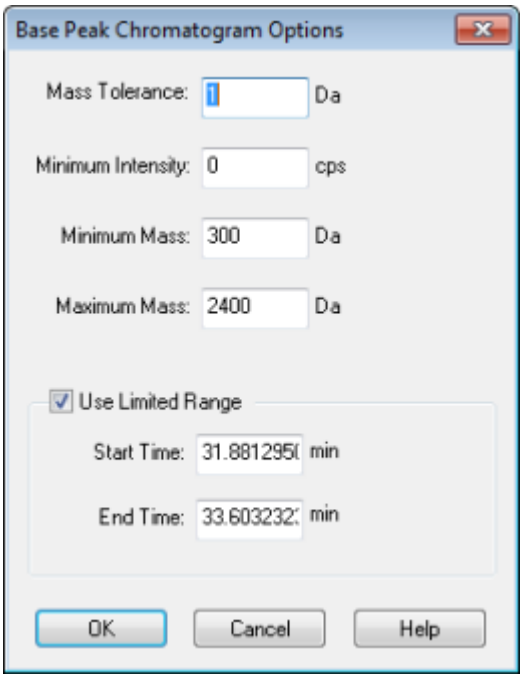
4. Click **OK**.
   An XIC of the selection opens below the chromatogram pane. The experiment information at the top of the pane includes the masses and the maximum intensity in counts per second.

Generate BPCs

BPCs can be generated only from single-period, single-experiment data.

1. Open a data file.
2. Select an area within a TIC.
   The selection is shown in blue.
3. Click **Explore** > **Show** > **Show Base Peak Chromatogram.**
   The selections are shown in the **Start Time** and **End Time** fields.

Figure 5-8 Base Peak Chromatogram Options



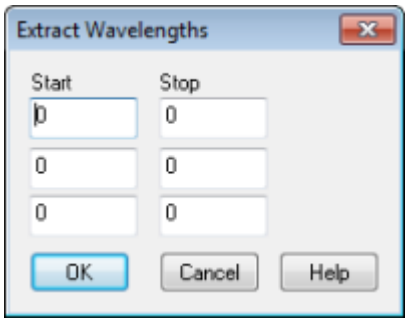
4. In the **Mass Tolerance** field, type the value to indicate the mass range used to find a peak. The software finds the peak using a value twice the typed range (± the mass value).
5. In the **Minimum Intensity** field, type the intensity below which peaks are ignored by the algorithm.
6. In the **Minimum Mass** field, type the mass at the beginning of the scan range.
7. In the **Maximum Mass** field, type the mass at the end of the scan range.
8. To set the start and end times, select the **Use Limited Range** check box and do the following:
   - In the **Start Time** field, type the time when the targeted range of the experiment starts.
   - In the **End Time** field, type the time when the targeted range of the experiment ends.
9. Click **OK**.
   The BPC is generated in a new pane.

Generate XWCs

An XWC is a wavelength chromatogram created by taking intensity values at a single wavelength, or by taking the sum of the absorbance for a range of several wavelengths. Up to three ranges can be extracted from a DAD spectrum to generate the XWC. For more information about using the available icons, refer to the table: Table 5-5.

1. Open a data file that contains a DAD spectrum.
2. Right-click anywhere in the pane and then click **Extract Wavelengths**.

Figure 5-9 Extract Wavelengths Dialog



3. Type **Start** and **Stop** values.
4. Click **OK**.
   The XWC is shown in a pane below the DAD spectrum.

Show DAD Data

Like mass spectrometer data, DAD data can be viewed in chromatogram or spectrum form. Users can view the DAD spectrum for a single point in time, or for a range of time as a Total Wavelength Chromatogram (TWC).

1. Open a data file containing data acquired with a DAD.
   The TWC, which is analogous to a TIC, opens in a pane below the TIC.
2. In the TWC pane, click a point to select a single point in time, or highlight an area of the spectrum to select a range of time.
3. Click **Explore** > **Show** > **Show DAD Spectrum.**
   The DAD spectrum opens in a pane below the TWC. The Y-axis shows the absorbance and the X-axis shows the wavelength.

Tip! If the pane with the TWC is closed, then click a point anywhere in the TWC to open it again. Click **Explore** > **Show** > **Show DAD TWC.**

Generate TWCs

A TWC is a less commonly used chromatogram. It shows the total absorbance (mAU) as a function of time. The TWC provides a way of viewing an entire data set in a single pane. It consists of the summed absorbances of all ions in a scan plotted against time in a chromatogram. If the data contains results from multiple experiments, then a TWC for each experiment can be created below the TWC that represents the sum of all of the experiments.

A TWC shows total absorbance (mAU) on the Y-axis plotted against time on the X-axis. For more information about using the available icons, refer to the table: Table 5-5.

1. Open a data file that contains a DAD spectrum.
2. Click **Explore** > **Show** > **Show DAD TWC.**
   The TWC is shown in a pane below the DAD spectrum.

Tip! Right-click inside the pane containing the DAD spectrum and then click **Show DAD TWC**.

Adjust the Threshold

The threshold is an invisible line drawn parallel to the X-axis of a graph that sets a limit below which the software will not include peaks in a spectrum. The line has a handle, represented by a blue triangle to the left of the Y-axis. Click the blue triangle to view a dotted line that represents the threshold. The threshold can be raised or lowered, but changing the threshold value does not change the data. The software does not label any peaks in the region that lies below the threshold.

1. Open a data file.
2. Do one of the following:
   - To increase the threshold, drag the blue triangle up the Y-axis.
   - To decrease the threshold, drag the blue triangle down.
   - Click **Explore** > **Set Threshold.** In the Threshold Options dialog that opens, type the threshold value and then click **OK**.
   - Click **Explore** > **Threshold.**

   The graph updates to show the new threshold. Peak labeling and the peak list are also updated.

Tip! To view the current threshold value, move the pointer over the threshold handle.

Graphs

The same data can be examined in different ways. Data can also be kept for comparison purposes before performing processing operations such as smoothing or subtraction.

A window contains one or more panes arranged in such a way that all the panes are fully visible and that they do not overlap.

Panes might be of a variable or fixed size. Panes are automatically tiled within the window and are arranged into column and row format. If the size of a window is changed, then the panes

within the window change in size to accommodate the new size. A window cannot be sized to the point where any of the panes become smaller than their minimum size.

Two or more windows or panes containing similar data can be linked, for example, spectra with similar mass ranges. As one pane or window is zoomed in, the other pane zooms in simultaneously. For example, the user can link an XIC to the BPC from which the XIC was extracted. Zooming in the BPC also zooms the XIC, so that both chromatograms show the same magnification.

Manage Data

- Use the following menu options or icons to manage data in graphs.

Table 5-5 Graph Options

To Do This	Use This Menu Option	Or Click This Icon
Copy a graph to a new window	Select the graph to copy. Click **Explore** > **Duplicate Data** > **In New Window.**	
Rescale a graph to its original size	Select the graph. Click **Explore** > **Home Graph.**	
Move a pane	• Select the graph. Click **Window** > **Move Pane.** • Select the pane or window and then drag it to the new position. This position can be inside the same window or within another window. A four-headed arrow is shown when the cursor is on the boundary of the active window or pane. • If the pane is at the top or bottom of the target pane, then the pane moves above or below that pane, respectively. • If the pane is at the left or right of the target pane, then the pane moves to the left or right of that pane, respectively. • If the pane is at any other position, then the pane moves to the target row. The drop shadow of the pane as the pane is moved indicates its new position.	

Table 5-5 Graph Options (continued)

To Do This	Use This Menu Option	Or Click This Icon
Link panes	a. With the two graphs open, click one to make that pane active. b. Click **Explore** > **Link** and then click the other pane.	
Remove linking	Close one of the panes. Click **Explore** > **Remove Link.**	
Delete a pane	Select the graph. Click **Window** > **Delete Pane.**	
Lock a pane	Select the graph. Click **Window** > **Lock Panes.**	
Hide a pane	Select the graph. Click **Window** > **Hide Pane.**	
Maximize a pane	Select the graph. Click **Window** > **Maximize Pane.**	
Tile panes	Select the graph. Click **Window** > **Tile all Panes.**	

Zoom In on the Y-axis

1. Move the pointer to the left of the Y-axis on either side of the area to be expanded and then drag away from the starting point in a vertical direction while holding the left mouse button. A box is drawn along the Y-axis representing the new scale.

   Note: Take care when zooming in on the baseline. Zoom in too far and the zoom-in box closes.

2. Release the mouse button to draw the graph to the new scale.

   Tip! To return the Y-axis of the graph to the original scale, double-click either axis. To return the entire graph to the original scale, click **Explore** > **Home Graph.**

Zoom In on the X-axis

1. Move the pointer under the X-axis to either side of the area to be expanded and then drag away from the starting point in a horizontal direction while holding the left mouse button.
2. Release the mouse button to draw the graph to the new scale.

Tip! To return the X-axis of the graph to the original scale, double-click the X-axis. To return the entire graph to the original scale, click **Explore** > **Home Graph.**

Analyze and Process Quantitative Data 6

This section describes how to use the Analyst software to analyze and process quantitative data. Data can also be processed using the MultiQuant software or the SCIEX OS software. We recommend that the MultiQuant software or SCIEX OS software be used to quantitate data. Refer to the documentation that comes with the MultiQuant software or SCIEX OS software.

Use the sample files found in the `Example` folder to learn how to select samples for quantitation, how to select preset queries and create table-specific queries, and how to analyze the acquired data. For more information about the following topics, refer to the document: *Advanced User Guide*.

- Metric Plots
- Layout of a Results Table

Quantitative Analysis

Quantitative analysis is used to find the concentration of a specific substance in a sample. By analyzing an unknown sample and comparing it to standard samples, that is, samples containing the same substance with known concentrations, the software can calculate the concentration of the unknown sample. The process involves creating a calibration curve using the signal response or response ratio of the standards and then calculating the concentrations of the unknown samples. The calculated concentrations of all of the samples are added to a Results Table.

Quantitative analysis is most commonly performed using a Multiple Reactions Monitoring (MRM) scan. In an MRM scan, a precursor ion and a characteristic product ion are used to identify an MRM transition that is highly specific to the analyte. The MRM transition, coupled with the retention time for the analyte during liquid chromatography, provides the specificity required for quantitation.

Quantitation is accomplished through the use of validated MRM LC-MS/MS acquisition methods, acquisition of calibration standard curves, and the subsequent integration of the peaks related to the compounds of interest. The calibration curve relationship between signal response and concentration is used to determine the quantity of a particular analyte in an unknown sample.

Quantitation Methods

A quantitation method is a set of parameters used to generate peaks in a sample. The quantitation method can include parameters used to locate and integrate peaks, generate standard curves, and calculate unknown concentrations. A previously saved quantitation method

can be selected from the Quantitation menu in the batch. The user can create a quantitation method before data acquisition and then apply the method to the quantitative data automatically after the batch is complete. Alternatively, a quantitation method can be created and applied post-acquisition.

Three tools can be used to create a quantitation method: the Quantitation Wizard, the Build Quantitation Method, and Quick Quant.

Quantitation Wizard

With the Quantitation Wizard, a Results Table is generated at the same time as the quantitation method. Alternatively, an existing quantitation method can be used to quantitate different sets of data.

Build Quantitation Method

The Build Quantitation Method does not generate a quantitation Results Table, although the method can subsequently be used in the Quantitation Wizard to create a Results Table. The Build Quantitation Method can also be used to change existing quantitation methods. This is the most flexible way of creating a quantitation method. Refer to the section: Create a Method Using the Quantitation Method Editor.

