AB SCIEX TripleTOF® 5600/5600+ Instruments

System User Guide

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For research use only. Not for use in diagnostic procedures.

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Contents

This section contains general safety-related information, describes the symbols and conventions used in the documentation, and provides regulatory compliance information. It also describes potential hazards and associated warnings for the system, and the precautions that should be taken to minimize the hazards. In addition to this section, refer to the *Site Planning Guide.* It provides site requirements, including requirements for the mains supply, source exhaust, ventilation, compressed air, nitrogen, and the roughing pump.

General Safety Information

Before operating any instrument, become familiar with its operation and with the potential hazards. To prevent personal injury or instrument damage, read, understand, and obey all safety precautions. Warnings in this document and labels on the mass spectrometer are shown with international symbols. Failure to heed these warnings could result in serious injury.

This safety information is intended to supplement federal, state or provincial, and local environmental health and safety (EHS) regulations. The information provided covers instrument-related safety with regard to the operation of the mass spectrometer. It does not cover every safety procedure that should be practised. Ultimately, you and your organization are responsible for compliance with federal, state or provincial, and local EHS regulations and for maintaining a safe laboratory environment.

For more information, refer to the appropriate laboratory reference material and standard operating procedures.

Symbols and Conventions

The following conventions are used throughout the guide.

DANGER! Danger signifies an action which leads to severe injury or death.

WARNING! Personal Injury Hazard: A warning indicates an operation that could cause personal injury if precautions are not followed.

WARNING! Electric Shock Hazard: This symbol indicates a warning of electrical shock hazard. Read the warning and follow all precautions before performing any operation described in the guide. Failure to do so can result in serious injury.

WARNING! Burn Hazard: This symbol indicates a warning of potential burns from hot surfaces. Read the warning and follow all precautions before performing any operation described in the guide. Failure to do so can result in serious injury.

WARNING! Biohazard: This symbol indicates a warning of biohazardous materials. Read the warning and follow all precautions before performing any operation described in the guide. Failure to do so can result in serious injury.

Caution: A caution indicates an operation that could cause damage to the instrument or loss of data if precautions are not followed.

Tip! Provides useful information that helps apply the techniques and procedures in the text for a specific need, and provides shortcuts, but is *not essential* to the completion of a procedure.

Note: A note emphasizes significant information in a procedure or description.

Qualified Personnel

After installing the system, the FSE (Field Service Employee) uses the *Customer Familiarization Checklist* to train the customer on system operation, cleaning, and basic maintenance. Only qualified AB SCIEX personnel shall install and service the equipment. Only personnel qualified by AB SCIEX shall operate and maintain the equipment. Contact an AB SCIEX FSE for more information.

Equipment Use and Modification

Use the system indoors in a laboratory that complies with the environmental conditions recommended in the system *Site Planning Guide*. If the system is used in an environment or in a manner not prescribed by AB SCIEX, the protection provided by the equipment can be impaired.

Unauthorized modification or operation of the system may cause personal injury and equipment damage, and may void the warranty. Erroneous data may be generated if the system is operating outside the recommended environmental conditions or with unauthorized modifications. Contact an AB SCIEX representative for more information on servicing the system.

Shipping Crate Labels and Indicators

Table 1 Labels and Indicators on the Crate

External Labels and Indicators	Definition	Action
 or 	TIP N TELL Blue beads in the arrow indicate that the container was tipped or mishandled.	Write on the Bill of Lading and check for damage. Any claims for tipping require a notation.
	Shock Indicator The indicator is broken if the container has suffered a shock greater than the level marked on the indicator.	Write on the Bill of Lading and check for damage. Any claims for shock damage require a notation.

Regulatory Compliance

This system complies with the standards and regulations listed in this section. Applicable labels have been affixed to the system.

Australia and New Zealand

- **Electromagnetic Interference**—AS/NZ CISPR 11 (Class A)
- **Safety**—AS/NZ 61010-1

Canada

- **Electromagnetic Interference**—CAN/CSA CISPR11-04. This ISM device complies with Canadian ICES-001.
- **Safety**—CAN/CSA C22.2 No. 61010-1-04, CAN/CSA C22.2 No. 61010-2-061:04

Europe

- **Electromagnetic Compatibility—**Electromagnetic Compatibility Directive 2004/108/EC, as implemented in these standards:
  - EN 55011 (Class A)
  - EN 61326-1
- **Safety—**Low Voltage Directives 2006/95/EC as implemented in these standards:
  - EN 61010-1
  - EN 61010-2-061
- **WEEE—**Waste, Electrical, and Electronic Equipment Directive 2002/96/EEC, as implemented in EN 40519

United States

- **Electromagnetic Interference, FCC Part 15, Class A**—This equipment has been tested and found to comply with the limits for a Class A digital device, pursuant to Part 15 of the FCC (Federal Communications Commission Compliance) Rules. These limits are designed to provide reasonable protection against harmful interference when the equipment is operated in a commercial environment. This equipment generates, uses, and can radiate radio frequency energy and, if not installed and used in accordance with the operator's manual, can cause harmful interference to radio communications. Operation of this equipment in a residential area is likely to cause harmful interference in which case you will be required to correct the interference, at your own expense. Changes or modifications not expressly approved by the manufacturer could void your authority to operate the equipment.
- **Safety**—UL 610101-1-04

International

- **Electromagnetic Compatibility**—IEC 61326-1; CEI/IEC CISPR 11
- **Safety**—IEC 61010-1; IEC 61010-2-061

For more information, refer to the Declaration of Conformance included with the system.

Symbols and Labels on the Mass Spectrometer

Table 2 Labels on the Mass Spectrometer

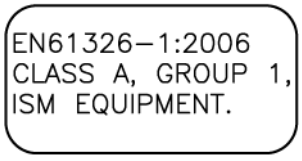
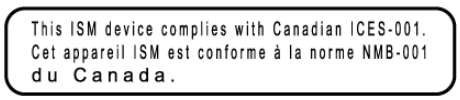
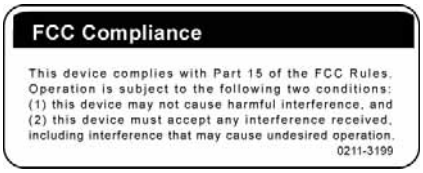
External Labels	Definition
	High Voltage
	**WARNING: NO USER SERVICEABLE PARTS INSIDE.** REFER SERVICING TO QUALIFIED PERSONNEL.
	WARNING: To avoid risk of injury, ensure turbo pump clamps are mounted with manufacturer's specified torque setting. Please contact your Factory Authorized Service Representative for assistance prior to replacement.
	EN61326—1:2006 CLASS A, GROUP 1, ISM EQUIPMENT
	This ISM device complies with Canadian ICES-001. Cet appareil ISM est conforme à la norme NMB-001 du Canada.
	FCC Compliance. This device complies with Part 15 of the FCC Rules. Operation is subject to the following conditions: (1) this device may not cause harmful interference, and (2) this device must accept any interference received, including interference that may cause undesired operation. 0211-3199

Table 2 Labels on the Mass Spectrometer (Continued)

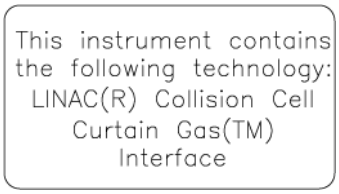
External Labels	Definition
	Do not dispose of equipment as unsorted municipal waste (WEEE).
FOR RESEARCH USE ONLY. NOT FOR USE IN DIAGNOSTIC PROCEDURES.	This mass spectrometer is for research use only. It is not intended for use in diagnostic procedures.
	This instrument contains the following technology: LINAC® Collision Cell Curtain Gas™ Interface
	**WARNING**: Hot Surface Hazard.
	Operator Guide
	Follow operating instructions (mandatory)
	Alternating Current
A	Amperes (current)
	High voltage. Electrical Shock Hazard
	On (Mains supply)
	Off (Mains supply)
	Protective Earth (ground)
V	Volts (voltage)

Table 2 Labels on the Mass Spectrometer (Continued)

External Labels	Definition
V-A	Volts - Amperes (power)
W	Watts (power)

Occupational Health and Safety Symbols

This section describes some occupational health and safety symbols found in the laboratory environment.

Table 3 Chemical Hazard Symbols

Safety Symbol	Description
	Biohazard
	Corrosive or Caustic Chemical Hazard
	Explosion Hazard
	Oxidizing Chemical Hazard
	Poison Hazard
	Reactive Chemical Hazard
	Toxic Chemical Hazard

Table 4 Mechanical Hazard Symbols

Safety Symbol	Description
	Automated Machinery Hazard
	Crushing Hazard — From Above

Table 4 Mechanical Hazard Symbols (Continued)

Safety Symbol	Description
	Crushing Hazard — From Side
	Fire Hazard
	Hot Surface Hazard
	Laser Radiation Hazard
	Lifting Hazard
	Magnetic Hazard
	Puncture Hazard

Table 5 Pressurized Gas Hazard Warning Symbols

Safety Symbol	Description
	Pressurized Gas Hazard

Mains Supply

WARNING! Electrical Shock Hazard: Use only qualified personnel for the installation of all electrical supplies and fixtures, and make sure that all installations adhere to local regulations.

The mass spectrometer power consumption is 2400 VA (50 Hz or 60 Hz) at 240 VAC.

An external line transformer is not needed for the mass spectrometer or roughing pump.

Caution: Potential Instrument Damage: Do not unpack or connect any components. The AB SCIEX FSE will unpack, connect, and configure the system for the proper operating voltage.

For information on system electrical specifications, refer to the *Site Planning Guide*.

Protective Earth Conductor

The mains supply should include a correctly installed protective earth conductor that must be installed or checked by a qualified electrician before connecting the mass spectrometer.

WARNING! Electrical Shock Hazard: Do not intentionally interrupt the protective conductor. Any interruption of the protective earth conductor is likely to make the installation dangerous.

Laboratory Ventilation

The venting of fumes and disposal of waste must be in accordance with all federal, state, provincial, and local health and safety regulations. The system shall be used indoors in a laboratory that complies with the environmental conditions recommended in the *Site Planning Guide* for the system. The source exhaust system must be vented either to an external fume hood or to an external exhaust system as recommended in the *Site Planning Guide* for the system.

Environmental Conditions

Use qualified personnel for the installation of electrical mains, heating, ventilation, and plumbing supplies and fixtures. Make sure that all installations follow local bylaws and biohazard regulations. For more information about the required environmental conditions for the system, refer to the *Site Planning Guide* for the mass spectrometer.

DANGER! Explosion Hazard: Do not operate the system in an environment containing explosive gases. The instrument is not designed for operation in an explosive environment.

WARNING! Asphyxiation Hazard: Take extreme care to vent exhaust gases properly. The use of instruments without adequate ventilation to outside air may constitute a health hazard. In addition, certain procedures required during the operation of the instrument may cause gases to be discharged into the exhaust stream; under these conditions, inadequate ventilation may result in serious injury.

WARNING! Radiation Hazard, Biohazard, Toxic Chemical Hazard: Make sure the mass spectrometer is connected to the local exhaust system and ducted to control hazardous emissions. The system should only be used in a well-ventilated laboratory environment in compliance with local regulations and with appropriate air exchange for the work performed.

Note: In the USA, OSHA 29 CFR Part 1910-1450 requires 4 to12 air changes per hour in laboratories.

WARNING! Biohazard: For biohazardous material use, always apply local regulations for hazard assessment, control, and handling. This instrument or any part is not intended to act as a biological containment safety cabinet.

Instrument Disposal (Waste Electrical and Electronic Equipment)

Do not dispose of system components or subassemblies, including computer parts, as unsorted municipal waste. Follow local municipal waste ordinances for proper disposal provisions to reduce the environmental impact of WEEE (waste, electrical, and electronic equipment). To make sure that you safely dispose of this equipment, contact an FSE for instructions.

European Union customers: Contact a local AB SCIEX Customer Service office for complimentary equipment pick-up and recycling.

System Information 1

The AB SCIEX TripleTOF® 5600/5600+ system is designed for the qualitative and quantitative analysis of chemical species. The system includes a mass spectrometer, a DuoSpray™ ion source, the optional calibrant delivery system (CDS), and a computer running the Analyst® TF software.

Theory of Operation

Mass spectrometry measures the mass-to-charge ratio of ions to identify unknown compounds, to quantify known compounds, and to provide information about the structural and chemical properties of molecules.

The AB SCIEX TripleTOF 5600/5600+ system has a series of quadrupole filters that transmit ions according to their mass-to-charge (m/z) value. The first quadrupole in this series is the QJet® ion guide, which is located between the orifice plate and the Q0 region. The QJet ion guide does not filter ions, but focuses them before they enter the Q0 region. By prefocusing the larger ion flux created by the wider orifice, the QJet ion guide increases instrument sensitivity and improves the signal-to-noise ratio. In the Q0 region, the ions are again focused before passing into the Q1 quadrupole.

The Q1 quadrupole sorts the ions before they enter the Q2 collision cell. In the Q2 collision cell, the internal energy of the ions is increased though collisions with gas molecules to the point that molecular bonds break, creating product ions. This technique allows users to design experiments that measure the m/z of product ions to determine the composition of the parent ions.

After passing through the Q2 collision cell, the ions enter the TOF region for additional mass analysis, and then enter the detector. In the detector, the ions create a current that is converted into a voltage pulse. These voltage pulses are counted, and the number of pulses leaving the detector is directly proportional to the quantity of ions entering the detector. The instrument monitors the voltage pulses and converts the information into a signal. The signal represents the ion intensity for a particular m/z value and the instrument displays this formation as a mass spectrum.

Data Handling

The Analyst TF software requires a computer running the Windows operating system. The computer with the associated system software works with the system controller and associated firmware to control the instrument and data acquisition. During system operation, the acquired data is sent to the Analyst TF software where it can be displayed as either full mass spectra, intensity of single or multiple ions versus time, or total ion current versus time.

System Overview

Figure 1-1 to Figure 1-2 show the mass spectrometer components and connections.

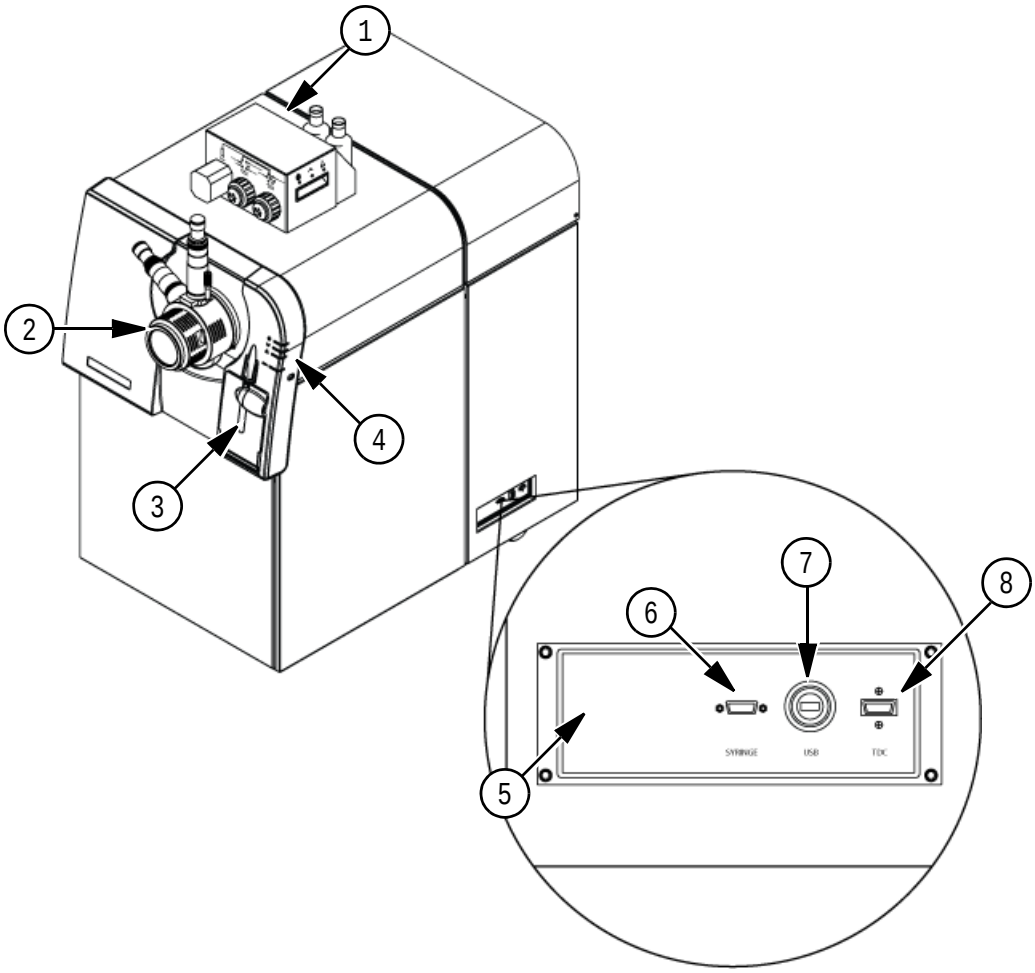


Figure 1-1 Front and right side

Item	Description	For more information...
1	Optional CDS	Refer to the *CDS Operator Guide.*
2	DuoSpray™ ion source	Refer to DuoSpray™ Ion Source User Reference on page 83
3	Syringe pump	Refer to Adjust the Integrated Syringe Pump Position on page 23.
4	Dress panel LEDs	Refer to Dress Panel LEDs on page 20.
5	TDC bulkhead	Contact an AB SCIEX FSE.
6	InfiniBand cable connection for the TDC card	Contact an AB SCIEX FSE.
7	USB cable connection for the USB-GPIB card	Contact an AB SCIEX FSE.