Quick Quant

Quick Quant is not recommended for quantitation of results.

Quick Quant is part of the Batch Editor. Use Quick Quant to add compound concentrations before acquiring data. Because a sample has not been acquired, a representative sample cannot be selected, nor can peaks be reviewed. With this feature, only the method components are defined.

To use a previously saved quantitation method, select it from the **Quantitation** menu in the batch. For instructions on creating a batch, refer to the section: Create and Submit a Batch.

About Results Tables

Results tables summarize the calculated concentration of an analyte in each unknown sample based on the calibration curve. Results tables also include the calibration curves as well as statistics for the results. The user can customize the results tables and view the results tables in layouts.

The data from a results tables can be exported to a txt file for use in other applications, such as Microsoft Excel. The user can also export data in the table or just the data in the visible columns.

Quantitation Methods and Results Tables

For the following procedures, use the sample data that is installed in `Example/Triple Quad` folder. The folder contains the data files, Mix_Batch_1 and Mix_Batch_2. These sample files

are used to demonstrate the usefulness of metric plots to isolate problematic samples. The ions scanned were reserpine (609.3/195.0), minoxidil (210.2/164.2), tolbutamide (271.1/91.1) and rescinnamine (635.3/221.2), which is the internal standard. Mix_Batch_1 contains no errors, but Mix_Batch_2 contains a QC sample to which the internal standard was added twice (sample QC2).

Create a Method Using the Quantitation Method Editor

Prerequisites
• Select the project or subproject that contains the data to be quantified. Refer to the section: Change Between Projects and Subprojects

1. Make sure that the `Example` project is selected.
2. On the Navigation bar, under **Quantitate**, double-click **Build Quantitation Method**.
   The Select Sample dialog opens.
3. Double-click the **Triple Quad** folder in the **Data Files** list.
4. Select **Mix_Batch_2. wiff**.
   The samples in the selected data file are shown in the **Samples** list.

   Note: If the **Compound ID** field was populated for the samples and internal standards in the acquisition method, then in the Internal Standards table, when a value is selected in the **Q1/Q3** field, the **Name** field is automatically populated.
5. Select a sample that provides a detectable signal to select integration parameters that fit the entire batch and then click **OK**.
6. In the Internal Standards table, in the **Name** column, select **rescinnamine**. In **Q1/Q3** column, select **635.3/221.2**.
7. In the Analytes table, do the following:
   a. In the **Name** column, select **minoxidol** for the **Q1/Q3** column masses of **210.2/164.188**, **tolbutamide** for **271.3/91.146**, and **reserpine** for **609.4/195.039**.
   b. In the **Internal Standard** column, from the list, select the **rescinnamine** as internal standard to be associated with each analyte.
   c. Delete **635.4/221.185** from the **Q1/Q3** column in the Analytes table.

   Note: If the **Compound ID** field was populated for the samples and internal standards in the acquisition method, then in the Analytes table, the **Name** field and **Q1/Q3** field are populated.
8. Open the Integration tab.
   The preset integration parameters are suitable for most peaks.

9. If the integration is not suitable, then change the algorithm. Refer to the section: Manually Integrate Peaks.
10. Click **Show or Hide Parameters** () to show the additional integration algorithms.
11. Open the Calibration tab.
    The preset parameters are suitable for these samples. User can change the fit, weighting, and regression parameter depending on the specific applications.
12. Save the quantitation method.
    The new method can be used when a batch is created in the Batch Editor or when the Quantitation Wizard is used to generate a Results Table.

Tip! The quantitation method can only be used in the current project unless it is copied to another project. To do this, click **Tools** > **Project** > **Copy Data**. A new project must be created and selected to be available for use.

Create a Results Table Using the Quantitation Wizard

Prerequisites
• Select the project or subproject that contains the data to be quantified. Refer to the section: Change Between Projects and Subprojects

1. On the Navigation bar, under **Quantitate**, double-click **Quantitation Wizard**.
   The Create Quantitation Set - Select Samples page opens.
2. In the **Available Data Files** list, double-click the **Triple Quad** folder.
3. Select **Mix_batch_2. wiff**.
4. Click **Add All**.

Note: We recommend that users do not process or report results from any sample for which acquisition was abnormally or unexpectedly terminated.

5. Click **Next**.
   The Create Quantitation Set - Select Settings & Query page opens.
6. Click **Select Existing: Query** in the **Default Query** section.
7. Select **Accuracy 15%** from the **Query** list.

Note: To create a query at the same time, refer to the section: Create a Results Table Using the Quantitation Wizard.

Note: It is the responsibility of the user to evaluate and validate the query to be used for specific applications.

8. Click **Next**.
   The Create Quantitation Set - Select Method page opens.
9. Click **Choose Existing Method**.
10. Select **PK Data_Mix.qmf** from the **Method** list.
11. Click **Finish**.
    The Results Table opens.

Tip! To add or remove samples in the Results Table, click **Tools** > **Results Table** > **Add/ Remove Samples.**

12. Review the sample type, actual concentration, peak integration, calibration curves, statistics pane, metric plot for the internal standard, and other information related to data quantitation.
13. Save the Results Table.

Note: We recommend that users do not change datafile (wiff) names if a Results Table includes samples from that file.

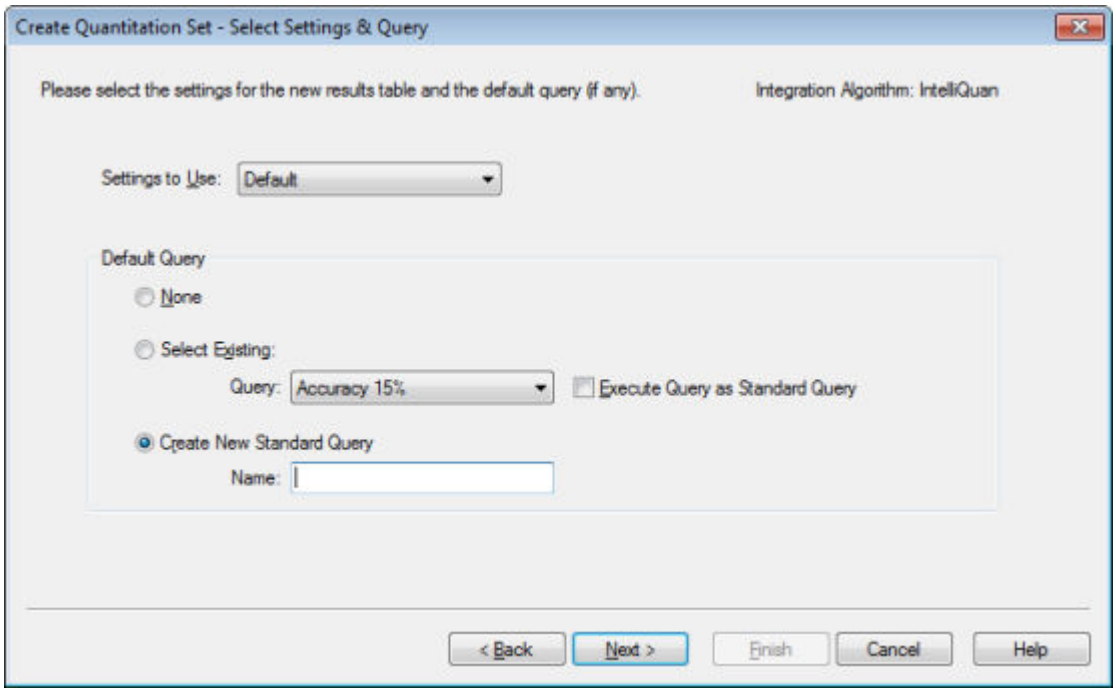
Tip! Well-formatted reports can be created from a Results Table using the Reporter software. We recommend that the user validate the results if a Reporter template that contains a query is used. Refer to the section: Reporter Software.

Create a Standard Query (Optional)

Advanced users can create a query and a standard query numerous ways. The following is one example.

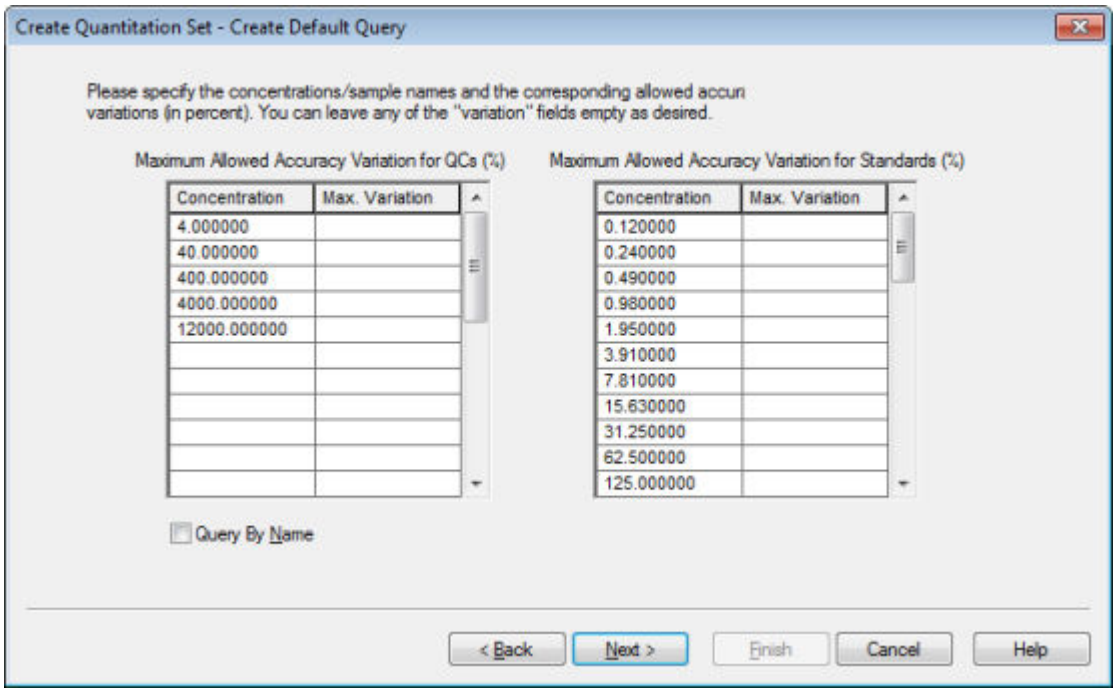
1. On the Navigation bar, under **Quantitate**, double-click **Quantitation Wizard**.
   The Create Quantitation Set - Select Samples page opens.
2. Select samples to be used as part of the quantitation set.
3. Click **Next**.
   The Select Settings & Query page opens.
4. In the **Default Query** section, select **Create New Standard Query**.
5. Type a query name.

Figure 6-1 Create Quantitation Set — Select Settings & Query Page



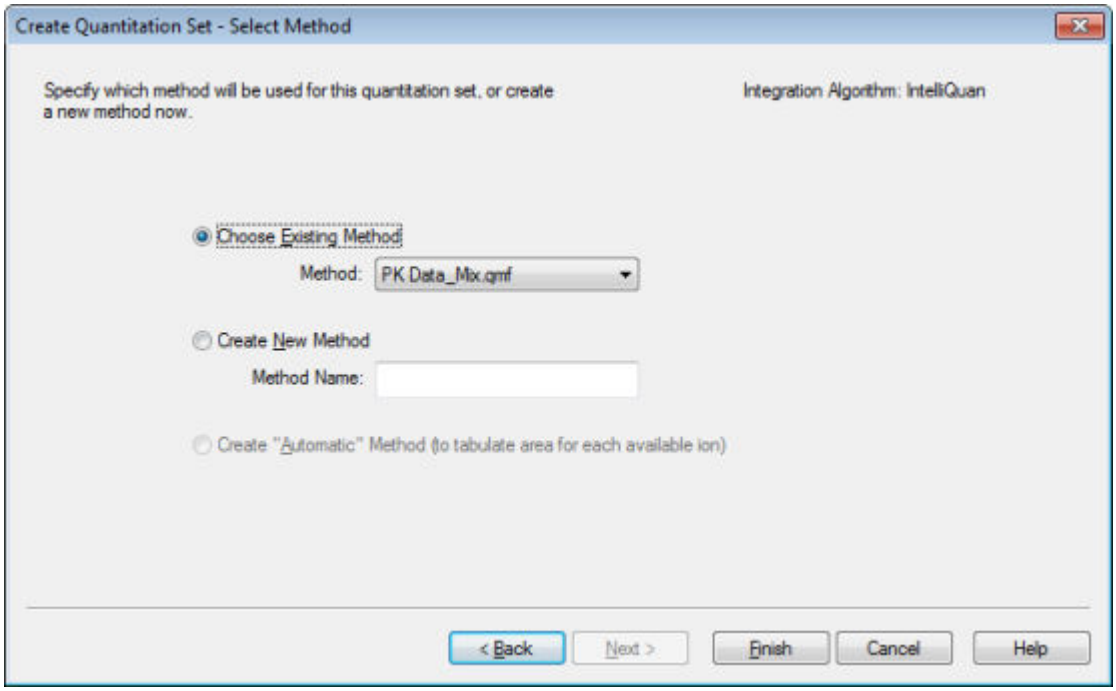
6. Click **Next**.

Figure 6-2 Create Quantitation Set — Create Default Query Page



7. In the **Maximum Allowed Accuracy Variation for QCs (%)** table in the **Max. Variation** column, type the maximum allowable percent of variation for each QC, for example 5 is ± 5%, in the same row as the corresponding concentration. If the concentrations were not specified during acquisition, then they are not shown. In this case, type them in the **Concentration** column.
8. In the **Maximum Allowed Accuracy Variation for Standards (%)** table, in the **Max. Variation** column, type the maximum allowable percent of variation for each standard, for example 10 is ±10%, in the same row as the corresponding concentration. If the concentrations were not specified during acquisition, then they are not shown. Type the concentrations in the **Concentration** column.
9. Click **Next**.

Figure 6-3 Create Quantitation Set — Select Method Page



10. Select or create a method.
11. Click **Finish**.
    The query is applied as a standard query. The query results are shown as a Pass or Fail entry in the **Standard Query Status** column of the Results Table.

Tip! To return to the full view, right-click and then click **Full**.

Peak Review and Manual Integration of Peaks

Use peak review to survey the peaks that the software has identified and then redefine the peak or the start and end points where required.

After identifying the analytes and internal standards that the software must find, the software searches for the peaks in the samples. When the software identifies a peak, it shows the chromatograms for each analyte and internal standard in the Create Quantitation Method: Define Integration page of the Standard Wizard or on the Integration tab of the Full Method Editor. The user can confirm the peaks that are found or change the quantitation method to better define the peaks. We recommend that users manually review all integration results.

Review Peaks

During peak review, the user might want to view a peak in its entirety or to examine the baseline to find out how well the software found the start and end points of the peak. The automatic zooming feature can be used to do either.

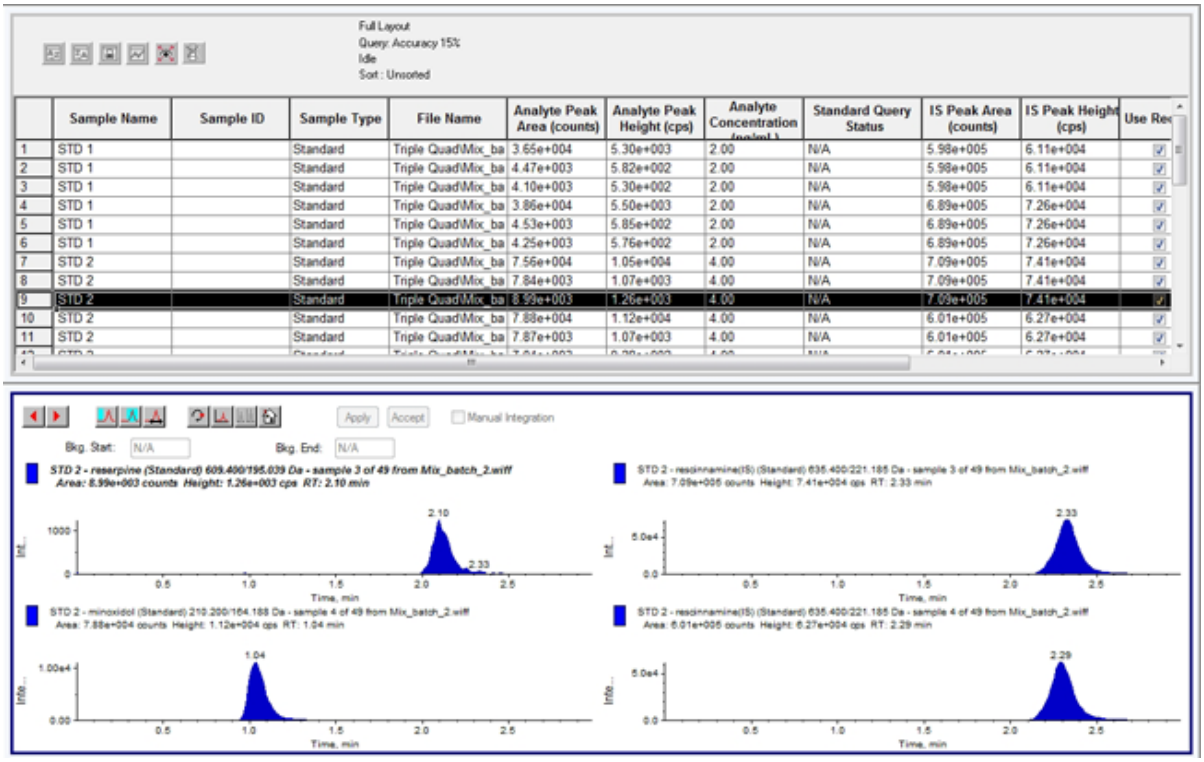
To help the software find a peak, define the exact start and end points of the peak and background manually. These changes will apply only to that individual peak unless the global method is updated.

Note: We recommend that manually integrated results be validated.

Tip! To review an individual peak, right-click on a point on the curve and then click **Show Peak**. The software opens the Peak Review window with the selected peak.

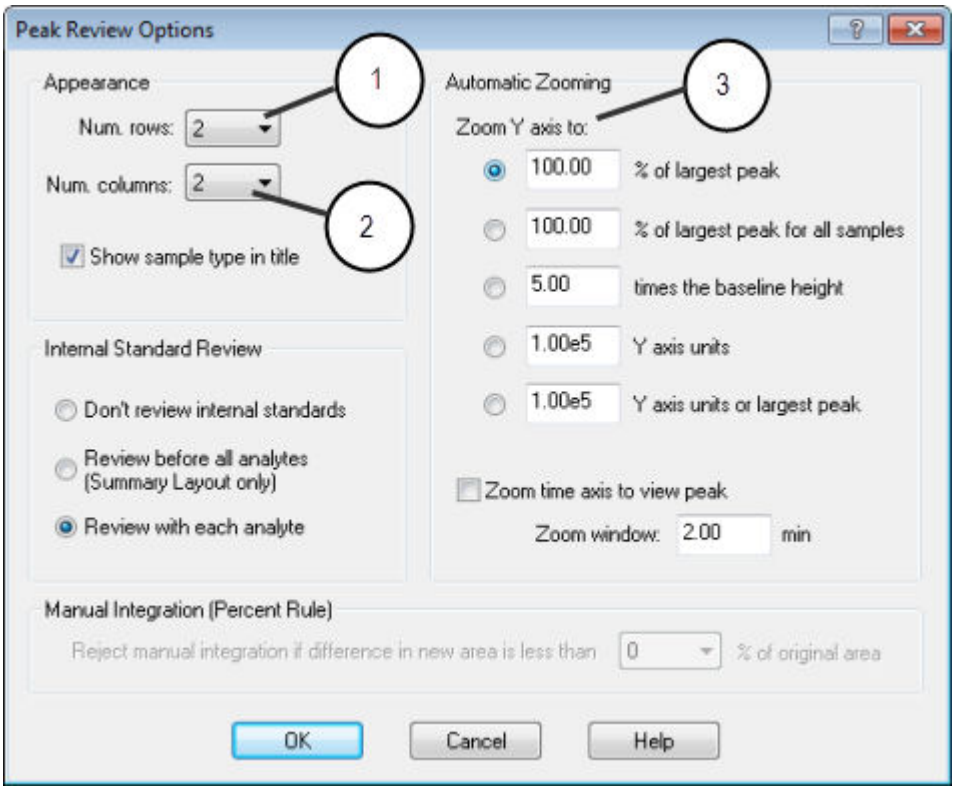
1. Right-click the Results Table and then click **Analyte**.
2. Select an analyte.
3. Click **Tools** > **Peak Review** > **Pane.**
   The peaks are shown below the Results Table with only the peaks listed in the Results Table.

Figure 6-4 Peak Review



4. Right-click the pane and then click **Options**.
   The Peak Review Options dialog opens.
5. In the **Appearance** section, change **Num. rows** to **1** and **Num. columns** to **2**.
6. In the **Automatic Zooming** section, click **Zoom Y axis to: 100% of largest peak** to show the entire peak.

Figure 6-5 Peak Review Options Dialog

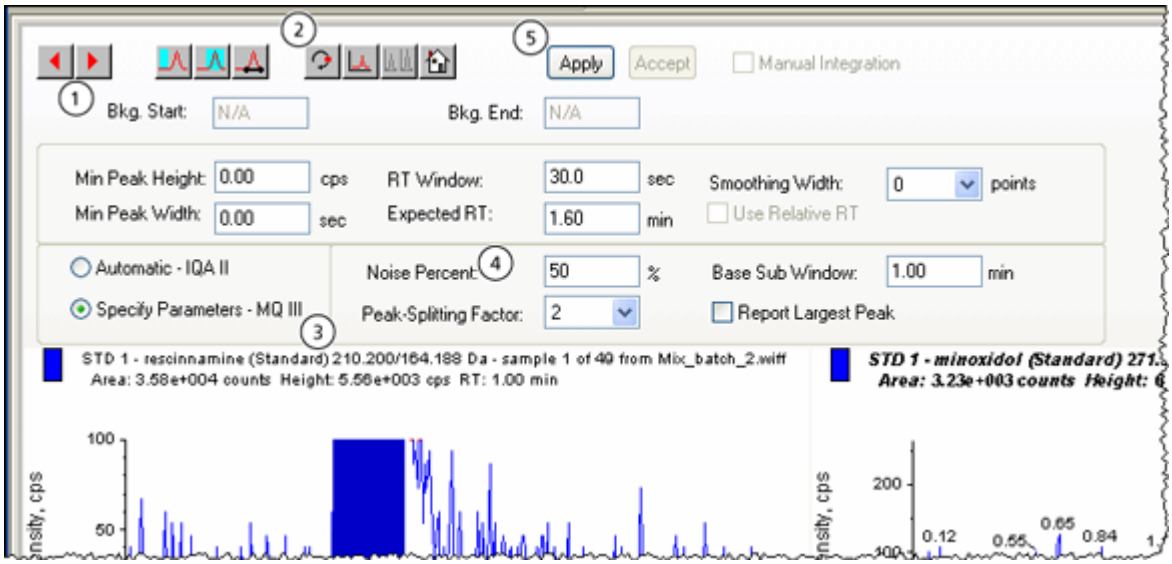


Item	Definition
1	Number of rows
2	Number of columns
3	**Zoom Y-axis to** 100% **of largest peak** to show the entire peak

7. Click **OK**.
8. To move through the peaks, click the right-pointing arrow. Refer to the figure: Figure 6-6.
9. Go to the second injection of standard 3.
   In this example, the peak can be integrated closer to the baseline by selecting the **Specify Parameters** option.