Figure 1-1 Front and right side (Continued)

Item	Description	For more information...
8	Serial (RS-232) cable connection for the syringe pump	Contact an AB SCIEX FSE.

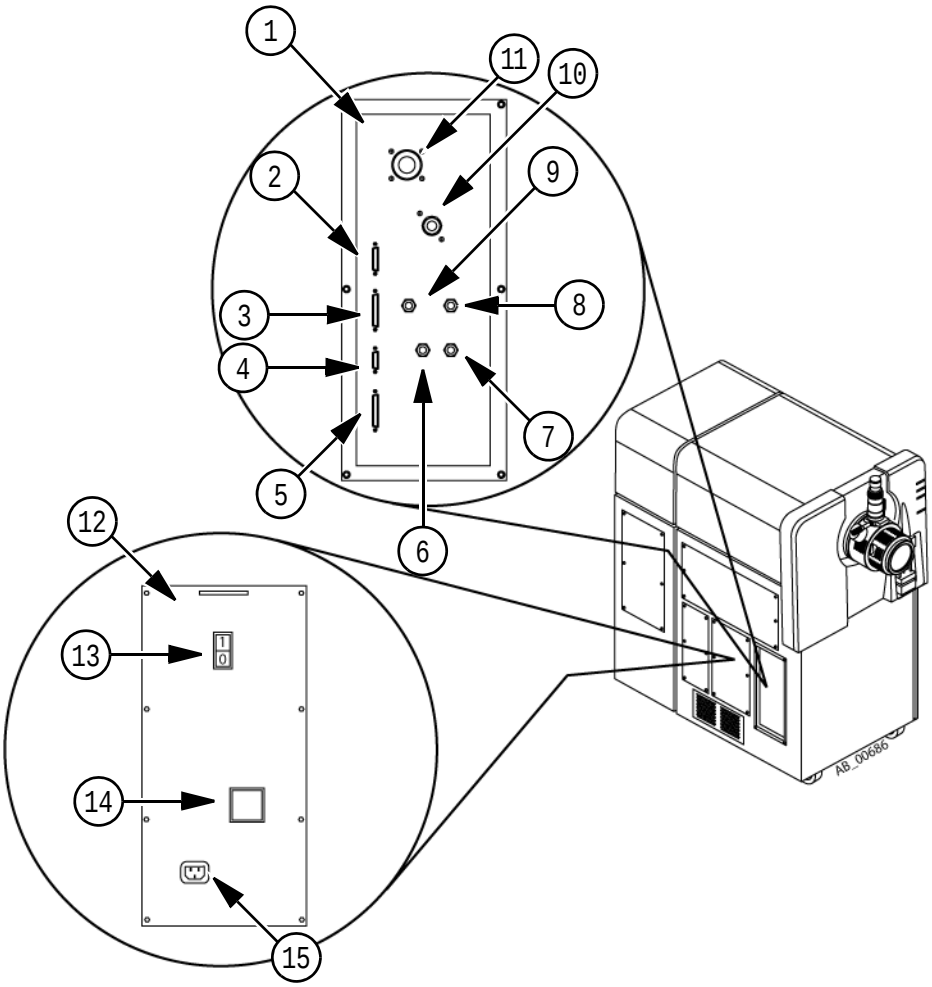


Figure 1-2 Left side view

Item	Description	For more information...
1	Gas and vacuum bulkhead	Contact an AB SCIEX FSE.
2	Calibrant control connection	See the *CDS Operator Guide*.
3	AUX IO connection. The optional LC system start signal connects to this port.	Contact an AB SCIEX FSE.
4	External control connection. This port is intended for future use.	Contact an AB SCIEX FSE.
5	Sources connection. Some ion sources connect to this port.	Contact an AB SCIEX FSE.
6	Curtain Gas™ (nitrogen) supply connection	Contact an AB SCIEX FSE.

Figure 1-2 Left side view (Continued)

Item	Description	For more information...
7	Gas 1 and Gas 2 (zero) supply connection	Contact an AB SCIEX FSE.
8	Source exhaust gas (zero air or nitrogen) supply connection	Contact an AB SCIEX FSE.
9	CAD gas (nitrogen) supply connection	Contact an AB SCIEX FSE.
10	Source exhaust waste connection	Contact an AB SCIEX FSE.
11	Roughing pump vacuum connection	Contact an AB SCIEX FSE.
12	AC distribution panel	Contact an AB SCIEX FSE.
13	Instrument power switch	Refer to Start Up the System on page 20.
14	Cover over circuit breaker	Refer to Start Up the System on page 20. Use the power switch rather than the circuit breaker to shut down the system.
15	Mains supply cable	Refer to Start Up the System on page 20.

Dress Panel LEDs

Table 1-1 Dress Panel LEDs

Instrument LED	Color	Name	Description
	Green	Power	Lit when the mass spectrometer is turned on.
	Green	Vacuum	Lit when the proper vacuum has been achieved; and flashing if the system is not at the proper vacuum level (during pumpdown and venting.)
	Red	Fault	Lit when the mass spectrometer encounters a system fault.
	Green	Syringe Pump Status	Lit when the syringe pump is running.

Start Up the System

Note: Before operating the instrument, read the safety information in the Safety and Regulatory Information.

Before the system is turned on, make sure the site requirements specified in the *Site Planning Guide* are met. This guide includes information on the mains supply and connections, source exhaust, compressed air, nitrogen, roughing pump, ventilation, exhaust, and site clearance.

Use the following procedures if you need to turn on or shut down the system. You may need to shut down the system to perform maintenance.

1. Make sure there is clear access to the mass spectrometer AC mains power cord. The cord must be accessible in order to disconnect the instrument from the AC mains power supply.
2. Make sure the 4 L drain bottle is connected to the Exhaust Waste connection on the rear of the instrument and to the laboratory ventilation system.
3. Make sure that the mains supply cable is plugged in to the instrument.
4. Make sure that the mass spectrometer and roughing pump mains supply cable are plugged into the 200 to 240 V electrical mains supply.
5. Make sure that the Ethernet cable is connected to both the instrument and the computer.
6. Turn on the roughing pump.
7. Remove the cover on the circuit breaker switch on the left side of the mass spectrometer, when viewed from the front (refer to Figure 1-2 on page 19), and then turn on the circuit breaker.
8. Replace the cover over the circuit breaker switch and then tighten the screw holding the cover until it is finger tight.
9. Turn on the instrument power switch. Refer to Figure 1-2 on page 19.
10. Turn on the computer, if it was turned off.
11. Start the software.

Shut Down the System

1. Complete or stop any ongoing scans. For more information, refer to Stop Sample Acquisition on page 61.

   Caution: Potential Instrument Damage: Turn off the sample flow before you shut down the mass spectrometer.

2. Turn off the sample flow to the mass spectrometer and disconnect the sample lines from the peripheral device to the ion source. Leave the source connected for proper venting.
3. In the Analyst TF software, deactivate the hardware profile, if it is active, and then close the Analyst TF software.
4. Turn off the instrument power switch on the left side of the instrument (refer to Figure 1-2 on page 19).
5. Turn off the roughing pump.
6. Wait 15 minutes.
7. Remove the cover on the circuit breaker switch on the left side of the mass spectrometer (refer to Figure 1-2 on page 19), and then turn off the circuit breaker.
8. Replace the cover over the circuit breaker switch and then tighten the screw holding the cover until it is finger tight.

Use the Integrated Syringe Pump

Edit the Hardware Profile for the Integrated Syringe Pump

Make sure that the serial (RS-232) cable is connected between the computer and mass spectrometer.

Make sure the syringe pump is seated properly to avoid damaging the syringe. For more information about creating and editing hardware profiles, refer to Create a Hardware Profile on page 29.

1. In the Navigation bar, under **Configure**, double-click **Hardware Configuration**.
2. Create or edit the hardware profile containing the instrument.
3. In the **Devices in current profile** box, select the mass spectrometer and click **Setup Device**.
4. In the **Configuration** tab, select **Use integrated syringe pump**.

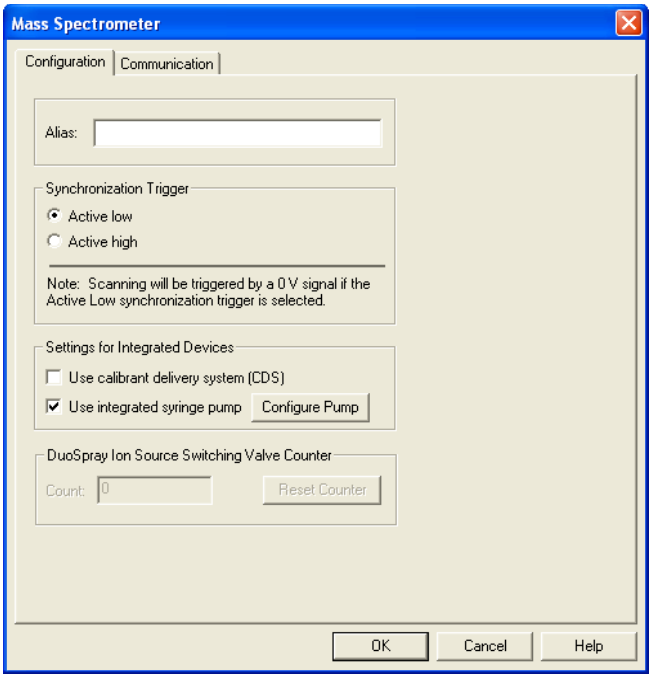


Figure 1-3 Mass Spectrometer dialog

5. Click **Configure Pump**.

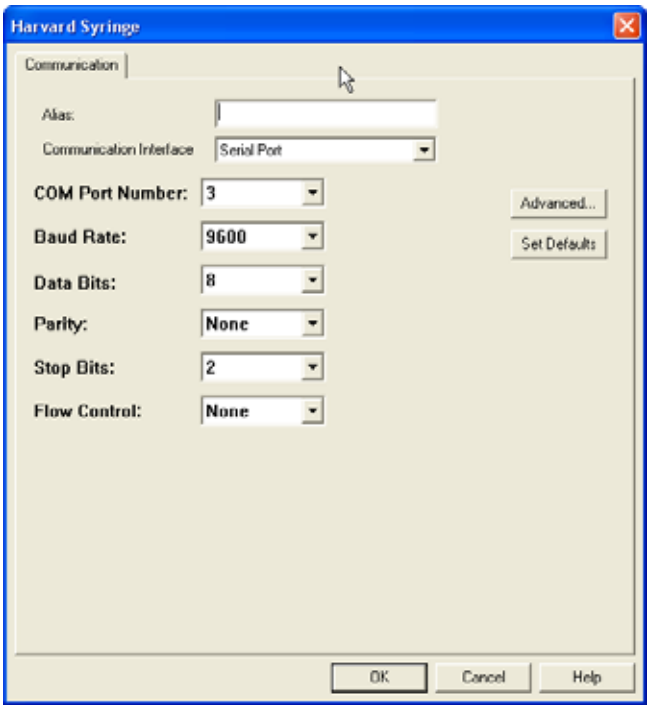


Figure 1-4 Harvard Syringe dialog

6. Select the COM port for the connection to the syringe pump.
7. Click **OK** until the Hardware Configuration Editor dialog box appears.
8. Activate the hardware profile.

Adjust the Integrated Syringe Pump Position

1. Press the Release button on the right side of the syringe pump to lower the base and then insert the syringe as shown in Figure 1-5.

   Make sure that the end of the syringe is flush against the base and that the shaft of the syringe rests in the cutout.

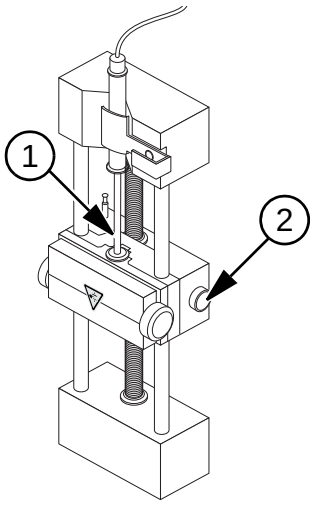


Figure 1-5 Lowering the syringe

Item	Description
1	Syringe plunger.
2	Release button. Press to raise or lower the base.

2. Adjust the post, shown in Figure 1-6, so that it triggers the automatic syringe stop before the syringe plunger hits the glass syringe.

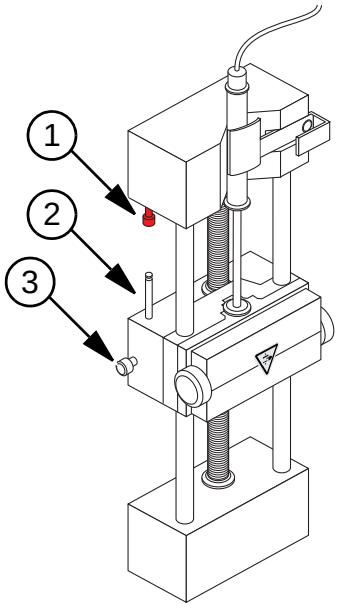


Figure 1-6 Safety stop

Item	Description
1	Automatic syringe stop. After the post hits the automatic syringe stop, the syringe pump stops.

Figure 1-6 Safety stop (Continued)

Item	Description
2	Post. Adjust the height to prevent the syringe plunger from hitting the syringe during sample infusion.
3	Post lock screw. Tighten the screw after you have adjusted the height of the post.

3. Turn the side screws as shown in Figure 1-7 to secure the syringe.

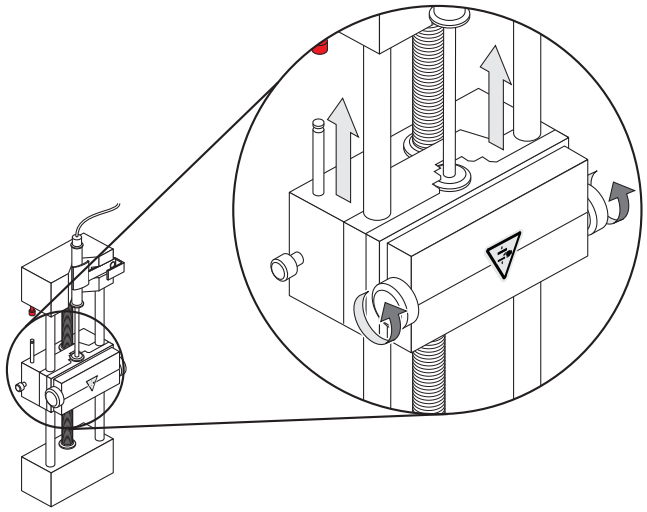


Figure 1-7 Syringe pump

4. In the Analyst TF software, on the Navigation bar, double-click **Manual Tuning**.
5. Click **Start Syringe**.
6. To stop the syringe pump, click **Stop Syringe**.

Configure the Integrated Syringe Pump

1. In the Navigation bar, under **Acquire**, double-click **Build Acquisition Methods**.
2. In the Acquisition method pane, click the **Syringe Pump** icon.

   The Syringe Pump method properties tab opens in the Acquisition Method Editor pane.
3. In the **Syringe Diameter (mm)** field, type the syringe diameter.
4. In the **Flow Rate** field, type the flow rate.
5. In the **Unit** list, select the units of flow.
6. Save the file.

Reset the Syringe Pump

If the Analyst TF software stops communicating with the syringe pump, you can reset the syringe pump.

- Use a paper clip or similar tool to press the reset button, shown in Figure 1-8.