Tip! To move to a specific peak in the Peak Review pane, select the corresponding row in the Results Table.

Figure 6-6 Peak Review Pane



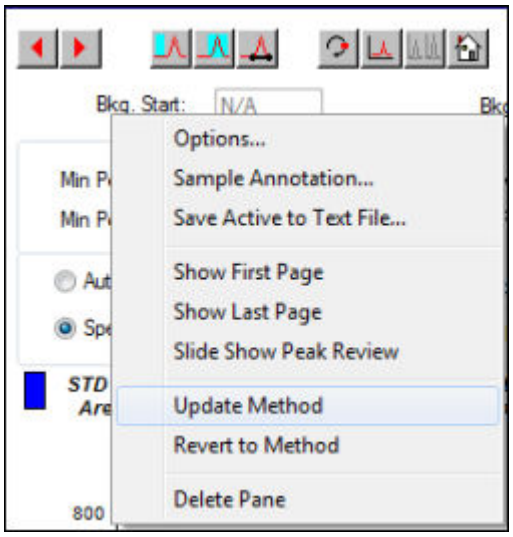
Item	Definition
1	Arrows: Click to move through the peaks.
2	**Show or Hide Parameters**: Click to show the integration parameters.
3	Integration parameters: Click to change the parameters.
4	**Noise Percentage**: Type a noise percentage.
5	**Apply**: Click to integrate the parameters.

10. Click **Show or Hide Parameters** twice.
11. Click **Specify Parameters - MQ III**.
12. Change the **Noise Percent** value.
13. Click **Apply**.
    The peak is integrated closer to the baseline.
14. If the change does not improve the peak integration, then adjust the **Noise Percent** parameter until the optimal value is found.

Note: The **Update Method** option only updates the algorithm values for that specific analyte (or internal standard) and not all analytes.

15. To update the algorithm for all peaks, right-click in the pane and then click **Update Method**.

Figure 6-7 Update Method



Manually Integrate Peaks

Manually integrating peaks should be done last, to limit person-to-person variability. Manually integrate peaks only if all the peaks have not been found after the algorithm parameters have been adjusted and updated. We recommend that users validate the results to determine whether manual integration is acceptable for specific applications.

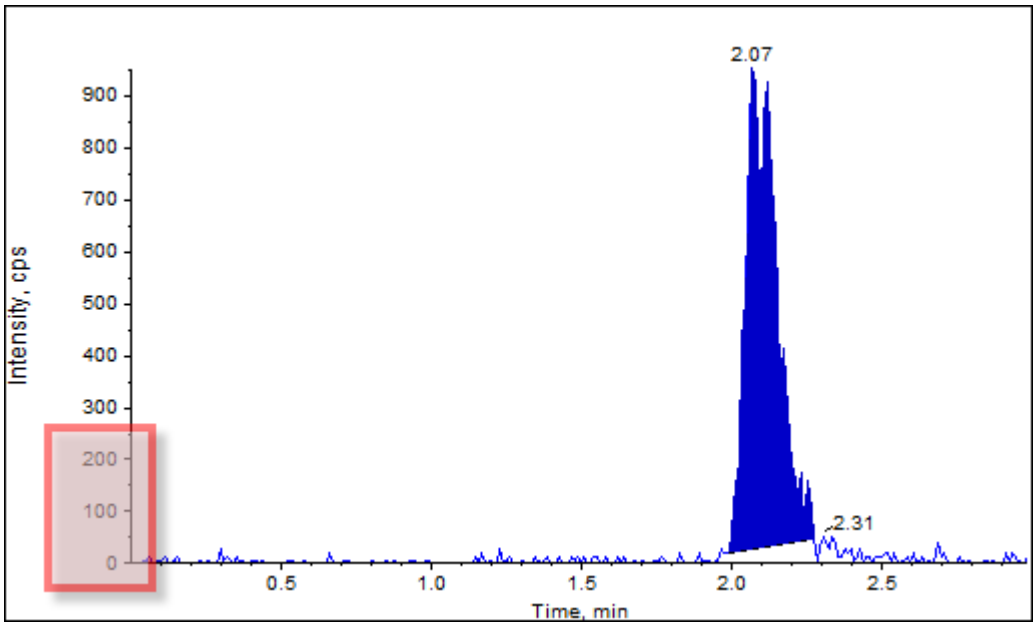
Note: Peaks that are manually integrated, or where the algorithm was changed for only that peak, are identified in the **Record Modified** column of the Results Table, as are peaks that have algorithm parameter changes for a sample that are not applied to the entire analyte group.

1. In the **Peak Review** pane, click **Manual Integration Mode**.

Figure 6-8 Peak Review Pane: Manual Integration Mode

2. Zoom in on the lower 10% of the peak.

Figure 6-9 Peak Review Pane: Zooming in on a Peak



3. Move the cross-hair to where the start of the peak is to be defined and then drag the cross-hair to where the end of the peak is to be defined.
   The software shades the area bounded by the base and sides of the peak. Peak parameters are gray because they are no longer applicable because the peak was drawn manually.
4. Do one of the following:
   - To make this change permanent, click **Accept**.
   - To discard the changes, clear the **Manual Integration** check box.

Tip! If a peak was correct as originally selected, right-click the peak and then click **Revert to Method**.

Calibration Curves

Use calibration curves to find the calculated concentration of samples, including quality control (QC) samples. QC samples are added to a batch to estimate the data quality and accuracy of standards in the batch. QC samples have known analyte concentrations but are treated as unknowns so that the measured concentrations can be compared to the actual value.

The calibration curve is generated by plotting the concentration of the standard against its area or height. If an internal standard is used, then the ratio of the standard concentration or internal standard is plotted against the ratio of the standard peak height or area to the internal standard peak height or area. The area or height ratio of a sample is then applied to this curve to find the concentration of the sample, as shown in the Results Table. A regression equation is generated

by this calibration curve according to the regression that was specified. The regression equation is used to calculate the concentration of the unknown samples.

For information on using the Calibration Curve right-click menu, refer to the section: Calibration Curve.

View Calibration Curves

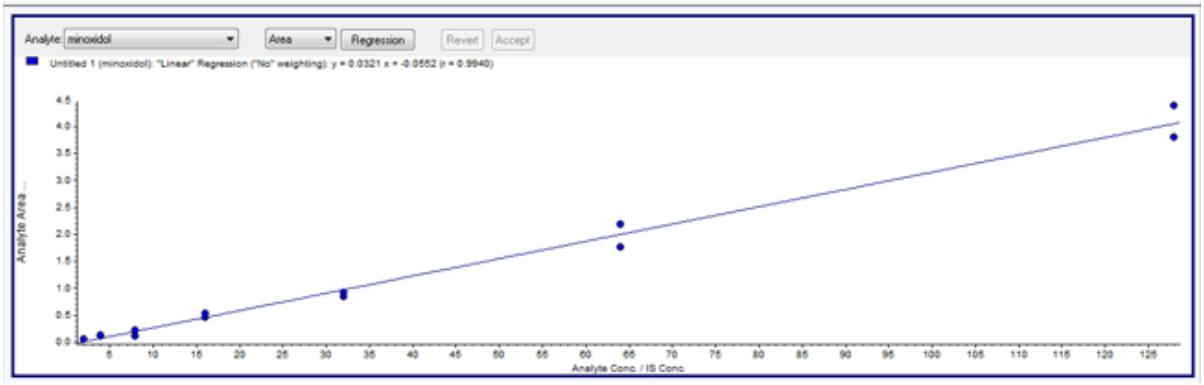
The user can view the calibration curve and change the regression options in an open Results Table. If two or more Results Tables are open, then the calibration curves can be overlaid. To overlay curves, make sure that the method used to create the tables is the same.

Plot a calibration curve to see the curve used for regression. The **Calculated Concentration** column in the Results Table reflects any changes resulting from the fit of the curve to the points of the standard.

Note: This option is available only when a Results Table is open in the workspace.

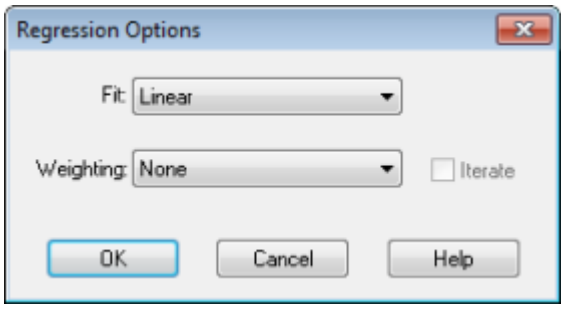
1. Open a Results Table.
2. Click **Tools** > **Calibration** > **Pane.**
   The Calibration Curve pane containing the calibration curve opens.

   Figure 6-10 Calibration Curve



3. If there is more than one analyte, then use the following steps to view the calibration curve for another analyte:
   a. From the **Analyte** list, select an analyte.
   b. If required, from the next list, select **Area** or **Height**.
4. To change the regression options for the calibration curve, do the following:
   a. Click **Regression**.

Figure 6-11 Regression Options Dialog



b. Select **Linear** in the **Fit** list.

c. Select **1 / x** in the **Weighting** list.

d. Click **OK**.

The calibration curve opens. The user can review individual peaks on the curve or exclude points from the curve to produce a better curve.

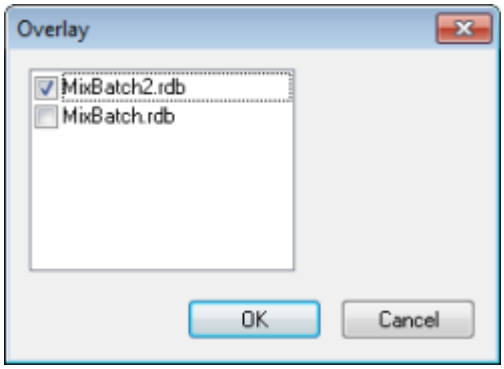
5. If required, repeat these steps to create a more appropriate curve.
6. To save the changes, click **Accept**.

Overlay Calibration Curves

Tip! To examine the curve for one table more closely, right-click the curve and then click **Active Plot**. Select the curve to be plotted on top.

1. With two or more open Results Tables, view a calibration curve for one of the tables.
2. Right-click the calibration curve and then click **Overlay**.

Figure 6-12 Overlay Dialog



3. Select the tables to overlay with the current curve.

4. Click **OK**.
   The software plots the curves for all selected tables on the same graph.

Sample Statistics

Use the Statistics window to view the statistics for samples, typically for standards and quality controls (QCs). The data from each available batch in the Results Table opens in tabular form in the grid and a row of data is shown for each standard or QC concentration.

View the Statistics for Standards and QCs

When more than one Results Table is open, statistical information about the standards and QCs for additional batches can be shown in the Statistics window. This facilitates comparison of results between batches and identification of trends in the standards or QCs.

1. Open a Results Table.
2. Click **Tools** > **Statistics.**
3. Select **Concentration** from the **Statistics Metric** list.
4. Select an analyte in the **Analyte Name** field.
5. Select **Standard** in the **Sample Type** field.
   The results are shown.
6. Examine the **%CV** and **Accuracy** columns.
   The **%CV** shows the coefficient of variance between the measurements of a single parameter, for example the area. **Accuracy** shows how close the plotted point is to the interpolated value.
7. If required, select the **Display Low/High values** check box and then examine the **Low**, **High** values, and **Mean** for each row in the grid. Each row represents standards that have the same concentration levels.
8. Select another analyte.
   The results are shown on a per-analyte basis.
9. To check for quality control (QC) variations at the same concentration levels, select **QC** in the **Sample Type** field.

Compare Results Between Batches

When more than one Results Table is shown, obtain statistical information about the standards and QCs for additional batches in the Statistics window. Normally results are compared between batches to look for trends in the standards or QCs or to verify that the method is valid.

For two or more open Results Tables, compare results in the Statistics window. Both sets of statistics are shown in the Statistics window.

The number of analytes and the analyte names must be the same for the data to be combined in the Statistics pane.

1. Open a Results Table.
2. Click **Tools** > **Statistics.**
3. Do one of the following:

   - To arrange the results by **Results Table**, select **Group By Batch** in the **Conc. as Rows** list.
   - To arrange the results in order of concentration, select **Group By Concentration** in the **Conc. as Rows** list.
   - To arrange the results in order of concentration without a row showing the statistics for each group or batch, select **Group By Concentration (no All)** in the **Conc. as Rows** list.

   The software sorts the results. At the end of each batch or group, one or two additional rows are shown: **All** (statistics for all Results Tables in that group) and **Average** (statistics on the statistics for that batch or group).

Reporter Software 7

The Reporter software extends the reporting functionality available in the Analyst software.

We recommend that users validate the results if a modified Reporter template or one that contains a query is used.

The Reporter software can be used to create custom reports with Microsoft Word and Excel (2013, 2016, or Office 365). The Reporter software has the following features:

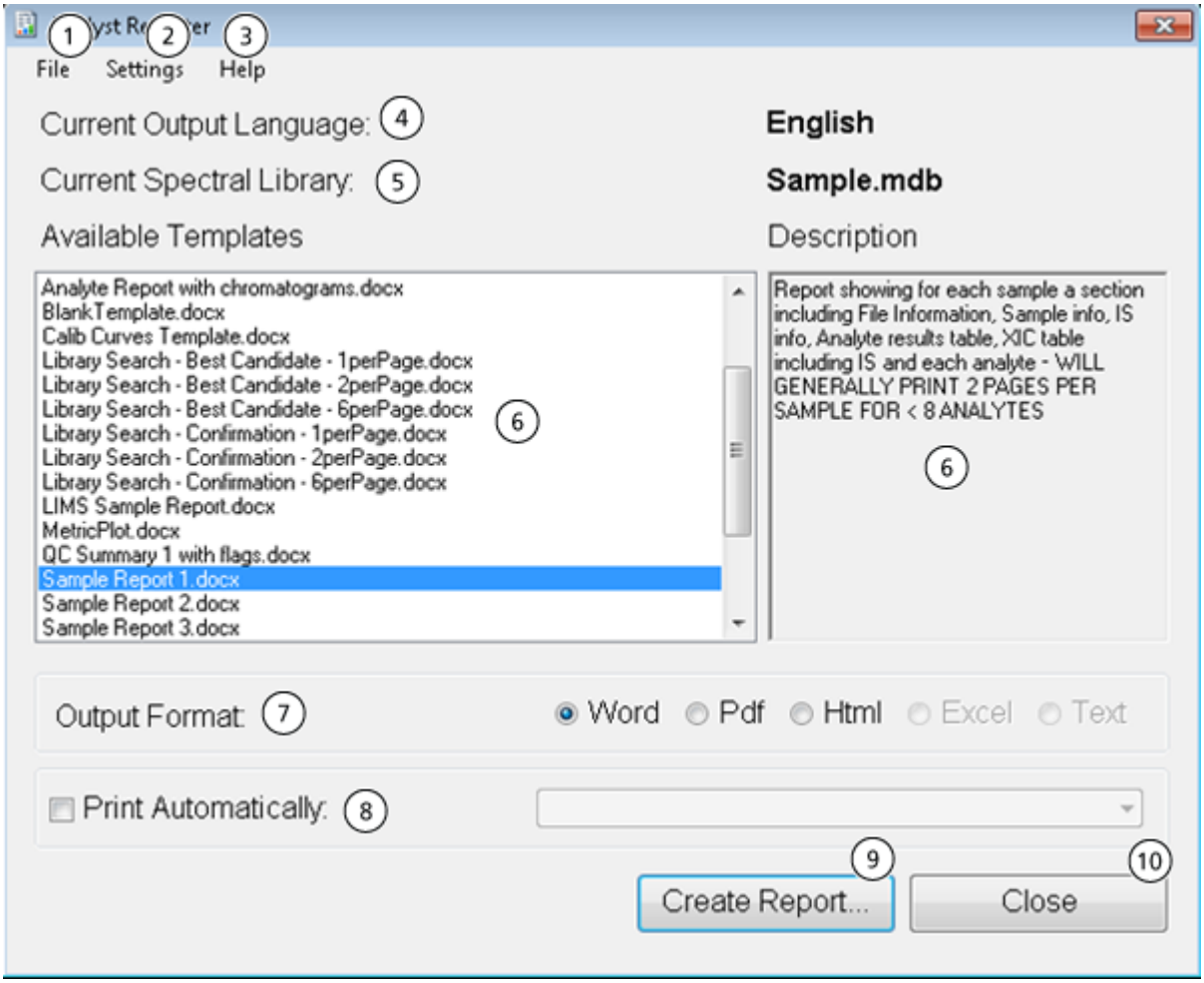
- Provides a variety of reports that use the data available in a Results Table, in file information, and in quantitative peak review windows.
- Provides a variety of reports that present MS/MS library search results. The user can configure the Reporter software to search against any MS/MS spectral library that uses the Analyst software (mdb) format.
- Uses Microsoft Word templates to provide the format information needed when generating reports. These templates can be created or modified to provide customized report formats.
- Contains a blank starting template that can be used in the Reporter software editing environment to design report templates to meet most reporting requirements.
- Automates report generation through the use of the Autoquan Reporter batch script.
- Automatically prints, exports to Adobe Portable Document Format (pdf), and delivers results by e-mail.
- Attaches processing scripts to report templates to expand both the content and automation level for various workflow requirements.
- Generates reports from custom software applications that use the available Analyst software programming libraries.

Reporter software can be used as follows:

- Within the Analyst software to manually generate a report or set of reports.
- By a batch script to automate report generation within a batch. Users can generate reports on a sample-by-sample basis, either during or after batch acquisition.
- By applications that do not use the Analyst software.

Analyst Reporter User Interface

Figure 7-1 Analyst Reporter



Item	Option	Description
1	**File** > **Exit**	Exits the program and releases all resources.
2	**Settings** > **Select Output Language**	Sets the language dictionary that will be used to replace language tags within a report template. Templates that contain language tags can be used to generate reports in any language. The language tags are replaced with text from a matching tag in the dictionary file for the selected language. These dictionary files are contained in the folder: `C:\Program Files (x86)\AB SCIEX\AnalystReporter\Resources\Languages`.

Item	Option	Description
2	**Settings** > **Select Library**	Browse to a spectral library. This library will be used for matching and scoring MS/MS data from Results Tables that contain data from information dependent acquisition (IDA) triggered MS/MS scan types.
2	**Settings** > **Select Template Folder**	Sets the folder from which the available templates will be read. To return to the default template folder, select the **Default** option.
3	**Help** > **About**	Shows information about the version of Reporter software currently installed.
4	**Current Output Language**	Shows the currently selected language dictionary used for replacing language tags within a report template. To select a language dictionary, click **Settings** > **Select Output Language.**
5	**Current Spectral Library**	Shows the currently selected spectral library. To select a spectral library, click **Settings** > **Select Library.**
6	**Available Templates** and **Description**	Shows a list of available report templates. Select a template to show a description of the template. To change the folder from which available templates are read, select **Settings** > **Select Template Folder** > **Browse.**

Item	Option	Description
7	**Output Format**	Shows the output formats that are supported by the Reporter software. Only formats that are compatible with the selected report template are enabled. • **Word**: Microsoft Word document (docx) is produced. This document can be viewed by Microsoft Word 2010 and above. • **PDF**: A report is created directly in PDF format. • **HTML**: Microsoft Word is used to generate an HTML file. Associated image files are stored in a folder with the same name as the HTML file. • **Excel**: A plain text file (csv) is produced. Report templates that contain values separated by commas can be opened in Microsoft Excel, where each value will be shown in a separate cell. Only templates that are specifically marked as text-compatible can be used for this output format. • **Text**: A plain text document (txt) is produced. Only templates that are specifically marked as text compatible can be used for this output format.
8	**Print Automatically**	After the report has been created it is printed to the selected printer. Select any available printer.
9	**Create Report**	Creates the report in the selected output format using the selected report template.
10	**Close**	Exits the program and releases all resources.

Generate Reports

The Reporter software extracts numerical data from the Results Table and sample and graphical information from the wiff file.

Tip! To avoid long processing times at the end of the acquisition for reports that can be generated on a sample-by-sample basis, generate the reports automatically using a batch script during acquisition. For more information about batch scripts, refer to the document: *Scripts User Guide*.

1. Open a **Results Table**.
2. Under **Companion Software**, double-click **Reporter**.

The **Analyst Reporter** opens.

3. In the **Available Templates** field, select the applicable report template.
4. Click the **PDF** output format.
   The Word option is pre-selected and the report is automatically saved in the current project Results folder. If the PDF output format is not selected, then the report is created and opened in Word or printed as selected, but the report is not saved. This lets the user edit the report in Word before saving the original report.
5. Select either one document containing all samples or multiple documents with one sample in each.
6. (Optional) Select the **Print Automatically** check box to print the reports automatically on a pre-selected printer.
   The default printer set in Windows is used unless a different printer is selected. The Reporter software keeps the selected printer between operations. If the printer is set to a PDF printer driver, then the Reporter software generates PDF file versions of the created reports automatically.
7. Click **Create Report**.
   The screen shows various progress indicators as the software opens the template and populates it with data from the Results Table. Some reports can take seconds to generate, others can take longer. A large data set with many MRM transitions or a large number of graphics might result in reports of several hundred pages that take hours to generate.

Parameters and Scan Types A

This section describes the different parameters and scan types that can be used for analysis.

About Instrument Parameters

Source-dependent parameters, compound-dependent parameters, and detector parameters are all configured in the Analyst software and applied at specific points to the ion path. Users should understand what each parameter controls and how it affects resolution, intensity, and peak shape, so that optimal results are achieved during sample analysis. Users should also consider how changing the value of one parameter can affect another parameter further along the ion path.

Source-Dependent Parameters

These parameters might change depending on the ion source being used.

Ion Source Gas 1 (GS1): The GS1 parameter controls the nebulizer gas. The nebulizer gas helps generate small droplets of sample flow and affects spray stability and sensitivity.

Ion Source Gas 2 (GS2): The GS2 parameter controls the auxiliary, or turbo, gas. It is used to help evaporate the solvent to produce gas phase sample ions.