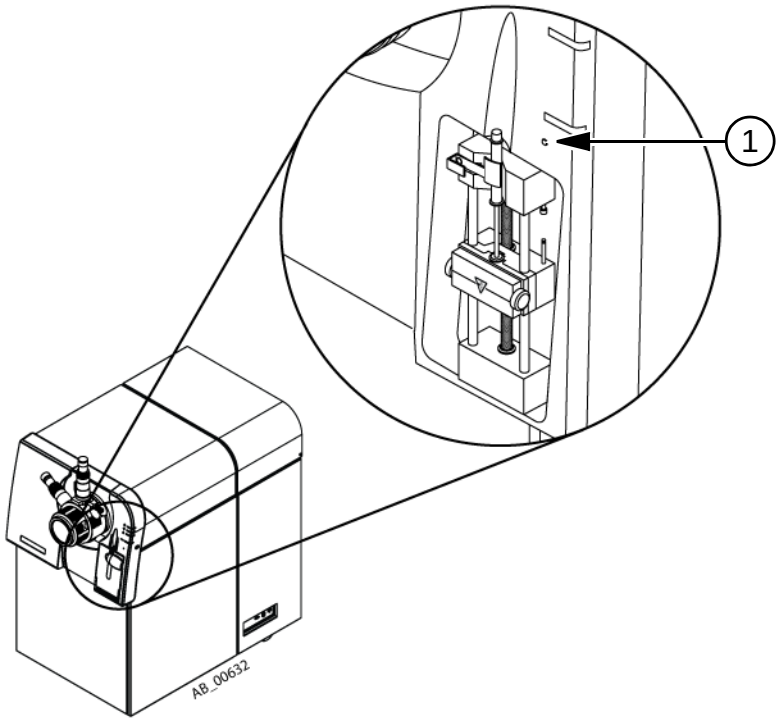


Figure 1-8 Syringe pump reset button

Item	Description
1	Reset button

Instrument Safe Fluids

These fluids can safely be used with the mass spectrometer:

- Methanol (0% to 100%)
- Acetonitrile (0% to 100%)
- Water
- Formic acid (0% to 1%)
- Ammonium acetate (1 mM to 5 mM)
- Ammonium formate (1 mM to 5 mM)
- Acetic acid (0% to 1%)

Sample Workflows

Table 2-1 Instrument Setup

Step	To do this...	Find the information in...	What does it do?
1	Create a hardware profile.	Create a Hardware Profile on page 29	Each hardware profile must include a mass spectrometer. Only devices included in the active hardware profile can be used when creating acquisition methods.
2	Create projects to store data.	Create Projects and Subprojects on page 35	Before starting an experiment, decide where to store the files related to the experiment. Using projects and subprojects helps manage data better and to compare the results more easily.
3	Optimize the instrument.	Optimize the Instrument on page 39	This is the process of optimizing the resolution, optimizing instrument parameters, and calibrating the instrument to obtain the best sensitivity and performance from the mass spectrometer.

Table 2-2 Sample Acquisition Workflow

Step	To do this...	Find the information in...	What does it do?
1	Create projects to store data.	Create Projects and Subprojects on page 35	Before starting an experiment, decide where to store the files related to the experiment. Using projects and subprojects helps manage data better and compare the results more easily.

Table 2-2 Sample Acquisition Workflow (Continued)

Step	To do this...	Find the information in...	What does it do?
2	Create an acquisition method.	Basic Acquisition Methods on page 41	To analyze samples, create an acquisition method for the mass spectrometer and any LC devices. An acquisition method indicates which peripheral devices to use, when to use them to acquire data, and the associated parameters.
4	Create and submit a batch.	Create and Submit a Batch on page 51	After creating an acquisition method, to run samples, create an acquisition batch and submit the batch to the Acquisition Queue.
5	Acquire data.	Create and Submit a Batch on page 51	Running samples involves managing the acquisition queue and monitoring instrument and device status. To submit samples and acquire data, use the Queue Manager. The Queue Manager displays queue, batch, and sample status, and allows users to manage samples and batches in the queue.
6	Analyze data in Explore mode. **—OR—** Analyze data and print reports using companion software.	Analyzing and Processing Data on page 65 MultiQuant™ software/ PeakView® software	Users can use many tools in Explore mode to view and process the acquired data, such as customizing graphs with peak labels and captions, displaying contour plots, and saving spectra in the library. Use the MultiQuant software or PeakView software to analyze data. For more information, refer to the documentation that comes with the software.

Table 2-3 Experienced User Workflow

Step	To do this...	Find the information in...
1	Mass calibrate the instrument.	Mass Calibration Tutorial located in **Start > Programs > AB SCIEX > Analyst® TF 1.6 Software > Hardware and Software Guides**
2	Optimize the instrument for an analyte of interest.	Manual Optimization Tutorial located in **Start > Programs > AB SCIEX > Analyst® TF 1.6 Software > Hardware and Software Guides**

Hardware Profiles

A hardware profile tells the software what instrument and peripheral devices to use, and how the instrument and the devices are configured and connected to the computer.

Each hardware profile must include a mass spectrometer and only peripheral devices included in the active hardware profile can be used when creating acquisition methods. Before creating an acquisition method, make sure that all devices used in the method are included in the hardware profile. In the configuration options for the mass spectrometer, ensure that the syringe pump or the CDS is enabled if it will be used during acquisition. Enable both the syringe pump and the CDS if both will be used during acquisition.

The peripheral devices configured in the active hardware profile and selected in the Add/Remove Device Method dialog appear as icons in the Acquisition Method Browser pane.

For information about setting up the physical connections, refer to the *Peripheral Devices Setup Guide*. For a list of the supported peripheral devices, refer to the *Software Installation Guide* for the Analyst® TF 1.6 software.

Create a Hardware Profile

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

1. In the Navigation bar, under **Configure,** double-click **Hardware Configuration**.
2. In the **Hardware Configuration Editor** dialog (Figure 2-1), click **New Profile.**

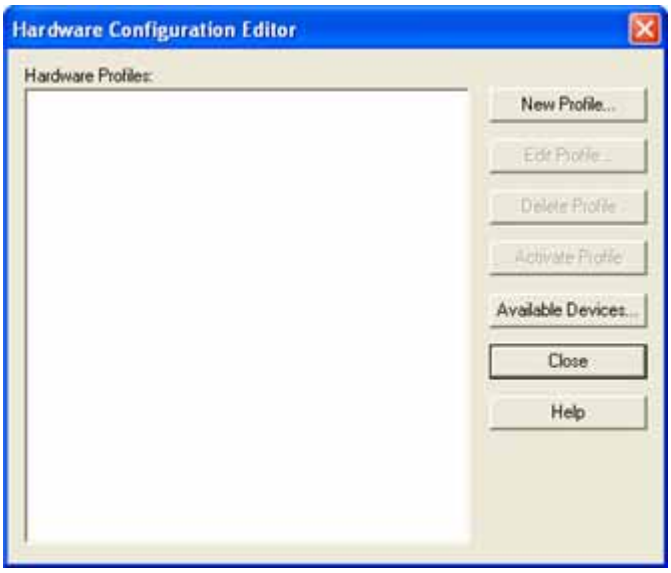


Figure 2-1 Hardware Configuration Editor dialog

3. In the **Profile Name** field (Figure 2-2), type a name for the profile. For example, TripleTOF5600+Shimadzu.

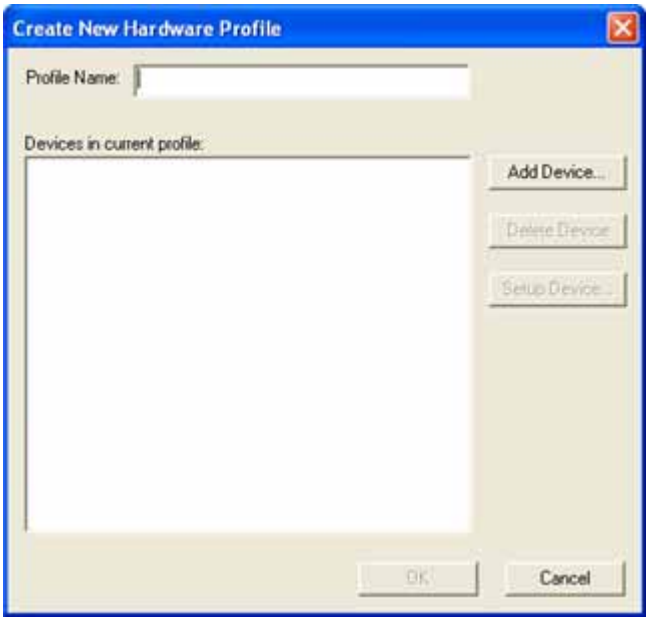


Figure 2-2 Create New Hardware Profile dialog

4. Click **Add Device.**

   In the **Available Devices** dialog, in the **Device Type** field, Mass Spectrometer is the preset value (Figure 2-3).

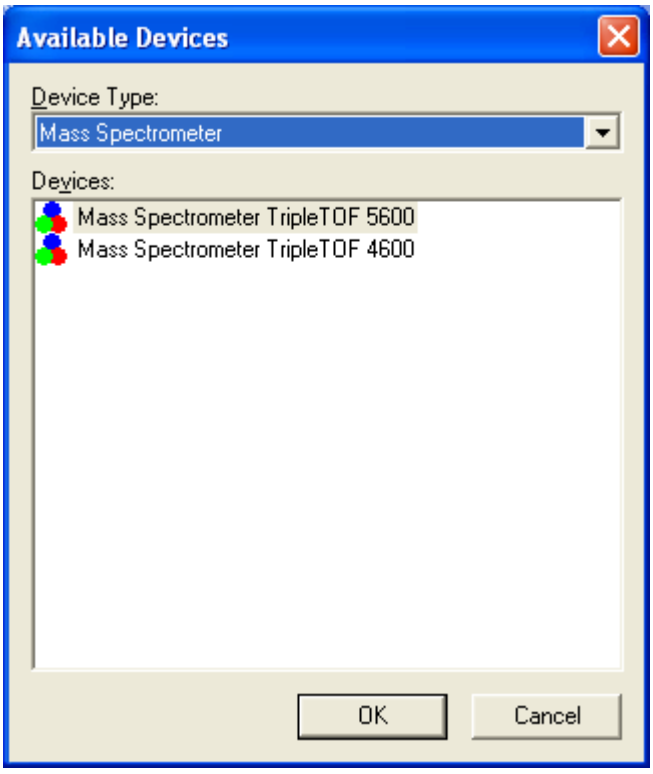


Figure 2-3 Available Devices dialog

5. In the **Devices** list, select the **Mass Spectrometer TripleTOF 5600** instrument and then click **OK.**
6. In the **Devices in current profile** list, select the instrument.
7. Click **Setup Device**.
8. (Optional) On the **Configuration** tab (Figure 2-4), in the **Settings for Integrated Devices** section, select the **Use calibrant delivery system (CDS)** check box.

9. (Optional) If using an integrated syringe pump, select **Use integrated syringe pump.**

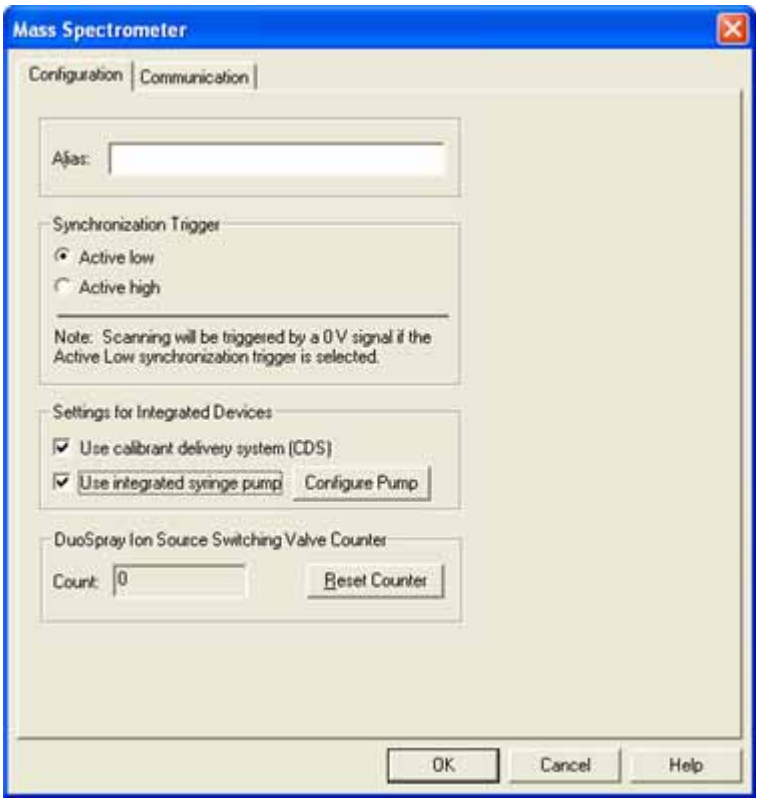


Figure 2-4 Configuration tab

10. Click **OK** to return to the **Create New Hardware Profile** dialog.
11. Click **Add Device** and then add and configure each peripheral device that is used with the instrument. Refer to Add Peripheral Devices to Hardware Profiles on page 33.
12. Ensure all changes are accepted and then click **OK.**
13. To activate the hardware profile, in the Hardware Configuration Editor, click the hardware profile and then click **Activate Profile.**

    A green check mark appears next to the profile.

Tip! A hardware profile does not have to be deactivated before activating another. Click a hardware profile and then click **Activate Profile**. The other profile is deactivated automatically.

14. Click **Close**.
15. Next steps: Either create projects and subprojects or optimize the instrument.
    - Create Projects and Subprojects on page 35.
    - Instrument Tuning and Calibrating on page 39.

Add Peripheral Devices to Hardware Profiles

Peripheral devices must be configured to enable the software to communicate with them.

Configuring the peripheral devices requires two procedures: setting up the physical connections and configuring the software to communicate with the peripheral devices.

When the software is installed, the driver required for each peripheral device is also installed (except if the peripheral devices are controlled through AAO devices; the user has to install the associated driver.) After the peripheral devices are physically connected to the computer, set up the appropriate configuration information.

1. Open the Hardware Configuration Editor.
2. In the **Hardware Profiles** list, if required, deactivate the hardware profile.
3. Click **Edit Profile**.
4. Click **Add Device**.
5. In the **Available Devices** dialog, in the **Device Type** list, select the device.
6. Click **OK**.

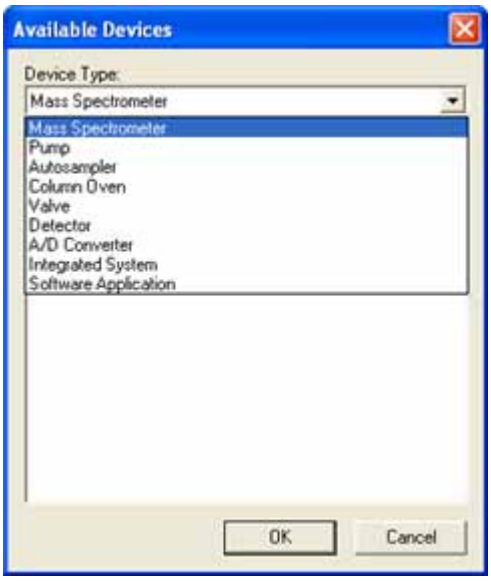


Figure 2-5 Device Type list

7. In the **Devices in the current profile** list, select the peripheral device
8. Click **Setup Device**.

   A dialog containing configuration values for the peripheral device opens.

Note: The Alias box may also be referred to as the Name box and may be found on another tab, under Alias.

9. In the **Alias** field, type a name or other identifier for the device.
   - If the device uses a serial connection to the acquisition station, in the COM Port Number list, select the COM port to which the device is connected.

- If the device uses Ethernet communication, type the IP address assigned to the device or use the corresponding host name for the address.
- If the device uses a GPIB board as a communication interface, do not change the settings for the GPIB board.

The rest of the preset values for the device are likely appropriate; do not change them. For information about the Configuration and Communication tabs, refer to the Help.

10. To restore the device preset values, on the **Communication** tab, click **Set Defaults**.
11. To save the instrument configuration, click **OK**.
12. Repeat step 4 to step 11 for each device.
13. To save the changes to the hardware profile, click **OK**.
14. To activate the hardware profile, click **Activate Profile**.

    The check mark should turn green. If a red x appears then there is an issue with the hardware profile activation. For more information, refer to Troubleshoot Hardware Profile Activation.

Troubleshoot Hardware Profile Activation

If a hardware profile fails to become active, a dialog appears indicating which device in the profile failed. A failed profile may be due to communications errors.

1. Read the error message generated. Depending on the message, there may be an issue with a device or how the communication is set up.
2. Verify that the device has power and is turned on.
3. Verify that the COM port assigned to the device is correct.
4. Verify that the communication settings with the peripheral device (for example, dip switch settings) are set correctly and match the settings on the **Communication** tab.
5. Turn off the peripheral device.
6. Wait 10 seconds.
7. Turn the device back on.

   Wait until all peripheral device power-up activities are complete before trying to activate the hardware profile again. Some peripheral devices may require 30 seconds or more to complete their power-up activities.
8. Activate the hardware profile.
9. If the issue persists, delete the failing profile and then create a new one.
10. If the issue still persists, contact AB SCIEX technical support.

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**.
2. In the **Project** name field, type a project name.
3. To use subprojects in this project, select the required folders in the **Projects folders** list and then use the arrow buttons to move them to the **Subproject folders** list (Figure 2-6).

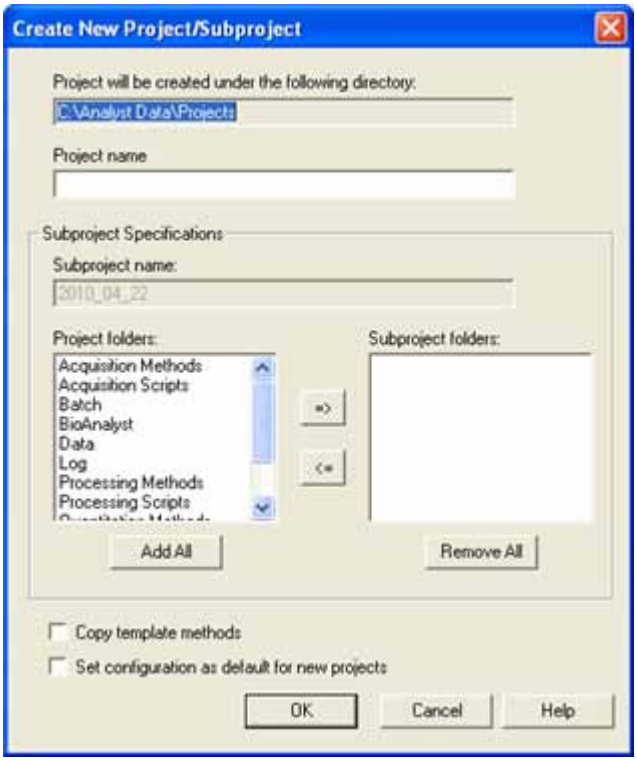


Figure 2-6 Create New Project/Subproject dialog

Note: Users cannot create a new subproject for a project that was not originally created with a subproject.

4. (If subprojects are used.) In the **Subproject name** field, type a name for the first subproject or use the existing date.
5. (Optional) To copy the template methods from the API Instrument > Acquisition Methods > template folder into the new folder, select **Copy template methods**.
6. (Optional) To use this project and subproject folder organization for all new projects, select the **Set configuration as default for new projects** check box.

   All new projects will be created with this folder configuration.
7. Click **OK**.

Create a New Subproject

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

1. On the Project toolbar, 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.
4. Click **OK**.

Copy a Subproject

Note: The user can copy a subproject from another project that has existing subprojects. If the copied subprojects contain folders that also exist in the project folder, then the software uses the project level folders.

1. Click **Tools > Project > Copy Subproject**.
2. In the **Copy Subproject** dialog, click **Browse** to navigate to the subproject source.
3. In the **Source Subproject** list, select the desired subproject.
4. Click **Browse** to navigate to the subproject destination field.
5. In the **Target Subproject** field, type the name for the copied subproject.
6. Do one of the following:
   - To copy all folders and files from the source subproject into the destination subproject, select the **Copy Contents** check box.
   - To copy only the folders in the same structure into the destination subproject, make sure that the **Copy Contents** check box is cleared.
7. Click **Copy**.

Switch Between Projects and Subprojects

- On the software toolbar (Figure 2-7), from the project list, click the required project or subproject.

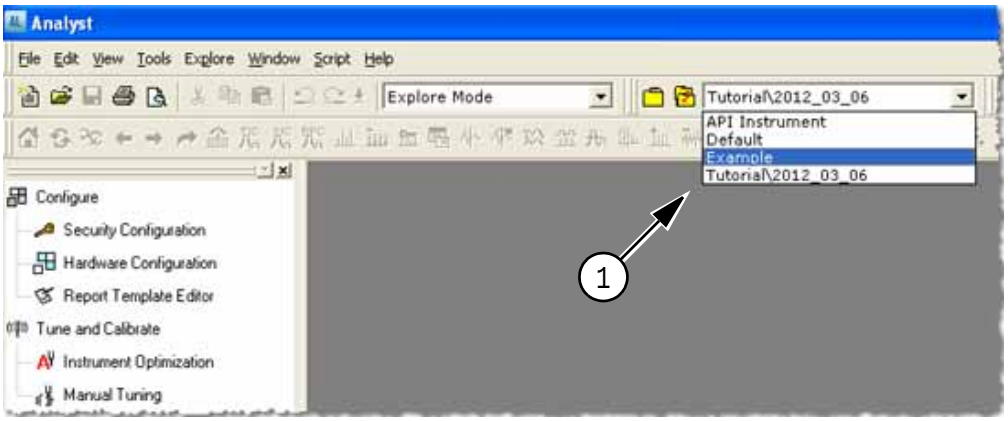


Figure 2-7 Project List

Item	Description
1	Project list showing a folder, Tutorial, and the Tutorial folders subfolders.

Installed Project Folders

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

API Instrument Project

The API Instrument project is unique and very important to the proper functioning of the instrument. The API Instrument project contains the information required for tuning and calibrating the instrument. This information includes parameter settings files, reference files, instrument data files that contain calibration and resolution information, and the acquisition methods used during automatic tuning. The API Instrument project 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 project in the Tuning Cache folder and named with the date and time they were created. The Tuning Cache is automatically purged when it reaches 2 GB.

Default Project

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

Example Project

The Example project contains sample methods and data files. Users can practice working with the Explore mode using the example data files. The example files are sorted into subfolders by instrument type and application area.

Back up the API Instrument Project

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

1. To create the backup, copy the API Instrument project, paste it to a different location, preferably to another computer, and then rename the folder. Use the date and an instrument reference if there is more than one instrument when the folder is named.
2. To recover the folder, rename the current API Instrument folder, copy the backup into the Projects folder and then change its name back to API Instrument.

Table 2-4 Icons on the Toolbar

Icon	Name	Function
	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, the software uses the project level folders.

Run the Verify Performance Only option at any time; however, tune the instrument only if a loss of sensitivity or resolution is noticed. For more information about tuning and calibration, refer to the *Advanced User* Guide.

For tuning the system, use the following solutions that come with the installation kit:

For positive mode:

- For optimizing TOF MS - MSMS high resolution or MSMS High Sensitivity, use the Tuning Solution.
- For Q1calibration, use the PPG POS solution.

In negative mode:

- For optimizing TOF MS - MSMS High Resolution or MSMS High Sensitivity, use Taurocholic acid.

Note: AB SCIEX recommends that after using the Taurocholic acid, repeat the channel alignment using the PPG 3000 solution.

- For Q1calibration, use the PPG 3000 solution.

Required material

- Tuning solutions that are supplied in the Standards Chemical Kit shipped with the system. If needed, a new Kit can be ordered from AB SCIEX.
- Gas-tight syringes (1.0 ml is recommended)
- PEEK (red) sample tubing

Prerequisites

- Make sure that a printer is configured.
- Make sure that the spray is stable and that the proper tuning solution is being used.

Optimize the Instrument

The following procedure shows how to verify the performance of the instrument. For more information on using the other instrument performance options, refer to the Help.

1. In the Navigation bar, under **Tune and Calibrate**, double-click **Manual Tuning**.
2. Run a TOF MS or Product ion scan type and confirm that there is a stable TIC and that the peaks of interest are present in the spectrum.
3. In the Navigation bar, under **Tune and Calibrate**, double-click **Instrument Optimization**.

4. Select a tuning solution. Make sure that the tuning solution matches the reference table.
5. The **Verify Performance Only** check box is preselected. Click **Next**.

   For this example, leave this option selected. If the report indicates that the instrument needs tuning, then run Instrument Optimization again and select one or more scan modes to optimize.
6. Make sure that the ion source and syringe parameters are suitable.

Note: Users can also use the CDS to inject the solution. Make sure the tuning solution matches the configuration in the reference table. Set the appropriate flow rate and then click CDS Inject.

Note: Ensure that the correct Calibrant Valve Position is selected in the Reference Table Editor for the chosen reference table. CDS can select from up to four different positions, A to D.

7. Click **GO**.

   The Verifying Performance screen appears. After the process has completed, the Results Summary appears showing the resolution and intensity for each scan mode.

An acquisition method consists of the method for the mass spectrometer and for liquid chromatography (LC) devices. Users can easily create an acquisition method using the Method Wizard.

The Acquisition Method Editor can also be used to create acquisition methods and to add a sequence of periods and experiments for the instrument and devices.

Users can use the SWATH™ acquisition feature, available in both the Method Wizard and the Acquisition Method Editor, to create SWATH acquisition methods. For more information, refer to the *Advanced User Guide*.

Create an Acquisition Method using the Method Wizard

The acquisition method can be saved in an existing project.

Tip! To copy the Method Wizard template methods into the Acquisition Methods folder in the project folder, select the Copy method templates check box in the Create New Project or Subproject dialog. To open this dialog, click **Tools > Project > Create Project or Create Subproject**.

1. Make sure that a hardware profile containing the mass spectrometer and peripheral devices is active.
2. On the software toolbar, make sure that the appropriate project is selected.
3. On the Navigation bar, in **Acquire** mode, double-click **Method Wizard**.

   The Method Wizard appears.

   Tip! Move the cursor over the interface to view tool tips and procedures.

4. From the **Choose MS Method** list, select **TOF MS (+)**.
5. From the **Choose LC Method** list, select the LC method that was created for the hardware profile.
6. Type a name for the method and then press **Enter**.
7. Click **Next**.
8. On the **Ion Source Parameters** tab, verify the values, editing them if necessary, and then click **Next**.
9. On the **TOF MS** tab, verify the values, editing them if necessary, and then click **Finish**.

Tip! If required, users can further edit the acquisition method using the Acquisition Method Editor. In **Acquire** mode, click **File > Open** and then open the method that was created using the Method Wizard.

10. Next steps: The newly created acquisition method can now be used to acquire data for preliminary analysis.

Create Acquisition Methods using the Acquisition Method Editor

Tip! If users are creating a new acquisition method file from an existing file, some or all of the peripheral device methods in the acquisition method may be used.

Only devices configured in the active hardware profile appear in the Acquisition Method Browser pane. Any devices added to the hardware profile must also be added to existing acquisition methods. For more information about devices, refer to the *Peripheral Devices Setup Guide.*

1. Make sure that a hardware profile containing the mass spectrometer and peripheral devices is active.
2. In the Navigation Bar, under **Acquire**, double-click **Build Acquisition Method**.

   The Method Editor appears with a method template based on the active hardware profile.
3. In the **Acquisition Method Properties** tab, select a **Synchronization Mode**. For more information about synchronization modes, refer to the Help.
4. In the **Acquisition method** pane, click **Mass Spectrometer**.
5. In the **MS** tab, select a scan type.
6. Type values in the fields as required. For more information refer to About Instrument Parameters on page 45.
7. In the **Advanced MS** tab, type values in the fields as required. For more information refer to About Instrument Parameters on page 45.
8. Click **Edit Parameters**.
9. On the **Source/Gas** tab, specify values in the fields as required.
10. On the **Compound** tab, specify values in the fields as required and then click **OK**.
11. Click a device icon.
12. Select the parameters for the devices as required.
13. Add any additional periods and experiments. For more information, refer to Add an Experiment and Add a Period.
14. Click **File** > **Save**.

Add an Experiment

1. Right-click the period where an experiment needs to be added and then click **Add experiment**.

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

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

2. In the **Acquisition Method Editor** pane, select the appropriate device or instrument parameters.

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.

Copy an Experiment into a Period

Prerequisite: Multi-period method

- 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. This is useful when the same or similar experiments are added to an acquisition method.

Scan Techniques

The system is a versatile and reliable system for performing liquid chromatography mass spectrometry analysis on liquid sample streams to identify, quantify, and examine polar compounds.

The system uses the following mass spectrometry techniques to analyze samples:

- Two modes of single mass spectrometry (MS):
  - Quadrupole-based single mass spectrometry (for Q1 calibration only)
  - Time-of-flight-based single mass spectrometry
- Two modes of tandem mass spectrometry (MS/MS):
  - Product ion mass spectrometry
  - Precursor ion mass spectrometry

Single Mass Spectrometry

Single mass spectrometry (MS) is used to analyze charged molecules to find the molecular weight and amount of detected ions. Individual ions detected by MS can indicate the presence of a target analyte.

Quadrupole-Based Single Mass Spectrometry

In a quadrupole-based single mass spectrometry (Q1 MS) scan, the system functions as a traditional quadrupole mass spectrometer. In this mode, the system generates single mass spectrometric information using the first quadrupole (Q1) section of the instrument.

Time-of-Flight Single Mass Spectrometry

In a time-of-flight single mass spectrometry (TOF MS) scan, the system generates mass spectrometric information by pulsing ions into a flight tube and recording their precise arrival time at the detector. Ions with a greater mass-to-charge ratio take longer to travel the flight tube.

Tandem Mass Spectrometry

The technique of MS/MS is well-suited to mixture analysis because the characteristic product ion spectra can be obtained for each component in a mixture without interference from the other components, assuming that the product ions have a unique m/z ratio.

Use MS/MS for targeted analysis by monitoring specific precursor/product ions while the sample is eluting. This type of analysis is more specific than single MS, which only discriminates on the basis of the mass-to-charge ratio.

Product Ion Mass Spectrometry

In a product ion scan (Product Ion), the system generates mass spectrometric information by selecting a particular precursor ion window in Q1, fragmenting in Q2 (a collision cell) and pulsing the ions (fragment ions) into a flight tube and recording their precise arrival time at the detector. Product ions can provide information on the molecular structure of the original (precursor) ions.

Precursor Ion Mass Spectrometry

In a precursor ion scan, the system detects precursor ions that generate a specific product ion. The instrument uses Q1 in mass resolving mode to scan over the mass range of interest, while the TOF section records product ion spectra for each precursor ion. The Q1 mass spectrum shows all precursor ions that produce the product ion of interest.

About Spectral Data Acquisition

Spectral data can be acquired in one of the following modes, as shown in Table 4-1. Spectral Data can only be acquired from Q1 and Precursor Ion scan types.

Table 4-1 Spectral Data Acquisition

Mode	Description
Profile	The preset value is 0.1 Da. Profile data is the data generated by the instrument and corresponds to the intensity recorded at a series of evenly spaced discrete mass values. For example, for the mass range 100 Da to 200 Da and step size 0.1, the instrument scans from 100 Da to 200 Da in 0.1 Da increments (e.g. 100.0, 100.1, 100.2, 100.3… up to 200.0).
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 (less data steps are made) but with the loss of peak shape information.

About Instrument Parameters

The working parameters are the set of instrument parameters currently being used.

- **Ion Source-dependent (Source and gas) parameters**: These parameters can change depending on the ion source used.
- **Compound-dependent parameters**: These parameters consist mostly of voltages in the ion path. Optimal values for compound-dependent parameters vary depending on the compound being analyzed.
- **Detector parameters**: These parameters affect the detector. The Multi-Channel Plate is the detector in a TOF instrument and consists of four channels for ion detection. The total of the channels equals the ion intensity. This parameter can be optimized using Instrument Optimization.

The following figure shows the location of the parameters on the ion optics path.