Temperature (TEM): The TEM parameter controls the temperature of the turbo gas in the TurboIonSpray probe or the temperature of the probe in the heated nebulizer (or APCI) probe.

Curtain Gas (CUR): The CUR parameter controls the flow rate of the gas for the Curtain Gas interface. The Curtain Gas interface is located between the curtain plate and the orifice. It assists in solvent evaporation and prevents solvent droplets from entering and contaminating the ion optics. The gas flow should be maintained as high as possible without losing sensitivity.

IS (IonSpray Voltage): The IS parameter controls the voltage applied to the electrode that ionizes the sample in the ion source. It depends on the polarity and it affects the spray stability and the sensitivity. This parameter can be compound-dependent and should be optimized for each compound.

Nebulizer Current (NC): The NC parameter controls the current applied to the corona discharge needle in the APCI probe, used in the Turbo V and IonDrive Turbo V ion source. The discharge ionizes solvent molecules, which in turn ionize the sample molecules.

Interface Heater (ihe): The ihe parameter switches the interface heater on and off. Heating the interface helps maximize the ion signal and prevents contamination of the ion optics. This should always stay on. The button controlling the interface heater reads ON when the interface heater is on.

Interface Heater Temperature (IHT): The IHT parameter controls the temperature of the interface heater for the NanoSpray ion source or the OptiFlow Nano ion source, if it is supported by the system and is only available if the NanoSpray ion source or the OptiFlow Nano ion source is installed.

Compound-Dependent Parameters

The compound-dependent parameters consist mostly of voltages in the ion path. Optimal values for compound-dependent parameters vary depending on the compound being analyzed.

Quadrupole- and LIT-Mode Scan Parameters

The following parameters are available for optimization if you are running a quadrupole mode scan or an LIT-mode scan.

Declustering Potential (DP): The DP parameter controls the voltage on the orifice, which controls the ability to decluster ions between the orifice and the skimmer or, for systems with a QJet ion guide, between the orifice and the QJet ion guide. It is used to minimize the solvent clusters that might remain on the sample ions after they enter the vacuum chamber, and, if required, to fragment ions. The higher the voltage, the higher the energy imparted to the ions. If the DP parameter is too high, then unwanted fragmentation might occur.

Entrance Potential (EP): The EP parameter controls the potential difference between the voltage on Q0 and ground. The entrance potential guides and focuses the ions through the high-pressure Q0 region.

Collision Energy (CE): The CE parameter controls the potential difference between Q0 quadrupole and Q2 collision cell. It is used only in MS/MS-type scans. This is the amount of energy that the precursor ions receive as they are accelerated into the collision cell, where they collide with gas molecules and fragment.

CAD Gas (CAD): The CAD parameter controls the pressure of collision gas in the collision cell during Q3, MS/MS-type, and LIT scans. For Q3 scans, the collision gas helps to focus the ions as they pass through the collision cell; the preset for the CAD parameter is in fixed mode. For MS/MS-type scans, the collision gas aids in fragmenting the precursor ions. When the precursor ions collide with the collision gas, they can dissociate to form product ions. For LIT scans, the collision gas helps to focus and trap ions in the LIT.

Collision Cell Exit Potential (CXP): The CXP parameter controls the potential difference between RO2 and ST3 (for SCIEX 4000 systems and SCIEX 5000 systems). It is only used in Q3 and MS/MS-type scans, where it transmits the ions into Q3.

Ion Energy 1 (IE1): The IE1 parameter controls the potential difference between Q0 and RO1. Although this parameter does affect the sensitivity, it has a greater impact on peak shape, and it is considered a resolution parameter. IE1 is used in Q1, MS/MS-type, and LIT scans. This parameter should only be used by experienced users.

Ion Energy 3 (IE3): The IE3 parameter controls the potential difference between RO2 and RO3. Although this parameter does affect the sensitivity, it has a greater impact on peak shape, and it is considered a resolution parameter. IE3 is used in Q3 and MS/MS-type scans. This parameter should only be used by experienced users.

LIT Mode Scan Parameters

In addition to the compound-dependent parameters that are available on the Compound tab, several parameters are available on the MS tab or the Advanced MS tab for linear ion trap (LIT) mode scans that will affect results. Because parameters on the MS tab or the Advanced MS tab cannot be changed in real time, the best method of sample introduction for optimizing these parameters is infusion. The acquisition must be stopped between each parameter change.

Q0 Trapping: The **Q0 Trapping** parameter controls the storage of ions in the Q0 region. It is used to increase sensitivity and duty cycle by trapping ions in the Q0 region while ions are being mass-selectively ejected from the LIT. Fixed fill time must be used with this parameter.

Collision Energy Spread (CES): The **CES** parameter, in conjunction with the CE, determines which three discrete collision energies will be applied to the precursor mass in an EPI or MS3 experiment when CES is used. By entering a collision energy spread value, CES is automatically turned on.

Time Delayed Fragmentation Collision Energy (TDF CE): The **TDF CE** parameter controls the potential difference between RO2 and RO3 for TDF scans. This is the amount of energy that the precursor ions receive as they are accelerated into Q3, where they collide with gas molecules and fragment.

Note: The **TDF CE** parameter is only available for the 3200 QTRAP and 4000 QTRAP systems.

Q3 Cool Time: The **Q3 Cool Time** parameter controls the amount of time that the precursor ions are allowed to cool prior to collection of their product ions in TDF scans.

Q3 Entry Barrier: The **Q3 Entry Barrier** parameter controls the potential difference between RO2 and RO3. It is used to transfer the ions from Q2 into the LIT.

Excitation Energy (AF2): The **AF2** parameter is the voltage of the auxiliary frequency (Aux RF) applied to Q3 during MS3 scans. It is used to fragment the isolated second precursor ion.

MS/MS/MS Fragmentation Time: The **MS/MS/MS Fragmentation Time** parameter controls the amount of time that the excitation energy is applied in MS3 scans. It is used in combination with the excitation energy to fragment the isolated second precursor ion.

Multi-Charge Separation (MCS) Barrier: The **MCS Barrier** parameter controls the voltage used when eliminating the singly-charged ions from the LIT in an Enhanced Multi-Charge (EMC) scan.

Q3 Empty Time: The **Q3 Empty Time** parameter controls the amount of time that singly-charged ions are removed from the LIT in an EMC scan.

Fixed LIT Fill Time: The **Fixed LIT Fill Time** parameter controls the amount of time that the LIT fills with ions.

DFT (Dynamic Fill Time): **DFT** will dynamically calculate the length of time that ions are collected in the LIT based on the incoming ion signal. When DFT is turned on the signal is optimized to either increase sensitivity or minimize space-charging.

EXB (Exit Barrier): The **EXB** parameter controls the voltage on the exit lens. It is used in LIT scans to mass-selectively eject ions from the LIT. It affects the peak width, the peak shape, and the intensity of the ion signal.

AF3 (Trap RF Amplitude): The **AF3** parameter controls the zero-to-peak voltage of the auxiliary frequency (Aux RF) applied to Q3 when ejecting ions from the LIT. The AF3 parameter affects the peak width, the peak shape, and the intensity of the ion signal.

Detector Parameters

- **CEM (CEM)**: The CEM parameter controls the voltage applied to the detector. It is used to detect ions by amplifying ion signals by producing a cascade of electrons
- **DF (Deflector)**: The DF parameter controls the voltage applied to the deflector. It is used to direct ions into the detector. It is preset to fixed mode. Not applicable to the SCIEX 5500+ system, the SCIEX 6500 systems, or the SCIEX 6500+ systems.

Scan Types

You can perform quadrupole-mode and LIT-mode scans either individually or in combination when analyzing your sample.

Scan Techniques

MS: In MS scans, also referred to as single MS scans, ions are separated according to their mass-to-charge ratio (*m/z*). A single MS scan might be used to find the molecular weight of a compound. Single MS scans can also be referred to as survey scans. MS scans do not supply any information about the chemical composition of the ions, other than the mass. Do MS/MS or MS/MS/MS scans to get more information about the ions.

MS/MS: MS/MS scans are used to identify structural information. Selected ions go into the Q2 collision cell where they are collisionally activated to make characteristic product ions.

If enough energy is used, then the precursor ion fragments to make characteristic product ions.

MS/MS/MS: The linear ion trap (LIT) system MS/MS/MS scans go one step further than MS/MS scans. A fragment that is produced in the collision cell is fragmented further in the LIT to give more structural information about the molecular ion.

Quadrupole-Mode Scan Types

Triple quadrupole instruments have high-sensitivity Multiple Reaction Monitoring (MRM) capabilities required for quantitation experiments. In addition, they have highly specific scan types, such as precursor ion and neutral loss scans, which allow a more advanced search to be performed on the components of the samples.

Q1 MS (Q1): A full scan type using the first quadrupole (Q1). The ion intensity is returned for every mass in the scan range.

Q1 Multiple Ions (Q1 MI): A selective scan type using the Q1 quadrupole. The ion intensity is returned for the specified masses only.

Q3 MS (Q3): A full scan type using the third quadrupole (Q3). The ion intensity is returned for every mass in the scan range.

Q3 Multiple Ions (Q3 MI): A selective scan type using the Q3 quadrupole. The ion intensity is returned for the specified masses only.

MRM (MRM): An MS/MS scan in which a user-defined ion is isolated in the Q1 quadrupole, then fragmented in the Q2 collision cell. The Q3 quadrupole is then used to isolate a user-defined fragment ion that is recorded by the detector. This scan type is used primarily for quantitation.

Product Ion (MS2): An MS/MS full scan where the Q1 quadrupole isused to isolate and transmit a specific precursor ion and the Q3 quadrupole scans a defined mass range. Used to identify all of the fragment ions of a particular precursor ion.

Precursor Ion (Prec): An MS/MS scan where the Q3 quadrupole is fixed at a specified *m/z* ratio to transmit a specific product ion and the Q1 quadrupole scans a mass range. Used to confirm the presence of a precursor ion or, more commonly, to identify compounds sharing a common product ion.

Neutral Loss (NL): An MS/MS scan where both the Q1 quadrupole and the Q3 quadrupole scan a mass range, a fixed mass apart. A response is observed if the ion chosen by the Q1 quadrupole fragments by losing the neutral loss, the fixed mass, specified. Used to confirm the presence of a precursor ion or, more commonly, to identify compounds sharing a common neutral loss.

LIT-Mode Scan Types

Note: Linear ion trap features are only available on QTRAP-enabled systems.

The LIT-mode scans use the Q3 quadrupole as a linear ion trap. Ions are trapped and stored in the Q3 quadrupole before being scanned out, giving increased sensitivity. In addition, MS/MS/MS analysis can be performed in the linear ion trap, providing more information about the sample. LIT-mode scan types are typically used for qualitative measurements.

Enhanced MS (EMS): Ions are scanned in the Q1 quadrupole and then collected in the linear ion trap. These ions are scanned out of the Q3 quadrupole to produce single MS type spectra.

Enhanced Multi-Charge (EMC): This scan type is similar to the EMS scan except that before ions are scanned out of the linear ion trap, there is a delay period during which low-charge state ions, primarily singly-charged ions, are allowed to preferentially escape from the linear ion trap. When the retained ions are scanned out, the multiply-charged ion population dominates the resulting spectrum.