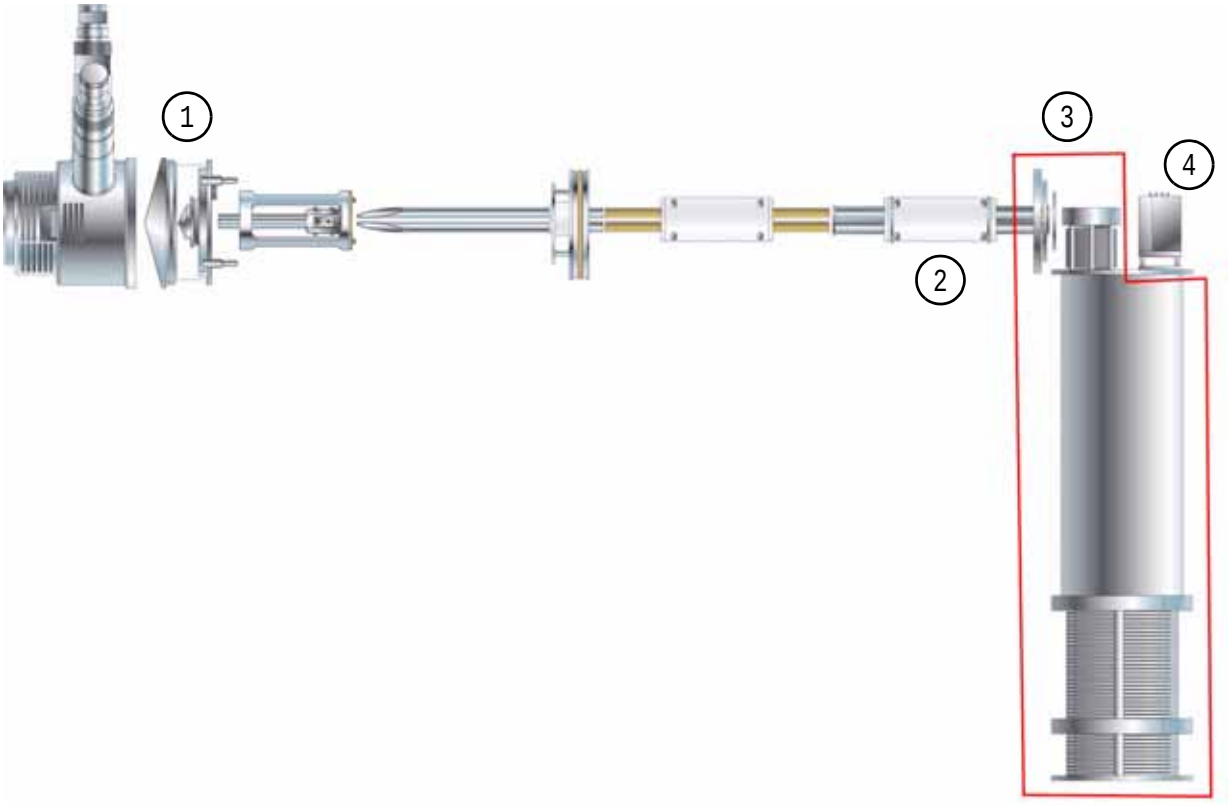


Figure 4-1 Ion optics path and parameters

Item	Parameter	Parameter type	Use	Scan type
1	Ion Source Gas 1 (Gas 1)	Source and Gas	The GS1 parameter controls the nebulizer gas. The nebulizer gas helps generate small droplets of sample flow and affects spray stability and sensitivity.	All
1	Ion Source Gas 2 (Gas 2)	Source and Gas	The GS2 parameter controls the flow of heater gas, which helps evaporate the solvent to produce gas phase sample ions.	All
1	Curtain Gas (CUR)	Source and Gas	The CUR parameter controls the gas between the curtain plate and the orifice plate. It prevents the contamination of the ion optics.	All
1	Temperature (TEM)	Source and Gas	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.	All

Figure 4-1 Ion optics path and parameters (Continued)

Item	Parameter	Parameter type	Use	Scan type
1	IonSpray Voltage Floating (ISVF)	Source and Gas	The ISVF parameter affects the stability of the spray and hence the signal sensitivity. This is the voltage applied to the needle that sprays the sample.	All
1	Nebulizer Current (NC)	Source and Gas	The NC parameter controls the current applied to the corona discharge needle in the APCI probe used in the TurboIonSpray® ion source when using the Heated Nebulizer probe. The discharge ionizes solvent molecules, which in turn ionize the sample molecules.	All
1	IHT (Interface Heater Temperature)	Source and Gas	The IHT parameter controls the temperature of the NanoSpray® interface heater and is only available if the NanoSpray ion source and interface are installed. The optimal heater temperature depends on the type of sample being analyzed and the solvent used. If the heater temperature is too high, the signal degrades. Typically, heater temperatures are in the 130 to 180 °C range. The maximum heater temperature that can be set is 250 °C, but this is too high for most applications.	All
2	CAD Gas	Compound	The CAD parameter controls the pressure of collision gas in the collision cell. 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. Use the preset value and optimize for the compound.	All

Figure 4-1 Ion optics path and parameters (Continued)

Item	Parameter	Parameter type	Use	Scan type
1	DP (Declustering Potential)	Compound	The DP parameter controls the voltage on the orifice, which affects the ability to decluster ions between the orifice and QJet® ion guide. It is used to minimize the solvent clusters that may 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, unwanted fragmentation may occur. Use the preset value and optimize for the compound.	TOF MS/MS
2	CE (Collision Energy)	Compound	The CE parameter controls the potential difference between Q0 and Q2 (collision cell). 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. Use the preset value and optimize for the compound.	Q1, MS/MS
2	CES (Collision Energy Spread)	Compound	The CES parameter, in conjunction with the Collision Energy (CE), determines the collision energy applied to the precursor ion in a Product Ion scan. The collision energy is ramped from low to high. For example, in positive mode, the collision energy will be ramped from CE – CES to CE + CES. By entering a CES value, collision energy spread is automatically turned on. Use the preset value and optimize for the compound.	Q1, MS/MS

Figure 4-1 Ion optics path and parameters (Continued)

Item	Parameter	Parameter type	Use	Scan type
3	Ion Release Delay (IRD)	Compound	The amount of time in milliseconds before the ion pulse. The default (11 msec) is calculated based on the TOF masses and can be adjusted by the operator. The range is typically 6 msec to 333 msec. This parameter is optimized using Instrument Optimization if the Enhanced Ion option is selected in the Advanced options. In general, the default values do not have to be changed.	MS/MS only, Enhanced
3	Ion Release Width (IRW)	Compound	This is the width, or duration, of the ion pulse in milliseconds and is calculated based on the IRD. The range is typically 5 to 328 msec with a default value of 10 msec. This parameter is optimized using Instrument Optimization if the Enhanced Ion option is selected in the Advanced options. In general, the default values do not have to be changed.	MS/MS only, Enhanced
4	MCP (CEM)	Detector	The CEM parameter controls the voltage applied to the detector. The voltage affects the detector response.	All

Acquisition Method Editor Icons

Table 4-2 Acquisition Method Editor Icons

Icon	Name	Function
	Mass Spec	Shows the MS tab in the Acquisition Method Editor.
	Period	Right-click to add an experiment, add an IDA Criteria Level, or delete the period.
	Autosampler	Opens the Autosampler Properties tab.

Table 4-2 Acquisition Method Editor Icons (Continued)

Icon	Name	Function
	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. For more information about the DAD, refer to View DAD Data on page 74.
	ADC	Opens the ADC Properties tab. For more information about the ADC, refer to Show ADC Data on page 67.

A batch is a collection of information about the samples to be analyzed. Batches tell the software the order in which to analyze the samples. For information about importing batches, refer to the *Advanced User Guide*.

Create and Submit a Batch

Use this workflow to create and submit a batch.

Set Queue Options

The queue goes one by one through the list, running each sample with the selected acquisition method. After all the samples have been acquired, the queue stops and the instrument goes into the Standby mode. In the Standby mode, the LC pumps and some instrument voltages are turned off.

The user can change the length of time the queue runs after the last acquisition has finished, before it puts the instrument into the Standby mode. For more information about the other fields in the Queue Options dialog, refer to the Help.

1. In the Navigation Bar, click **Configure**.
2. Click **Tools > Settings > Queue Options**.

   The Queue Options dialog opens.

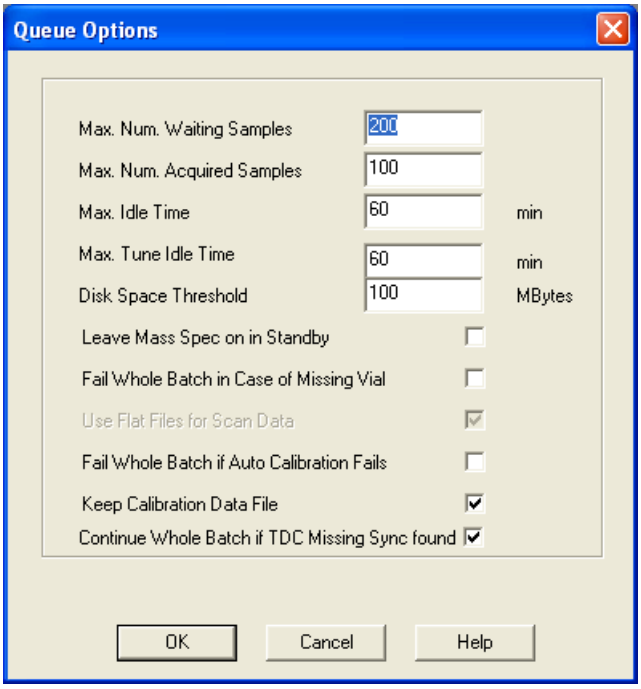


Figure 5-1 Queue Options dialog

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 length of time the queue will wait after acquisition is completed before going into Standby mode. The preset value is 60 minutes.

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

   If using an LC method, before the run is started, make sure that there is enough solvent in the reservoirs for the primary flow rate for all of the sample runs and the Max. Idle Time.
5. Select **Leave Mass Spec on in Standby** to keep the mass spectrometer running after analysis have been completed. This feature allows the heaters and gasses to continue running, even after devices have entered idle state, so that the source housing and front plate are kept free of contaminants.
6. Select **Fail Whole Batch in Case of Missing Vial** to fail the entire batch when a missing vial is encountered. If this option is not selected, only the current sample will fail and the queue will continue to the next sample.
7. Select **Fail Whole Batch if Auto Calibration Fails** to stop the batch if auto calibration fails.
8. Select **Keep Calibration Data File** to keep the calibration data file in a subfolder in the Data folder of the project from which samples are being submitted.
9. Select **Continue Batch when TDC Missing Sync found** to continue acquiring the entire batch when a TDC Missing Sync signal is encountered. If this check box is not selected, the current sample will fail and the queue will not proceed to the next sample when this signal is encountered.

Add Sets and Samples to a Batch

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

1. In the Navigation Bar, under **Acquire**, double-click **Build Acquisition Batch**.

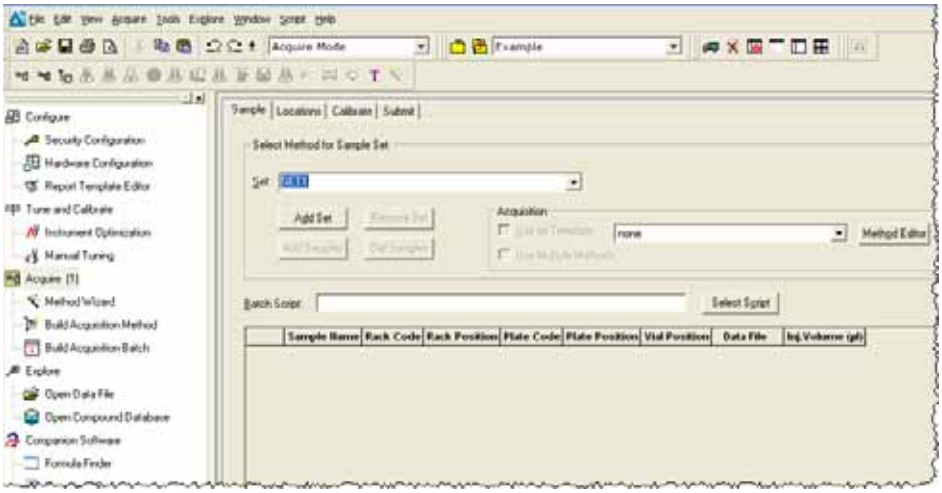


Figure 5-2 Batch Editor

2. In 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 5-3 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, in the **Number of digits** field, type the number of digits to include in the sample name.

For example, if 3 is typed, the sample names would be samplename001, samplename002, 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: AB SCIEX recommends using a new .wiff file for each sample.

11. In the **Sub Folder** field, type a name.

    The folder is stored in the Data folder for the current project. If the Sub folder field is left blank, 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 be added.
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. In the **Sample** tab, in the **Acquisition** section, select a method from the list.
15. In the **Vial Position** column, indicate the positions of the vials.

Tip! It is also possible to automatically fill in the samples from the Locations tab by clicking on the first and last vial within a set with the Shift key held down. These vials appear as red circles. On the Locations tab, multiple injections from the same vial can be done by holding down the Ctrl key while clicking the vial location. The red circle turns green.

16. To set sample locations, do one of the following:
    - Set Sample Locations in the Batch Editor on page 56.
    - Select Vial Positions using the Locations Tab (Optional) on page 57.

Set up Sample Calibration

The software can automatically schedule and execute the external auto calibration while samples are being acquired in batch mode. This ensures good mass accuracy is maintained throughout the acquisition.

If the CDS is not configured, calibration is done using an autosampler and users must supply the calibration method (*.dam) and the vial position of the calibrant sample.

1. In the **Batch Editor**, click the **Calibrate** tab.

2. In the **Calibrate Every _ Samples** field, type the number of samples to be acquired between calibration samples.
3. From the **Calibrant Reference Table**, select a table from the list of all calibrant reference tables available for the current polarity. Ensure that the selected reference table has the correct Calibrant Valve Position.
4. Set the **CDS Inject Flow Rate**.

   When the batch is submitted, the calibration samples are inserted into the queue. Each set starts with a calibration sample. The calibration method is named Cal_ plus the acquisition method name (for example, Cal_TOF.dam). If the CDS is configured, the software automatically creates a calibration method that matches the acquisition method that is used for the next sample in the queue. Calibration data is saved to a separate data file for each calibration sample. The calibration data file is saved in the subfolder Cal Data and named with Cal plus the time stamp and calibration sample index (for example, Cal200906261038341.wiff) if the Keep Calibration Data File was selected in the Queue Options dialog.

Note: Re-ordering or deleting samples in the queue may result in calibration samples being lost or no longer matching the following method.

Submit a Sample or a Set of Samples

1. In the **Batch Editor**, click the **Submit** tab.
2. If the Submit Status section contains a message about the status of the batch, do one of the following:
   - If the message indicates that the batch is ready for submission, proceed to step 3.
   - If the message indicates that the batch is not ready for submission, make the changes as indicated by the message.
3. Click **Submit**.

   The Acquisition dialog appears.
4. Save the file.

Change Sample Order

The order of the samples can be edited before they are submitted to the Queue.

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

Acquire Data

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

1. In the Navigation Bar, click **Acquire**.

2. Click **View > Sample Queue**.

   The Queue Manager opens with all submitted samples.

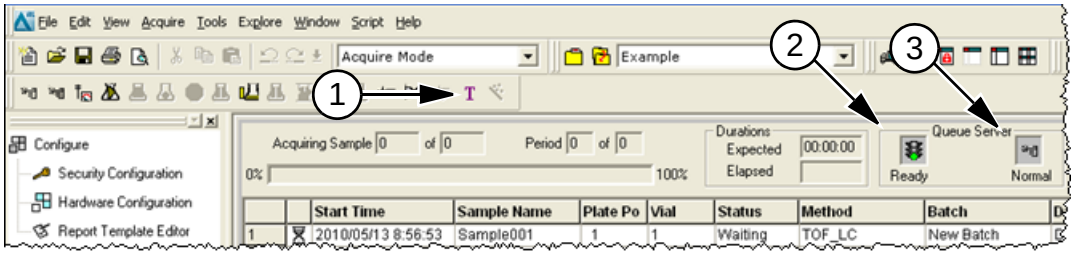


Figure 5-4 Queue Manager

Item	Description
1	The Tune icon should not be pressed in.
2	Queue status.
3	Queue Server should be in Normal mode. For more information, refer to Queue States on page 59.

3. Click **Acquire > Start Sample**.
4. Next steps: After the data has been acquired, it can be analyzed. Depending on the application, use the MultiQuant™ software, the MetabolitePilot™ software, or the PeakView® software. For more information, refer to the documentation that comes with the software.

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 on page 53.

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

1. In the **Sample** tab, in the **Set** list, select the set for which sample locations need to be specified.
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**, click the **Locations** tab.
2. In the **Set** list, select the set for which sample locations need to be specified.
3. In the **Autosampler** list, select the autosampler.

   The appropriate number of rack spaces for the autosampler is shown in the graphic rack display.
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 one of the rectangles, or select a rectangle and then click **Plate/ Autosampler View**.

   The circles depicting the wells or vials for the plate or tray appear.
6. To select whether samples are marked by row or column, click **Row/Column Selection**.

   If the button shows a red horizontal line, the Batch Editor marks the samples by row. If the button shows a red vertical line, the Batch Editor marks the samples by column.
7. Click the sample wells or vials in the order to be analyzed. Click a selected well or vial again to clear it.
8. Save the file.

Tip! To auto fill in the samples, hold down the Shift key and then click the first and last vial within a set. To perform multiple injections from the same vial, hold down the Ctrl key and then click the vial location. The red circle changes to a green circle.

Stop Sample Acquisition

The following procedure shows one way to stop sample acquisition. For more information on the other ways to stop sample acquisition, refer to Table 5-4. When a sample acquisition is stopped, the current scan finishes before the acquisition is stopped.

1. In the Queue Manager, click the sample in the queue after the point where acquisition should stop.
2. Click **Acquire > Stop Sample**.