Enhanced Product Ion (EPI): This scan type is used to obtain a high-quality MS/MS spectrum for a specific ion. The fragmentation is done in the Q2 collision cell and thus provides the information-rich MS/MS spectrum typical of collisionally activated dissociation (CAD) fragmentation. In this scan mode, the precursor ion to be fragmented is first selected in the Q1 quadrupole with a mass window that is 1 Da to 4 Da wide, filtering out all of the other ions. The precursor ion is fragmented by CAD gas in the Q2 collision cell. The fragment ions generated are captured in the linear ion trap and then scanned out at one of three scan speeds, depending on the required fragment ion resolution.

For IDA experiments, the **Product Of** field is set to 30 Da by default, and this value should not be changed.

Enhanced Resolution (ER): This scan type is similar to the EMS scan except that a small 30 Da mass window around the precursor mass is scanned out of the linear ion trap at the slowest scan rate to produce a narrow window of the best-resolved spectra.

MS/MS/MS (MS3): A precursor ion is selected by the Q1 quadrupole and fragmented with collisionally activated dissociation in the Q2 collision cell. The resulting product ions are all transmitted to the linear ion trap, where a single product ion is then isolated. The isolated ion is further fragmented in the linear ion trap, and the resulting product ions are scanned out of the trap at one of three scan speeds. As with any in-trap Collision Induced Dissociation (CID) technique, there is a low mass cut-off for the second MS/MS step because the lowest mass fragment and precursor must be simultaneously stable in the trap. For QTRAP systems, this results in the loss of ions lower than 28 percent of the mass of the precursor ion during MS3 experiments. This phenomenon is often referred to as the one-third cut-off rule.

Time Delayed Fragmentation (TDF): Product ions are generated and collected in the linear ion trap. During the first part of the collection period, the lower mass ions are not collected. During the second part of the collection period, all masses in the mass range of interest are collected. The resulting enhanced product ion spectra are similar to EPI scan type spectra. The nature of the spectra aids in the interpretation of the structure and fragmentation pathways of the molecule of interest. This scan type is only applicable to the 3200 QTRAP and 4000 QTRAP systems.

Toolbar Icons B

For additional toolbar icons, refer to the document: *Advanced User Guide*.

Table B-1 Tool Bar Icons

Icon	Name	Description
	**New Subproject**	Creates a subproject. Subprojects can only be created later in the process if the project was originally created with subprojects.
	**Copy Subproject**	Copies a subproject folder. Subprojects can be copied only from another project that has existing subprojects. If the same folders exist at both the project and subproject levels, then the software uses the project level folders.

Table B-2 Acquisition Method Editor Icons

Icon	Name	Description
	**Mass Spec**	Shows the MS tab in the Acquisition Method editor.
	**Period**	Adds an experiment, an **IDA Criteria Level**, or deletes the period.
	**Autosampler**	Opens the Autosampler Properties tab.
	**Syringe Pump**	Opens the Syringe Pump Properties tab.
	**Column Oven**	Opens the Column Oven Properties tab.
	**Valve**	Opens the Valve Properties tab.
	**DAD**	Opens the DAD Method Editor. Refer to the section: Show DAD Data.
	**ADC**	Opens the ADC Properties tab. Refer to the section: Show ADC Data.

Table B-3 Acquire Mode Icons

Icon	Name	Description
	**View Queue**	Shows the sample queue.
	**Instrument Queue**	Shows a remote instrument station.
	**Status for Remote Instrument**	Shows the status of a remote instrument.
	**Start Sample**	Starts the sample in the queue.
	**Stop Sample**	Stops the sample in the queue.
	**Abort Sample**	Aborts a sample acquisition in the middle of the processing of that sample.
	**Stop Queue**	Stops the queue before it has completed processing all of the samples.
	**Pause Sample Now**	Inserts a pause in the queue.
	**Insert Pause before Selected Sample(s)**	Inserts a pause before a specific sample.
	**Continue Sample**	Continues acquiring the sample.
	**Next Period**	Starts a new period.
	**Extend Period**	Extends the current period.
	**Next Sample**	Stops acquiring the current sample and starts acquiring the next sample.
	**Equilibrate**	Selects the method to be used to equilibrate the devices. This method should be the same as the method that was used with the first sample in the queue.
	**Standby**	Puts the instrument in **Standby** state.

Table B-3 Acquire Mode Icons (continued)

Icon	Name	Description
	**Ready**	Puts the instrument in **Ready** state.
	**Reserve Instrument for Tuning**	Reserves the mass spectrometer for tuning and calibrating.
	**IDA Method Wizard**	Starts the **IDA Method Wizard**.
	**Purge Modifier**	Starts the modifier purge from the modifier pump.

Icon	Name	Description
	**Calibrate from spectrum**	Opens the Mass Calibration Option dialog and uses the active spectrum to calibrate the mass spectrometer.
	**Manual Tune**	Opens the Manual Tune Editor.
	**Compound Optimization**	Optimizes for a compound using infusion by FIA.
	**Instrument Optimization**	Verifies the instrument performance, adjusts the mass calibration, or adjusts mass spectrometer settings.
	**View Queue**	Shows the sample queue.
	**Instrument Queue**	Shows a remote instrument.
	**Status for Remote Instrument**	Shows the status of a remote instrument.
	**Reserve Instrument for Tuning**	Reserves the instrument for tuning and calibrating.
	**IDA Method Wizard**	Starts the IDA Method Wizard.

Table B-4 Explore Quick Reference: Chromatograms and Spectrum

Icon	Name	Description
	**Open Data File**	Opens files.
	**Show Next Sample**	Goes to the next sample.
	**Show Previous Sample**	Goes to the previous sample.
	**Go To Sample**	Opens the Select Sample dialog.
	**List Data**	Shows the data in tables.
	**Show TIC**	Generates a TIC from a spectrum.
	**Extract Using Dialog**	Extracts ions by selecting masses.
	**Show Base Peak Chromatogram**	Generates a BPC.
	**Show Spectrum**	Generates a spectrum from a TIC.
	**Copy Graph to new Window**	Copies the active graph to a new window.
	**Baseline Subtract**	Opens the Baseline Subtract dialog.
	**Threshold**	Adjusts the threshold.
	**Noise Filter**	Shows the Noise Filter Options dialog, which can be used define the minimum width of a peak. Signals below this minimum width are regarded as noise.
	**Show ADC**	Shows ADC data.
	**Show Auxiliary Traces**	Opens the Select Auxiliary Trace Channel dialog
	**Show File Info**	Shows the experimental conditions used to collect the data.
	**Add arrows**	Adds arrows to the X-axis of the active graph.

Table B-4 Explore Quick Reference: Chromatograms and Spectrum (continued)

Icon	Name	Description
	**Remove all arrows**	Removes arrows from the X-axis of the active graph.
	**Offset Graph**	Compensates for slight differences in the time during which the ADC data and the mass spectrometer data were recorded. This is useful when overlaying graphs for comparison.
	**Force Peak Labels**	Labels all of the peaks.
	**Expand Selection By**	Sets the expansion factor for a portion of a graph to be viewed in greater detail.
	**Clear ranges**	Returns the expanded selection to normal view.
	**Set Selection**	Defines start and stop points for a selection. This feature provides more accurate selection than is possible by selecting the region using the cursor.
	**Normalize To Max**	Scales a graph to maximum size, so that the most intense peak is scaled to full scale, whether or not it is visible.
	**Show History**	Shows a summary of data processing operations performed on a particular file, such as smoothing, subtraction, calibration, and noise filtering.
	**Open Compound Database**	Opens the compound database.
	**Set Threshold**	Adjusts the threshold.
	**Show Contour Plot**	Shows selected data as either a spectrum graph or an XIC. Additionally, for data acquired by a DAD, a contour plot can show selected data as either a DAD spectrum or an XWC.
	**Show DAD TWC**	Generates a TWC of the DAD spectrum.
	**Show DAD Spectrum**	Generates a DAD spectrum.

Table B-4 Explore Quick Reference: Chromatograms and Spectrum (continued)

Icon	Name	Description
	**Extract Wavelength**	Extracts up to three wavelength ranges from a DAD spectrum to view the XWC.

Table B-5 Explore Toolbar Quick Reference: Overlaying Graphs

Icon	Name	Description
	**Home Graph**	Return the graph to the original scale.
	**Overlay**	Overlays graphs.
	**Cycle Overlays**	Cycles between overlaid graphs.
	**Sum Overlays**	Adds the graphs together.

Table B-6 Explore Toolbar Quick Reference: Fragment Interpretation Tool

Icon	Name	Description
	**Show Fragment Interpretation Tool**	Opens the Fragment Interpretation tool, which calculates the single, non-cyclic bond cleavage fragments from a mol file.

Table B-7 Navigation Icons on the Explore Toolbar

Icon	Name	Description
	**Open File**	Opens files.
	**Show Next Sample**	Navigates to the next sample.
	**Show Previous Sample**	Navigates to the previous sample.
	**GoTo Sample**	Opens the Select Sample dialog.
	**List Data**	Shows the data in tables.
	**Show TIC**	Generates a TIC from a spectrum.

Table B-7 Navigation Icons on the Explore Toolbar (continued)

Icon	Name	Description
	**Extract Using Dialog**	Click to extract ions by selecting masses.
	**Show Base Peak Chromatogram**	Generates a BPC.
	**Show Spectrum**	Generates a spectrum from a TIC.
	**Copy Graph to new Window**	Copies the active graph to a new window.
	**Baseline Subtract**	Opens the Baseline Subtract dialog.
	**Threshold**	Adjusts the threshold.
	**Noise Filter**	Opens the Noise Filter Options dialog that defines the minimum width of a peak. Signals below this minimum width are regarded as noise.
	**Show ADC**	Shows ADC data.
	**Show Auxiliary Traces**	Opens the Select Auxiliary Trace Channel dialog
	**Show File Info**	Shows the experimental conditions used to collect the data.
	**Add arrows**	Adds arrows to the X-axis of the active graph.
	**Remove all arrows**	Removes arrows from the X-axis of the active graph.
	**Offset Graph**	Compensates for slight differences in the time during which the ADC data and the mass spectrometer data were recorded. This is useful when overlaying graphs for comparison.
	**Force Peak Labels**	Labels all the peaks.
	**Expand Selection By**	Sets the expansion factor for a portion of a graph to view in greater detail.

Table B-7 Navigation Icons on the Explore Toolbar (continued)

Icon	Name	Description
	**Clear ranges**	Returns the expanded selection to normal view.
	**Set Selection**	Sets start and stop points for a selection. This provides more accurate selection than is possible by highlighting the region using the cursor.
	**Normalize to Max**	Scales a graph to maximum, so that the most intense peak is scaled is to full scale, whether or not it is visible.
	**Show History**	Shows a summary of data processing operations performed on a particular file, such as smoothing, subtraction, calibration, and noise filtering.
	**Open Compound Database**	Opens the compound database.
	**Set Threshold**	Adjusts the threshold.
	**Show Contour Plot**	Shows selected data as either a spectrum graph or an XIC. Additionally, for data acquired by a DAD, a contour plot can display selected data as either a DAD spectrum or an XWC.
	**Show DAD TWC**	Generates a TWC of the DAD.
	**Show DAD Spectrum**	Generates a DAD spectrum.
	**Extract Wavelength**	Extracts up to three wavelength ranges from a DAD spectrum to view the XWC.

Table B-8 Integration Tab and Quantitation Wizard Icons

Icon	Name	Description
	**Set parameters from Background Region**	Uses the selected peak.
	**Select Peak**	Uses the selected background.