   The queue stops after the current scan in the selected sample is complete. The sample status on the Queue Manager (Local) window changes to Terminated, and all others following in the queue are Waiting.
3. When ready to continue processing the batch, click **Acquire > Start Sample**.

Batch and Acquisition Method Editor Tips

Table 5-1 Tips

To do this...	...do this
To change all the values in a column simultaneously	click a column heading and then right-click. From the menu, use the Auto Increment and Fill Down commands to change the values in the column. This 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 if the Use Multiple Methods option is used.
To select more than one well or vial at a time	hold down the Shift key and then click the first and last well or vial in the range.

Batch Editor Right-Click Menu

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

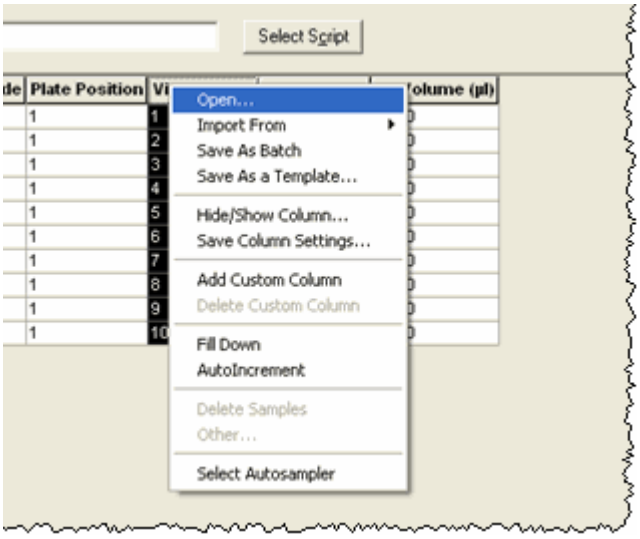


Figure 5-5 Batch right-click menu

Menu	Function
Open	Opens a batch file.
Import From	Imports a file.
Save As Batch	Saves the batch with a different name.
Save As a Template	Saves the batch as a template. Used with the Express View feature.

Figure 5-5 Batch right-click menu (Continued)

Menu	Function
Hide/Show Column	Hides or shows a column.
Save Column Settings	Saves the batch column settings.
Add Custom Column	Adds a custom column.
Delete Custom Column	Deletes a custom column.
Fill Down	Fills the same data into the selected cells.
Auto Increment	Automatically increments data into the selected cells.
Delete Samples	Deletes the selected row.
Select Autosampler	Selects an autosampler.

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.

Queue States

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

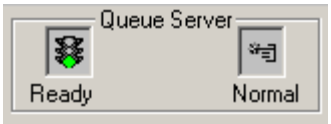


Figure 5-6 Queue Server indicator showing Normal mode

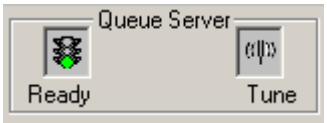


Figure 5-7 Queue Server indicator showing Tune mode

The first icon in Figure 5-6 shows the queue state. The second icon indicates whether the queue is in Tune mode (for tuning) or Normal mode (for running samples). Table 5-2 shows the various queue states.

Table 5-2 Queue States

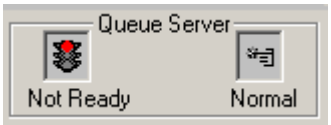
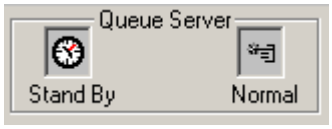
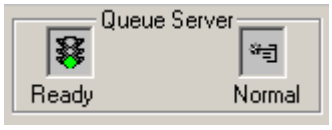
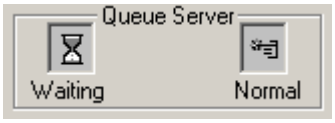
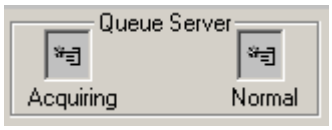
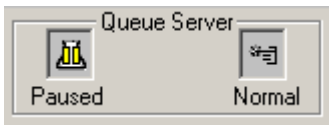
Icons	State	Definition
	Not Ready	In the Not Ready state, the hardware profile is deactivated and the queue is not accepting any sample submissions.

Table 5-2 Queue States (Continued)

Icons	State	Definition
	Standby	In the Standby state, the hardware profile has been activated, but all devices are idle. Pumps are not running and gases are turned off.
	Warming Up	In the Warming Up state, the instrument and devices are equilibrating, columns are being conditioned, the autosampler needle is being washed, and column ovens are reaching temperature. The period of equilibration is selected by the operator. From this state, the system can go to the Ready state.
	Ready	In the Ready state, 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	In the Waiting state, the system will automatically begin acquisition when the next sample is submitted.
	Prerun	In the Prerun state, 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	In the Acquiring state, the method is run and data acquisition occurs.
	Paused	In the Paused state, the instrument has been paused during acquisition.

View Instrument and Device Status Icons

Icons representing the instrument and each device in the active hardware configuration appear on the status bar in the bottom right corner of the window. The user can view the detailed status of an LC pump to check if the LC pump pressure is appropriate, or view the detailed status of the instrument to check the temperature of the ion source.

- On the status bar, double-click the icon for the device or instrument.

  The Instrument Status dialog opens.

Table 5-3 Instrument and Device Status (showing the instrument icon)

Status	Icon	Background color	Description
Idle		Green or yellow	The device is not running. If the background color is yellow, the device should be equilibrated before it is ready to run. If the background color is green, 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, from 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.

Note: For each status the background color can also be red. This situation means that the device encountered an error while in that status.

Queue Right-Click Menu

Right-click in the Queue table to access the following options.

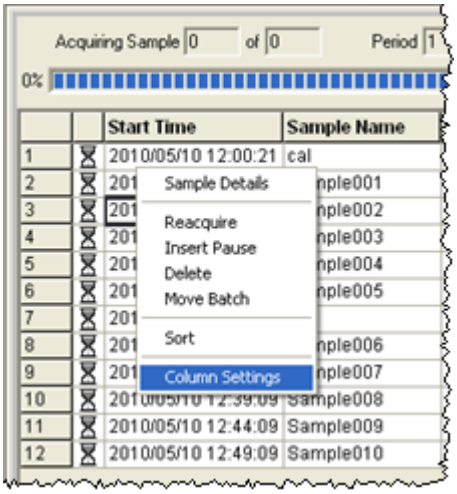


Figure 5-8 Queue Manager right-click menu

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 by the preselect column.
Column Settings	Changes the column settings.

Icon Quick Reference: Acquire Mode

Table 5-4 Acquire Mode Icons

Icon	Name	Function
	View Queue	View the sample queue.
	Instrument Queue	View a remote instrument station.
	Status for Remote Instrument	View the status of a remote instrument.
	Start Sample	Starts the sample in the queue.

Table 5-4 Acquire Mode Icons (Continued)

Icon	Name	Function
	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 the samples.
	Pause Sample Now	Inserts a pause in the queue.
	Insert Pause before Selected Sample	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 to start acquiring the next sample.
	Equilibrate	Click to select a method to use to equilibrate the devices. This method should be the same as the method used with the first sample in the queue.
	Standby	Puts the instrument in Standby mode.
	Ready	Puts the instrument in Ready mode.
	Reserve Instrument for Tuning	Reserves the instrument for tuning and calibrating.

Analyzing and Processing Data

6

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 *Advanced User Guide*.

- Labelling 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

Prerequisite: The Example project is selected.

1. In the Navigation Bar, under **Explore**, double-click **Open Data File**.

   The Select Sample dialog opens.
2. In the **Data Files** field, double-click **TOF.**
3. Select **Reserpine MSMS.wiff.**
4. In the **Samples** list, select a sample.
5. Click **OK**.

   The data acquired from the sample is shown. If data is still being acquired, the mass spectrum, DAD/UV trace, and TIC continue to update automatically.

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.

Navigate Between Samples in a Data File

Prerequisite: The Example project is selected.

Table 6-9 shows the navigation icons used in this procedure. If samples were saved in separate data files, then open each file individually.

1. In the Navigation Bar, under **Explore**, double-click **Open Data File**.
2. In the **Data Files** list, double-click **TOF**.
3. Select **Reserpine MSMS.wiff**.

4. To skip to the next sample in the data file, click the icon with the arrow pointing to the right.
5. To skip to a non-sequential sample, click the icon with the arrow curving to the right.
6. In the **Select Sample** dialog, in the **Sample** list, select the sample.
7. To go to the previous sample in the data file, click the icon with the arrow pointing to the left.

Show 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 HPLC device method (LC pump flow rate). In addition, it also contains the MS resolution and mass calibration tables used for the sample acquisition. Table 6-1 shows the software functionality available when the user views the file information.

Note: If data is acquired from more than one sample into the same .wiff file, the file information pane will not refresh automatically as the user scrolls through the samples. Close the file information pane and then reopen it 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.**

Table 6-1 Right-Click Menu for Show File Information Pane

Menu	Function
Copy	Copies the selected data.
Paste	Pastes data.
Select All	Selects all the data in the pane.
Save To File	Saves data in an .rtf file.
Font	Changes the font.
Save Acquisition Method	Saves the acquisition method as .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 pane.

Show Experimental Data in Tables

- With a data file open, click **Explore** > **Show** > **Show List Data**.

  The data is shown in a pane below the graph.

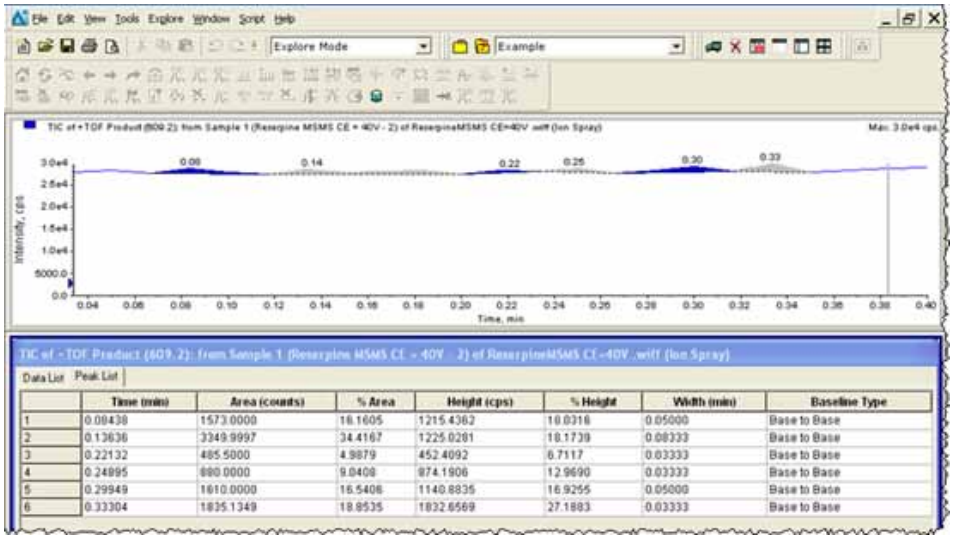


Table 6-2 Right-Click Menu for the Spectral Peak List Tab

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

Table 6-3 Right-Click Menu for the Chromatographic Peak List Tab

Menu	Function
Analyst Classic Parameters	Opens the Analyst Classic dialog.
IntelliQuan Parameters	Opens the Intelliquan dialog.
Save As Text	Saves the data as text file.
Delete Pane	Deletes the pane.

Show ADC Data

ADC (analog-to-digital converter) 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 have ADC data available, acquire the data and the mass spectrometer data simultaneously and save it in the same file.

Prerequisite: The Example project is selected.

1. In the Navigation Bar, under **Explore**, double-click **Open Data File**.

   The Select Sample dialog opens.

2. In the **Data Files** list, navigate to the file to open, and then select and pan a sample.

3. Click **Explore > Show > Show ADC Data**.

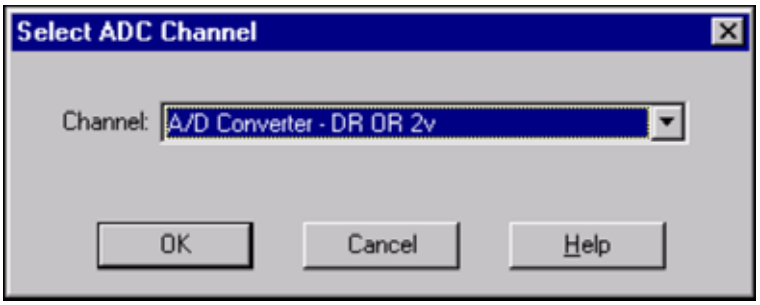


Figure 6-1 Select ADC Channel dialog

4. In the **Channel** list, select a channel.
5. Click **OK**.

   The ADC data opens in a new pane below the active pane.

Show Basic Quantitative Data

1. With a data file open, click **Explore > Show > Show List Data**.
2. In the **Peak List** tab, right-click and select **Show Peaks in Graph.**

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

Chromatograms

Table 6-4 Chromatograms

Types of chromatograms	Purpose
TIC (Total Ion Chromatogram)	A chromatographic display 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 appear as a TIC. If the experiment contains only one scan, it is shown as a spectrum. For more information about using the available icons, refer to Table 6-8. 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 with the TIC
XIC (Extracted Ion Chromatogram)	An ion 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.

Table 6-4 Chromatograms (Continued)

Types of chromatograms	Purpose
BPC (Base Peak Chromatogram)	Chromatographic plot that shows the intensity of the most intense ion within a scan versus time or scan number.
TWC (Total Wavelength Chromatogram)	A chromatographic display 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.
XWC (Extracted Wavelength Chromatogram)	A subset of TWC, an XWC shows the absorbance for a single wavelength or the sum of the absorbance for a range of wavelengths.
DAD (Diode Array Detector)	A UV detector that monitors the absorption spectrum of eluting compounds at one or more wavelengths.

Show TICs from a Spectrum

Prerequisite: The Example project is selected.

1. In the Navigation Bar, under **Explore**, double-click **Open Data File**.

   The Select Sample dialog opens.
2. In the **Data Files** list, open a file containing spectra.
3. 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**.

Show a Spectrum from a TIC

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.

Generate XICs

The user can generate XICs 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 that is under the x-axis. For more information about using the available icons, refer to Table 6-8.

There are several methods for extracting ions to generate an XIC, depending on whether chromatographic or spectral data is used. Table 6-5 contains a summary of methods that can be used with chromatograms and spectra.

Table 6-5 Summary of XIC Generation Methods

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

To generate an XIC using a selected range

1. In the Navigation Bar, under **Explore**, double-click **Open Data File**.

   The Select Sample dialog opens.

2. In the **Data Files** list, select a file containing spectra.
3. Click **OK**.
4. To select a range inside the pane, click and hold the left mouse button at the start of the range and then drag the cursor to the stop point and release.

   The selection is highlighted in blue.

5. Click **Explore > Extract Ions > Use Range**.

   An XIC of the specified 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.

To generate an XIC using the maximum peak

1. In the Navigation Bar, under **Explore**, double-click **Open Data File**.

   The Select Sample dialog opens.
2. In the **Data Files** list, select a file containing spectra.
3. Click **OK**.
4. Select a range.

   The selection is highlighted in blue.
5. 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.

To generate an XIC using base peak masses

1. In a BPC, select the peak from which to extract ions.

   The selection is highlighted in blue.
2. 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.

To extract ions by selecting masses

1. Open a spectrum or chromatogram.

2. Click **Explore > Extract Ions** > **Use Dialog**.

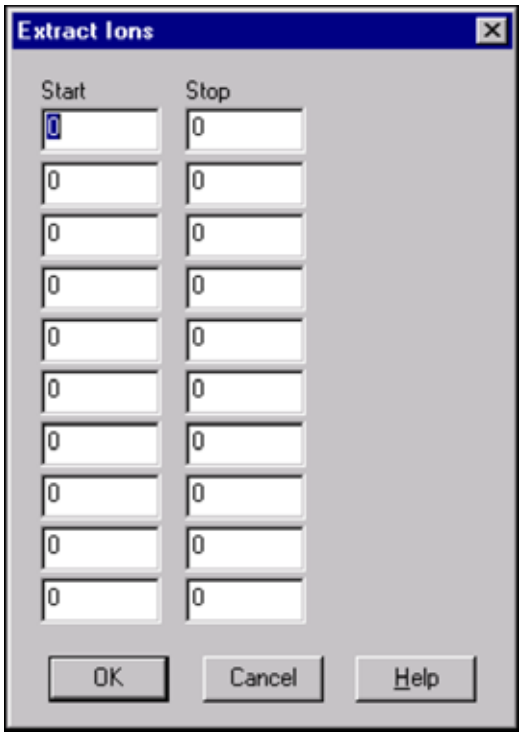


Figure 6-2 Extract Ions dialog

3. Type the values for each XIC to be created. If a stop value is not typed, then the range is defined by the start value.
   - In the **Start** field, type the start value (lower value) for the mass range to be extracted.
   - In the **Stop** field, type the stop value (higher value) for the mass range to be extracted.
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. For more information about using the available icons, refer to Table 6-8.