Table B-8 Integration Tab and Quantitation Wizard Icons (continued)

Icon	Name	Description
	**Manual Integration Mode**	Manually integrates peaks.
	**Show or Hide Parameters**	Shows or hides the peak-finding parameters.
	**Show Active Graph**	Shows the analyte chromatogram only.
	**Show Both Analyte and IS**	Shows the analyte and its associated chromatogram. Available only when an associated internal standard exists.
	**Use Default View for Graph**	Returns to the preset, view all data, view if, for example, the user has zoomed in on a chromatogram.

Table B-9 Results Table Icons

Icon	Name	Description
	**Sort Ascending by Selection**	Sorts the selected column in ascending order.
	**Sort Descending by Selection**	Sorts the selected column in descending order.
	**Lock Or Unlock Column**	Locks or unlocks the selected column. A locked column cannot be moved.
	**Metric Plot By Selection**	Creates a metric plot from the selected column.
	**Show all Samples**	Shows all of the samples in the Results Table.
	**Delete Formula Column**	Deletes formula columns.
	**Report Generator**	Opens the Reporter software.

Table B-10 Icon Quick Reference: Quantitate Mode

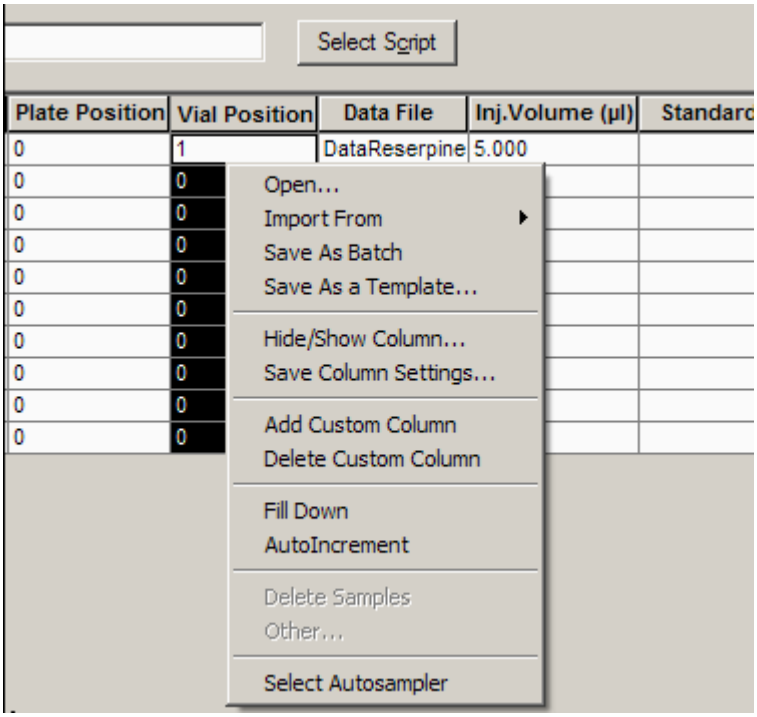
Icon	Name	Description
	**Add/Remove Samples**	Adds or removes samples from the Results Table.
	**Export as Text**	Saves the Results Table as a text file.
	**Modify Method**	Opens a wiff file.
	**Peak Review - Pane**	Opens peaks in a pane.
	**Peak Review - Window**	Opens peaks in a window.
	**Calibration - Pane**	Opens the calibration curve in a pane.
	**Calibration - Window**	Opens the calibration curve in a window.
	**Show First Peak**	Shows the first peak in the pane or window.
	**Show Last Peak**	Shows the last peak in the pane or window.
	**Show Audit Trail**	Shows the audit trail for the Results Table.
	**Clear Audit Trail**	Clears the audit trail for the Results Table. This functionality is not available.
	**Statistics**	Opens the Statistics window.
	**Report Generator**	Opens the Reporter software.

Right-Click Menus C

Batch Editor

Right-click the Batch Editor table to access the options.

Figure C-1 Batch Right-Click Menu



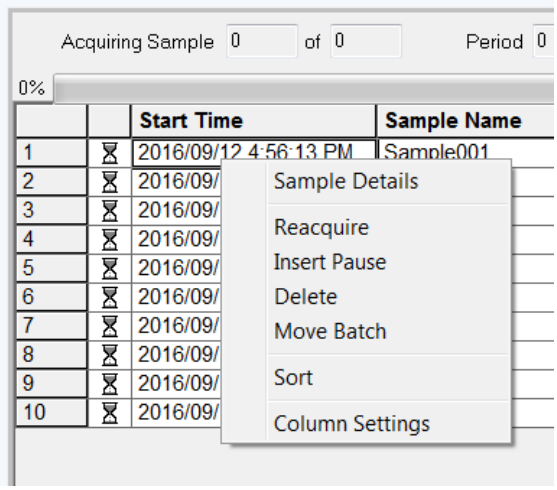
Menu	Function
Open	Opens a batch file.
Import From	Imports a batch from a file.
Save As Batch	Saves the batch with a different name.
Save As a Template	Saves the batch as a template.
Hide/Show Column	Hides or shows a column.
Save Column Settings	Saves the batch column settings.
Add Custom Column	Adds a custom column.

Menu	Function
Delete Custom Column	Deletes a custom column.
Fill Down	Copies the same data into the selected cells.
AutoIncrement	Automatically increments data in the selected cells.
Delete Samples	Deletes the selected row.
Select Autosampler	Selects an autosampler.

Queue

Right-click the Queue table to access the options.

Figure C-2 Queue Manager Right-Click Menu



Menu	Function
Sample Details	Opens the Sample Details dialog.
Reacquire	Acquires a sample again.
Insert Pause	Inserts a pause, in seconds, between two samples.
Delete	Deletes either the batch or the selected samples.
Move Batch	Moves the batch within the queue.
Sort	Sorts on the preselected column.
Column Settings	Changes the column settings.

Show File Information Pane Right-click Menu

Table C-1 Show File Information Pane Right-click Menu

Menu	Function
Copy	Copies the selected data.
Paste	Pastes data.
Select All	Selects all of the data in the pane.
Save To File	Saves data as an rtf file.
Font	Changes the font.
Save Acquisition Method	Saves the acquisition method as a dam file.
Save Acquisition Method to CompoundDB	Opens the Specify Compound Information dialog. Select the IDs and molecular weights to be saved in the compound database.
Delete Pane	Deletes the selected pane.

Chromatogram Panes

Table C-2 Right-click Menu for Chromatogram Panes

Menu	Function
List Data	Lists the data points and integrates the peaks found in chromatograms.
Show Spectrum	Generates a new pane containing the spectrum.
Show Contour Plot	Shows a color-coded plot of a dataset, where the color represents the intensity of the data at that point. Only certain MS modes are supported.
Extract Ions	Extracts a specific ion or set of ions from a selected pane and then generates a new pane containing a chromatogram for the specific ions.
Show Base Peak Chromatogram	Generates a new pane containing a base peak chromatogram.
Show ADC Data	Generates a new pane containing the ADC data trace, if acquired.
Show Auxiliary Traces	Opens the Select Auxiliary Trace Channel dialog.
Show UV Detector Data	Generates a new pane containing the UV data trace, if acquired.

Table C-2 Right-click Menu for Chromatogram Panes (continued)

Menu	Function
Spectral Arithmetic Wizard	Opens the Spectral Arithmetic Wizard.
Save to Text File	Generates a text file containing the data in a pane, which can be opened in Microsoft Excel or other programs.
Save Explore History	Saves information about changes to processing parameters, also called processing options, that were made when a wiff file was processed in Explore mode. The processing history is stored in a file with an eph (explore processing history) extension.
Add Caption	Adds a caption at the cursor location in the pane.
Add User Text	Adds a text box at cursor location in the pane.
Set Subtract Range	Sets the subtract range in the pane.
Clear Subtract Range	Clears the subtract range in the pane.
Subtract Range Locked	Locks or unlocks the subtract ranges. If the subtract ranges are not locked, then each subtract range can be moved independently. The subtract ranges are preset to locked.
Delete Pane	Deletes the selected pane.

Spectra Panes

Table C-3 Right-click Menu for Spectra Panes

Menu	Function
List Data	Lists the data points and integrates chromatograms.
Show TIC	Generates a new pane containing the TIC.
Extract Ions (Use Range)	Extracts a specific ion or set of ions from a selected pane and then generates a new pane containing a chromatogram for the specific ions.
Extract Ions (Use Maximum)	Extracts ions using the most intense peak in a selected area.
Save to Text File	Generates a text file of the pane, which can be opened in Microsoft Excel or other programs.

Table C-3 Right-click Menu for Spectra Panes (continued)

Menu	Function
Save Explore History	Saves information about changes to processing parameters, also called Processing Options, that were made when a wiff file was processed in Explore mode. The processing history is stored in a file with an eph (explore processing history) extension.
Add Caption	Adds a caption at the cursor location in the pane.
Add User Text	Adds a text box at the cursor location in the pane.
Show Last Scan	Shows the scan prior to the selection.
Select Peaks For Label	In this dialog, select the parameters to reduce peak labeling.
Delete Pane	Deletes the selected pane.
Add a Record	Adds records and compound-related data, including spectra, to the library. An active spectrum is required to perform this task.
Search Library	Searches the library without constraints or with previously saved constraints.
Set Search Constraints	Searches the library using the criteria typed in Search Constraints dialog.

Results Table

Right-click the Results Table to access the options shown in the following table.

Table C-4 Results Table Right-click Menu

Menu	Function
Full	Shows all the columns.
Summary	Shows specific columns.
Analyte	Shows a specific analyte.
Analyte Group	Creates an analyte group.
Sample Type	Shows samples of a specific type or all samples.
Add Formula Column	Adds a formula column. It is recommended that the user validate the results if a formula column is used.
Table Settings	Edits or selects a table setting.
Query	Creates or selects a query.

Table C-4 Results Table Right-click Menu (continued)

Menu	Function
Sort	Creates a sort or sorts by index.
Metric Plot	Creates a metric plot.
Delete Pane	Deletes the active pane.
Fill Down	Copies the same data into the selected cells.
Add Custom Column	Adds a custom column.
Delete Custom Column	the selected custom column.

Peak Review

Right-click the **Peak Review** window or pane to access the options shown in the following table.

Table C-5 Peak Review Right-click Menu

Menu	Function
Options	Opens the Peak Review Options dialog.
Sample Annotation	Opens the Sample Annotation dialog.
Save Active to Text File	Saves the selected peak as a text file.
Show First Page	Goes to the first sample.
Show Last Page	Goes to the last sample.
Slide Show Peak Review	Opens the slide show.
Update Method	Updates the algorithm for all peaks.
Revert to Method	Selects a redefined peak based on the current quantitation method.
Delete Pane	Deletes the active pane.

Calibration Curve

Right-click the Calibration window or pane table to access the options shown in the following table.

Table C-6 Calibration Curve Right-click Menu

Menu	Function
Exclude (Include)	Right-click a point and then click **Exclude** to exclude the point from the curve. Right-click a point and then click **Include** to include the point.
Exclude All Analytes (Include All Analytes)	Right-click a point and then click **Exclude All Analytes** to exclude all of the analytes from the curve. Right-click a point and then click **Include All Analytes** to include the points.
Show Peak	Reviews an individual peak.
Overlay	Overlays two graphs.
Active Plot	Determines which plot is active.
Legend	Shows the graph legend.
Log Scale X Axis*	Uses a log scale for the X-axis.
Log Scale Y Axis*	Uses a log scale for the Y-axis.
Delete Pane	Deletes the active pane.
Home Graph	Scales the graph to its original size
* A log scale arranges the data points in a more manageable view so that the effect of all points can be monitored simultaneously. For this view, select **Log Scale Y Axis** versus **Log Scale X** and not just the log of one axis.	

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