1. Select an area within a TIC.

   The selection is highlighted in blue.

2. Click **Explore > Show > Show Base Peak Chromatogram**.

   The selections are shown in the Start Time and End Time fields.

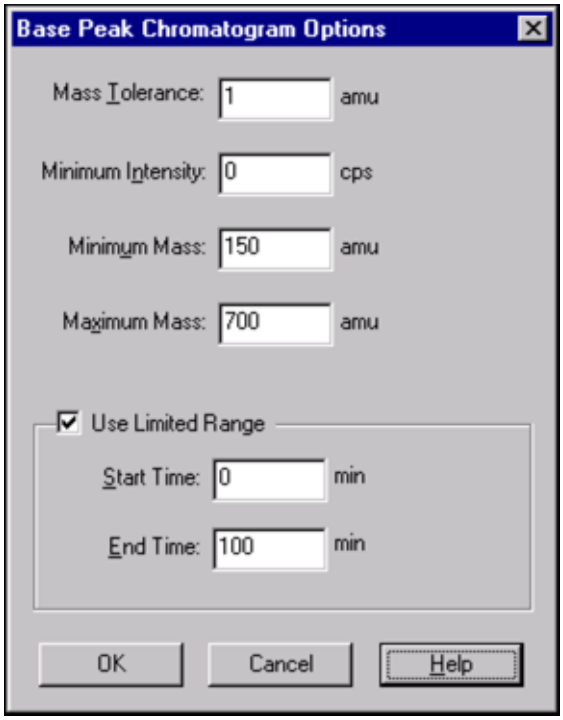


Figure 6-3 Base Peak Chromatogram Options dialog

3. In the **Mass Tolerance** field, type the value to dictate the mass range used to find a peak. The software finds the peak using a value twice the typed range (± the mass value).
4. In the **Minimum Intensity** field, type the intensity below which peaks are ignored by the algorithm.
5. In the **Minimum Mass** field, type the mass that determines the beginning of the scan range.
6. In the **Maximum Mass** field, type the mass that determines the end of the scan range.
7. 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 that determines the start of the experiment.
   - In the **End Time** field, type the time that determines the end of the experiment.
8. Click **OK**.

   The BPC is generated in a new pane.

Generate XWCs

The user can extract up to three ranges from a DAD spectrum to generate the XWC. For more information about using the available icons, refer to Table 6-8.

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

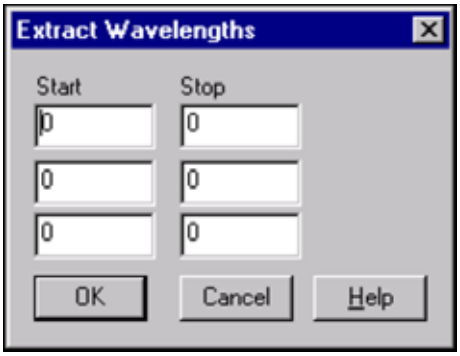


Figure 6-4 Extract Wavelengths dialog

3. Type start and stop values.
4. Click **OK**.

   The XWC opens in a pane below the DAD spectrum.

View DAD Data

The user can view DAD data in chromatogram or spectrum form, the same as mass spectrometer data.

1. Open a data file containing data acquired with a DAD.
2. The TWC, which is analogous to a TIC, opens in a pane below the TIC.
3. 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.
4. Click **Explore > Show > Show DAD Spectrum**.

   The DAD spectrum opens in a pane below the TWC. The y-axis shows absorbance and the x-axis shows wavelength.

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

Generate TWCs

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 Table 6-8.

1. Open a data file that contains a DAD spectrum.
2. Click **Explore > Show > Show DAD TWC**.

The TWC opens 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. Adjust the threshold using one of the following steps:
   - To raise the threshold, drag the blue triangle up the y-axis. To lower the threshold, drag the blue triangle down.
   - Click **Explore > Set Threshold**. In the **Threshold Options** dialog that opens, type the threshold value.
   - 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.

Table 6-6 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.
Show Contour Plot	Shows a color-coded plot of a data set, 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 an extracted chromatograph 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 UV data trace, if acquired.
Save to Text File	Generates a text file of the pane, which can be opened in Excel or other programs.

Table 6-6 Right-Click Menu for Chromatogram Panes (Continued)

Menu	Function
Save Explore History	The Explore History File records changes to processing parameters, also called Processing Options, when a .wiff file is 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 point in the pane.
Add User Text	Adds a text box at the cursor point 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.

Table 6-7 Right-Click Menu for Spectra Panes

Menu	Function
List Data	Lists the data points and integrates the peaks found in the spectrum.
Show TIC	Generates a new pane containing the TIC.
Extract Ions	Extracts a specific ion or set of ions from a selected pane and then generates a new pane containing a chromatograph for the specific ions.
Save to Text File	Generates a text file of the pane, which can be opened in Excel or other programs.
Save Explore History	The Explore History File records changes to processing parameters, also called Processing Options, when a .wiff file is 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 point in the pane.
Add User Text	Adds a text box at the cursor point 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.
Re-Calibrate TOF	Opens the TOF Calibration dialog.
Abscissa (Time)	Changes the view to display TOF values on the x-axis.
Delete Pane	Deletes the selected pane.
Add a Record	Add 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.
Search With Constraints	Searches using the Search Constraints dialog.

Data Processing

Graphical data can be processed many ways. This section provides information and procedures for using some of the most commonly used tools.

The user can zoom in on part of a graph to view a particular peak or an area in greater detail in both spectra and chromatograms. The user can also zoom in repeatedly to view smaller peaks.

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 they do not overlap.

Panes may be of 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, 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 would become smaller than its 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.

Table 6-8 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 graph to its original size	• Select the graph. Click **Explore > Home Graph**.	

Table 6-8 Graph Options (Continued)

To do this...	use this menu option...	...or click this icon
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 within 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, the pane moves above or below that pane, respectively. • If the pane is at the left or right of the target pane, the pane moves to the left or right of that pane, respectively. • If the pane is at any other position, the pane moves to the target row. The drop shadow of the pane as the pane is moved around indicates its new position.	
Link panes	1. With the two graphs open, click one to make that pane active. 2. 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. Position the pointer to the left of the y-axis and then drag vertically away from the starting point.

   A box is drawn along the y-axis representing the new scale.

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

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

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

Zoom in on the x-axis

1. Position the pointer under the x-axis to either side of the area to expands and then drag away from the starting point in a horizontal direction to expand the area of interest.
2. Release the mouse button to redraw the graph to the new scale.

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

Table 6-9 Explore Quick Reference: Chromatograms and Spectrum

Icon	Name	Function
	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	Views the data in tables.
	Show TIC	Generates a TIC from a spectrum.
	Extract Using Dialog	Extracts ions by selecting masses.

Table 6-9 Explore Quick Reference: Chromatograms and Spectrum (Continued)

Icon	Name	Function
	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	Click to use the Noise Filter Options dialog to define the minimum width of a peak. Signals below this minimum width are regarded as noise.
	Show ADC	Displays ADC data.
	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	Click to compensate 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 be viewed in greater detail.
	Clear ranges	Return the expanded selection to normal view.
	Set Selection	Click to type 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	Click to scale a graph to maximum, so that the most intense peak is scaled to full scale, whether or not it is visible.

Table 6-9 Explore Quick Reference: Chromatograms and Spectrum (Continued)

Icon	Name	Function
	Show History	View 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.
	Show DAD	Generates a DAD.
	Extract Wavelength	Extracts up to three wavelength ranges from a DAD spectrum to view the XWC.

The DuoSpray™ ion source combines a TurboIonSpray® probe and an APCI (atmospheric pressure chemical ionization) probe in a single ion source housing.

WARNING! Toxic Chemical Hazard: Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of poisonous or injurious materials used with the ion source. Any poisonous or injurious materials introduced into the equipment will be present in the ion source and exhaust output.

Introduction to the Ion Source

Figure 7-1 shows the parts of the ion source.

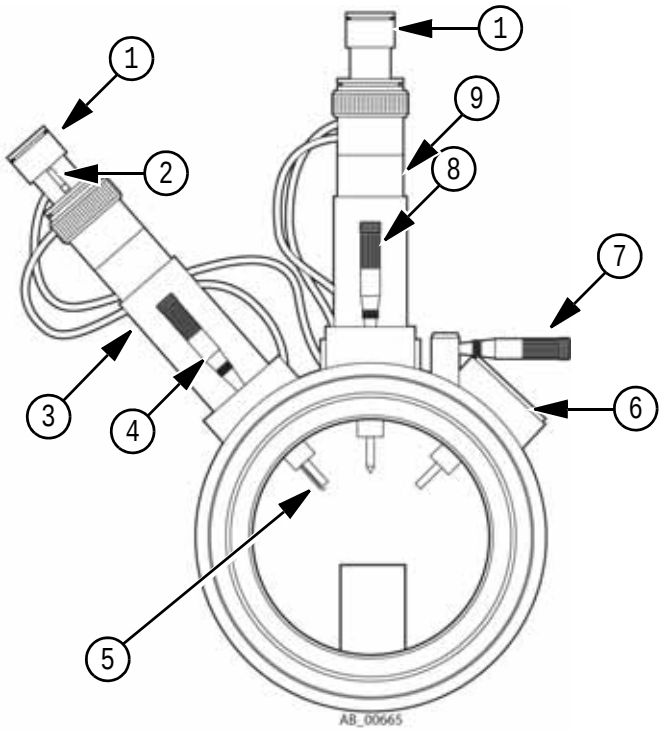


Figure 7-1 Parts of the ion source

Item	Description
1	Electrode adjustment nut
2	Corona discharge needle adjustment knob
3	APCI probe

Figure 7-1 Parts of the ion source (Continued)

Item	Description
4	Y-axis adjustment knob for the APCI probe, used to position the probe on the vertical axis for ion source sensitivity adjustments
5	Corona discharge needle, which ionizes the trace species, or sample gas. Primary ions, which are formed as a result of the discharge, are converted by collisional processes to final ion-molecule reaction products.
6	Turbo heater
7	X-axis adjustment knob for the TurboIonSpray probe, used to position the probe on the horizontal axis for ion source sensitivity adjustments
8	Y-axis adjustment knob for the TurboIonSpray probe, used to position the probe on the vertical axis for ion source sensitivity adjustments
9	TurboIonSpray probe

Probes

Choose the probe and method most suitable for the compound in the sample stream flow.

Table 7-1 Specifications of the Ion Source

Parameter	TurboIonSpray probe	APCI probe
Ion source temperature range	Probe temperature from ambient temperature to 750°C, depending on liquid flow	Probe temperature from 50°C to 750°C, depending on liquid flow
Liquid chromatography	Interfaces to any liquid chromatography system	
Nebulizer gas (Gas 1) Heater gas (Gas 2)	Refer to the *Site Planning Guide* for the mass spectrometer.	

The TurboIonSpray probe produces ions through ion evaporation. The APCI probe vaporizes the sample before inducing ionization through atmospheric pressure chemical ionization. This process is induced by a corona discharge needle as the ions pass through the ion source housing to the interface region.

All of the data acquired using the ion source is identified with an abbreviation representing the probe used to acquire the data (TIS for the TurboIonSpray probe, HN for the APCI probe).

TurboIonSpray Probe

The TurboIonSpray probe is suited for LC/MS/MS analyses. The sensitivity that is achieved with this technique is dependent on both flow rate and analyte. At higher flow rates, ionization efficiency increases, resulting in improved sensitivity. Compounds with extremely high polarity and low surface activity usually show the greatest sensitivity increases. The TurboIonSpray technique is mild enough to be used with labile compounds, such as peptides, proteins, and thermally labile pharmaceuticals.

When the heater is turned off, the TurboIonSpray probe functions as a conventional IonSpray™ ion source. It also functions with flow rates from 5 µL/min to 3000 µL/min and it vaporizes 100% aqueous to 100% organic solvents.

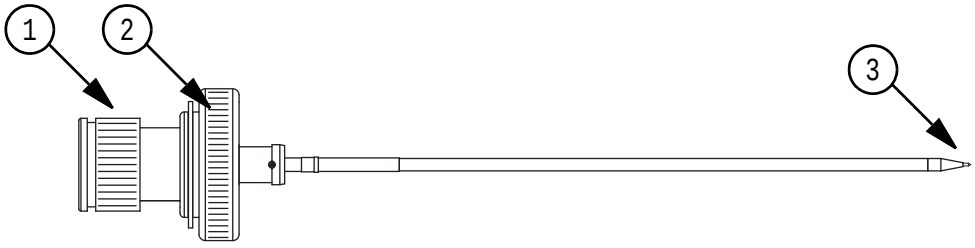


Figure 7-2 Parts of the TurboIonSpray probe

Item	Description
1	Electrode adjustment nut (black collar) that adjusts the extension of the electrode tip
2	Bronze retaining ring that fastens the probe to the probe tower on the ion source housing
3	Electrode tip through which samples are sprayed into the sample inlet area of the ion source

APCI Probe

The APCI probe is suitable for:

- Ionization of compounds that do not readily form ions in solution. These are usually non-polar compounds.
- Creation of simple APCI spectra for MS/MS experiments.
- High-throughput analyses of complex and dirty samples. It is less sensitive to ion suppression effects.
- Rapid sample introduction by flow injection with or without an LC column

The APCI probe can accept the entire effluent, without splitting, at flow rates from 50 µL/min to 3000 µL/min (through a wide bore column). It can vaporize volatile and labile compounds with minimal thermal decomposition. The rapid desolvation and vaporization of the droplets and entrained analyte minimizes thermal decomposition and preserves molecular identity for ionization by the corona discharge needle. Buffers are readily tolerated by the ion source without significant contamination and the flash vaporization of the sprayed effluent allows up to 100% water to be used without difficulty.

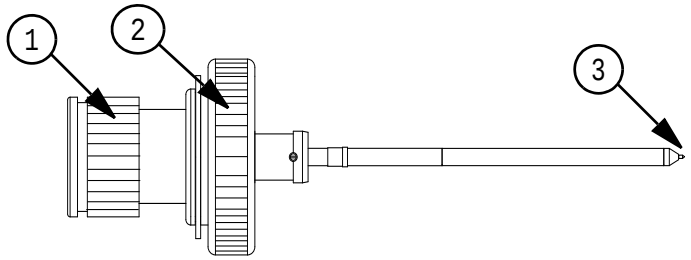


Figure 7-3 Parts of the APCI probe

Item	Description
1	Electrode adjustment nut (black collar) that adjusts the extension of electrode tip
2	Bronze retaining ring that fastens the probe to the probe tower on the ion source housing
3	Electrode tip through which samples are sprayed into the sample inlet area of the ion source

Gas and Electrical Connections

Gas and high-voltage electrical connections enter through the front plate of the interface and connect internally through the ion source housing. When the ion source is installed on the mass spectrometer, all of the electrical and gas connections are made.

Ion Source Latch

A latch disables the high-voltage power supply for the mass spectrometer and the source exhaust system if:

- The ion source housing is not installed or is improperly installed.
- A probe is not installed.
- The mass spectrometer senses a gas fault.

Source Exhaust System

WARNING! Toxic Chemical Hazard: Be sure to use the source exhaust system to safely remove sample vapor exhaust from the laboratory environment. For requirements for the source exhaust system, refer to the *AB SCIEX TripleTOF*® 5600/5600+ Instruments *Site Planning Guide*.

A passive pressure exhaust system removes ion source gases through a drain port without introducing chemical noise. The drain port connects through a drain chamber and a source exhaust pump to a drain bottle, and from there to a customer-supplied exhaust ventilation system. For more information on the requirements for the source exhaust system, refer to the *Site Planning Guide* for the mass spectrometer.

WARNING! Toxic Chemical Hazard: Vent the source exhaust system to an external fume hood or an external vent to prevent hazardous vapors from being released into the laboratory environment.

A pressure switch mounted on the source exhaust pump measures the pressure in the source exhaust line. If the pressure in the line rises above the set point while the probes are installed, the high-voltage power supply is turned off.

Installation

When the ion source is installed, the mass spectrometer recognizes the ion source and displays the ion source identification in the software.

The interior of the ion source is visible through the tempered glass windows on the side and end of the ion source housing. The ion source housing is connected to the vacuum interface housing and is held in position by two source latches.

WARNING! Electrical Shock Hazard: Install the ion source on the mass spectrometer as the last step in this procedure. High voltage is present when the ion source is installed on the equipment.

Required tools

- Ion source housing assembly
- Probes
- Ion source hardware kit (Do not discard the empty package. Use it to store the ion source when not in use.)

Install the Probe in the Ion Source Housing

Install the probes in the ion source housing before installing the ion source. Always remove the ion source from the mass spectrometer before exchanging probes. Refer to Remove the Ion Source on page 96.

If the probes are not properly installed in the ion source housing, then high-voltage power for the mass spectrometer and source exhaust system is turned off.

WARNING! Electrical Shock Hazard: Make sure that the ion source housing is completely disconnected from the mass spectrometer before proceeding.

WARNING! Electrical Shock Hazard: When installing the ion source, install the probe before installing the ion source on the mass spectrometer.

Caution: Potential Equipment Damage: Do not let the protruding electrode tip touch any part of the ion source housing, to avoid damaging the probe.

1. Adjust the black electrode adjustment nut on the probe to move the electrode tip inside the electrode tube.

   For optimum stability and performance, the electrode tip should extend between 0.5 mm and 1.0 mm from the end of the probe.Insert the probe into the tower.
2. Insert the APCI probe into the tower that is on the left side of the ion source when the glass window is facing you, inserting the raised plastic post into the groove on the probe.
3. Gently push down on the probe until the contacts engage with those in the tower.
4. Turn the bronze retaining ring over the probe and push it down to engage its threads with the threads on the tower.
5. Tighten the ring until it is finger-tight.
6. Insert the TurboIonSpray® probe into the tower on the top of the ion source, inserting the raised plastic post into the groove on the probe.
7. Gently push down on the probe until the contacts engage with those in the tower.
8. Turn the bronze retaining ring over the probe and push it down to engage its threads with the threads on the tower.
9. Tighten the ring until it is finger-tight.

Install the Ion Source

1. Make sure that the source latches on the side of the ion source are pointing up in the 12:00 position.
2. Align the ion source with the vacuum interface, making sure that the latches on the ion source are aligned with the sockets in the vacuum interface.
3. Push the ion source gently against the vacuum interface and then rotate the ion source latches, shown in Figure 7-1 on page 83, fully downwards to lock the ion source into place.

Connect the Sample Tubing and Cables for Sample Introduction with the TurboIonSpray Probe

If you are using the optional CDS, refer to the *CDS Operator Guide* to install the CDS and connect the tubing and cables.

WARNING! Toxic Chemical Hazard: Make sure that the sample tubing nut is tightened properly before operating this equipment. If the sample tubing nut is not tight, the sample may leak, and you may be exposed to dangerous chemicals.

WARNING! Electrical Shock Hazard: Do not bypass the grounding union connection. The grounding union provides safety grounding between the mass spectrometer and the sample introduction device.

1. Insert a 30 cm piece of red PEEK tubing into the sample tubing nut at the top of the TurboIonSpray probe.

2. Install the sample tubing nut on the fitting at the top of the TurboIonSpray probe.
3. Tighten the sample tubing nut until it is finger-tight.
4. Connect red PEEK tubing from the sample supply device to the grounding union on the ion source.
5. Connect the other end of the red PEEK tubing to the grounding union.

Tip! Refer to Figure 7-1 on page 83 for a picture on the parts referenced in this procedure.

Connect the Sample Tubing and Cables for Sample Introduction with the APCI Probe

If you are using the optional CDS, refer to the *CDS Operator Guide* to install the CDS and connect the tubing and cables.

WARNING! Toxic Chemical Hazard: Make sure that the sample tubing nut is tightened properly before operating this equipment. If the sample tubing nut is not tight, the sample may leak, and you may be exposed to dangerous chemicals.

WARNING! Electrical Shock Hazard: Do not bypass the grounding union connection. The grounding union provides safety grounding between the mass spectrometer and the sample introduction device.

1. Insert a 30 cm piece of red PEEK tubing into the sample tubing nut at the top of the APCI probe.
2. Install the sample tubing nut on the fitting at the top of the APCI probe.
3. Tighten the sample tubing nut until it is finger-tight.
4. Connect red PEEK tubing from the sample supply device to the grounding union on the ion source.
5. Connect the other end of the red PEEK tubing to the grounding union.

Tip! Refer to Figure 7-1 on page 83 for a picture of the parts referenced in this procedure.

Optimization

Optimize the ion source whenever the analyte, flow rate, or mobile phase composition changes.

Use appropriate analytical procedures and practices to minimize external dead volumes. Prefilter samples so that the capillary tubing in the sample inlets is not blocked by particles, precipitated samples, or salts.

Tip! It is easier to optimize signal and signal-to-noise with FIA or on-column injections.

Optimize the TurboIonSpray Probe

Optimize performance while injecting a known compound and monitor the signal of the known ion. Adjust the parameters to maximize the signal-to-noise ratio and signal stability.

Caution: Potential Equipment Damage: If the LC system connected to the mass spectrometer is not controlled by the Analyst® TF software, then do not leave the mass spectrometer unattended while in operation. The LC system can flood the ion source housing when the mass spectrometer goes into Standby mode.

Note: The IonSpray Voltage Floating (ISVF) is always applied to both the TurboIonSpray probe and the APCI probe simultaneously, and the Temperature (TEM) is always applied to both the turbo and APCI heaters simultaneously.

Table 7-2 Typical Values for Optimizing the TurboIonSpray Probe

Parameters	LC flow rate			Operational range
	5 µL/min to 50 µL/min	200 µL/min	1000 µL/min	5 µL/min to 3000 µL/min
Probe X-axis position	3 mm to 8 mm			0 mm to 10 mm
Probe Y-axis position	5 mm to 10 mm	0 mm to 5mm		0 mm to 13 mm
The optimal X-axis position is within 0 mm to 3 mm on either side of the orifice. The optimal Y-axis position is within 3.0 mm to 7.0 mm of the orifice.				

Run the Method

1. Start the Analyst TF software.
2. In the Analyst TF software, in **Tune and Calibrate** mode, double-click **Manual Tuning**.
3. Set the **Temperature (TEM)** parameter to **450** and let the ion source warm up for 30 minutes or until the ion source housing is warm to the touch.

   The 30-minute warm-up stage prevents solvent vapors from condensing in a cold probe.
4. Start the sample flow.
5. Run the method to be used to optimize the ion source.

Set the Starting Conditions

1. On the **Source/Gas** tab in the **Tune Method Editor**, type a starting value for **Ion Source Gas 1 (GS1)**.

   For LC pumps, use a value between 40 and 60 for GS1.
2. Type a starting value for **Ion Source Gas 2 (GS2)**.

For LC pumps, use a value between 30 and 50 for GS2.

Note: Gas 2 is used with higher flow rates typical with an LC system and in conjunction with increased temperature.

3. Type a starting value for **IonSpray Voltage Floating (ISVF)**.
4. In the **Curtain Gas (CUR)** field, type **20**.
5. On the Compound tab, in the **Declustering Potential (DP)** field, type **80**.

Adjust the TurboIonSpray Probe Position

At low flow rates, the probe can be adjusted to its lowest Y-axis position. For high flow rates, position the probe higher than the orifice. The curtain plate orifice should remain clear of solvent or solvent droplets at all times.

For multiply-charged proteins and peptides introduced at a few microliters per minute, position the sprayer nozzle higher than the curtain plate orifice.

1. Look through the window of the ion source housing to view the position of the probe.
2. Set the X-axis adjustment knob to 5 and the Y-axis adjustment knob to 5.
3. Infuse or inject the sample.
4. Monitor the signal in the software.
5. Use the X-axis adjustment knob to adjust the probe position in small increments until the best signal or signal-to-noise ratio is achieved.

   The TurboIonSpray probe may optimize slightly to either side of the orifice.
6. Use the Y-axis adjustment knob to adjust the probe position in small increments to achieve the best signal or signal-to-noise ratio.

Note: The vertical position of the probe depends on flow rate. At low flow rates, the probe should be closer to the orifice. At higher flow rates, the probe should be farther away.

WARNING! Toxic Chemical Hazard: Make sure that the electrode tip extends past the end of the probe, to prevent the escape of hazardous vapor from the ion source.

7. Adjust the black electrode adjustment nut on the probe to move the electrode tip relative to the sprayer tube. For optimal performance, the electrode should protrude 0.5 mm to 1.0 mm.

   After the probe is optimized, it needs only minor adjustment. If the probe is removed, or if the analyte, flow rate, or solvent composition changes, repeat the optimizing procedure after installation.

Optimize the Source/Gas Parameters

Optimize nebulizer gas (Gas 1) for best signal stability and sensitivity. The heater gas (Gas 2) helps in the evaporation of solvent, which helps to increase the ionization of the sample. Too high a temperature can cause premature vaporization of the solvent at the TurboIonSpray probe tip,

especially if the probe is too low, resulting in signal instability and a high chemical background noise. Similarly, a high heater gas flow could produce a noisy or unstable signal.

1. Adjust GS1 and GS2 in increments of 5 to achieve the best signal or signal-to-noise ratio.
2. Increase CUR until the signal starts to decrease.

Note: To prevent contamination, use the highest value for CUR possible without sacrificing sensitivity. Do not set CUR lower than 20.

3. Adjust ISVF in increments of 100 V to achieve the best signal or signal-to-noise ratio.

Note: If the ISVF is too high, a corona discharge can occur. It is visible as a blue glow at the tip of the TurboIonSpray probe. This will result in decreased sensitivity and stability of the ion signal.

Optimize the Turbo Heater Temperature

The quantity and type of sample affects the optimal TurboIonSpray probe temperature. At higher flow rates the optimal temperature increases.

WARNING! Toxic Chemical Hazard: Vent the source exhaust system to an external fume hood or an external vent to prevent hazardous vapors from being released into the laboratory environment.

- Adjust the TEM value in increments of 50°C to achieve the best signal or signal-to-noise ratio.

Optimize for the Compound

- Adjust the DP value in increments of 10 to achieve the best signal or signal-to-noise ratio. DP optimizes between 60 to 200.

Optimize the APCI Probe

Optimize performance by injecting a known compound and monitoring the signal of the known ion. Adjust the parameters to maximize the signal-to-noise ratio.

Table 7-3 Typical Values for Optimizing the APCI Probe

Parameter	Typical value	Operational range
Probe X-axis position	5 mm	Scale 0 mm to 10 mm
Probe Y-axis position	5 mm	Scale 0 mm to 13 mm
The optimal X-axis position is within 0 mm to 2 mm on either side of the orifice. The optimal probe Y-axis position is within 3.0 mm to 7.0 mm of the orifice.		

Run the Method

Caution: Potential Equipment Damage: Warm the ceramic heater slowly to avoid thermal shock to the heating element.

Caution: Potential Equipment Damage: If the LC system connected to the mass spectrometer is not controlled by the Analyst TF software, then do not leave the mass spectrometer unattended while in operation. The LC system can flood the ion source housing when the mass spectrometer goes into Standby mode.

1. Start the Analyst TF software.
2. In the Analyst TF software, in **Tune and Calibrate** mode, double-click **Manual Tuning**.
3. Set the **Temperature (TEM)** parameter to **450** and let the ion source warm up for 30 minutes or until the ion source housing is warm to the touch.

   The 30-minute warm-up stage prevents solvent vapors from condensing in a cold probe.
4. Start the sample flow.
5. Run the method to be used to optimize the ion source.

Set the Starting Conditions

1. On the **Source/Gas** tab in the **Tune Method Editor**, in the **Ion Source Gas 1 (GS1)** field, type **0**.

   Note: The value for the GS1 parameter, which is used by the TurboIonSpray probe, may influence performance of the APCI probe. You may need to adjust the GS1 parameter value to achieve optimal performance.

2. In the **Ion Source Gas 2** (**GS2**) field, type **20**.

   Note: Gas 2 is used as a nebulizer gas for the APCI probe.

3. In the **Curtain Gas (CUR)** field, type **20**.
4. Type a starting value for **IonSpray Voltage Floating (ISVF)**.
5. On the Compound tab, in the **Declustering Potential (DP)** field, type **80**.

Optimize Gas 1, Gas 2, and Curtain Gas™ Flow

1. Adjust GS1 and GS2 in increments of 5 to achieve the best signal or signal-to-noise ratio.
2. Increase CUR until the signal starts to decrease.

   Note: To prevent contamination, use the highest value for CUR possible without sacrificing sensitivity. Do not set CUR lower than 20.

Adjust the Corona Discharge Needle

When using the APCI probe, make sure that the corona discharge needle is pointing toward the orifice.

WARNING! Electrical Shock Hazard: Follow this procedure to avoid contact with the high voltages applied to the corona discharge needle and the curtain plate.

1. Use the slotted screwdriver to rotate the plastic screw on the top of the needle.
2. Look through the glass window to make sure that the needle is aligned with the tip facing the orifice.

Adjust the APCI Probe Position

Make sure that the curtain plate orifice remains clear of solvent or solvent drops at all times.

The position of the probe relative to the curtain plate orifice affects sensitivity and signal stability. For lower flow rates, position the probe closer to the orifice. For higher flow rates, position the probe farther away from the orifice.

1. Set the Y-axis adjustment knob to 10.
2. Monitor the signal in the Analyst TF software.
3. Use the Y-axis adjustment knob to adjust the probe in small increments until you achieve the best signal or signal-to-noise ratio.

   The APCI probe optimizes toward the orifice plate.

   After the probe is optimized, it needs only minor adjustment. If you remove the probe, or if the analyte, flow rate, or solvent composition changes, repeat the optimizing procedure after reinstallation.

Note: The position of the TurboIonSpray probe may influence performance of the APCI probe. You may need to adjust the TurboIonSpray probe position to achieve optimal performance.

Optimize the IonSpray Voltage Floating

- In positive mode, start at a value of 5500, and decrease in steps of 500 V; in negative mode, start at a value of –4500, and increase in steps of 500 V; continue adjusting until you achieve the best signal or signal-to-noise ratio.

  This parameter usually optimizes around 5500 V in positive mode. If you observe no changes in signal with increasing ISVF, then leave the ISVF at the lowest setting that provides the best signal or signal-to-noise ratio.

Note: If the ISVF is too high, a corona discharge can occur. It is visible as a blue glow at the tip of the TurboIonSpray probe. This will result in decreased sensitivity and stability of the ion signal.

Optimize the APCI Probe Temperature

The quantity and type of solvent affects the optimal APCI probe temperature. At higher flow rates, the optimal temperature increases.

WARNING! Toxic Chemical Hazard: Vent the source exhaust system to an external fume hood or an external vent to prevent hazardous vapors from being released into the laboratory environment.

- Adjust the TEM parameter in increments of 50°C to achieve the best signal or signal-to-noise ratio.

Optimize for the Compound

- Adjust the DP value in increments of 10 to achieve the best signal or signal-to-noise ratio. DP optimizes between 60 to 200.

Maintenance

To determine how often to clean the ion source or perform preventive maintenance, consider the following:

- Compounds tested
- Cleanliness of the preparation methods
- Amount of time an idle probe contains a sample
- Overall system run time

These factors can cause changes in mass spectrometer performance, indicating that maintenance is required.

Perform periodic gas leakage tests and general maintenance inspections to be sure of safe operation of the system. Clean the ion source regularly to keep it in good working condition.

Caution: Potential Instrument Damage: Use only the recommended cleaning method to avoid damaging the equipment.

Required tools

- 1/4 inch open-ended wrench
- 9/64 inch Allen key (supplied)
- 5 mm Allen key
- 2.5 mm Allen key
- Phillips screwdriver
- Slotted screwdriver

Clean the Probes

Flush the ion source periodically, regardless of the type of compounds sampled. Do this by setting up a method in the Analyst TF software specifically for performing a flushing operation.

1. Switch to a mobile phase that is 50:50 water:acetonitrile or 50:50 water:methanol.
2. Adjust the position of the TurboIonSpray and APCI probes so that they are as far from the orifice as possible.
3. In the Analyst TF software, set **Temperature (TEM)** to between 500 and 600, **Ion Source Gas 1 (GS1)** and **Ion Source Gas 2 (GS2)** to at least 40, and **Curtain Gas (CUR)** to the highest setting possible.
4. Wait until the TEM setpoint is reached.
5. Infuse or inject mobile phase through the sample tubing and probe at 1 mL/min for about 10 to 15 minutes.
6. Make sure that the probe and sample tubing are flushed thoroughly.

Remove the Ion Source

Always remove the ion source from the mass spectrometer before you perform any maintenance on the ion source or exchange probes.

WARNING! Hot Surface Hazard: Surfaces of the ion source become hot during operation. Let the ion source cool for at least 10 minutes before starting any maintenance procedures.

1. Stop any ongoing scans.
2. Shut down the sample stream.
3. Using the Analyst TF software, put the mass spectrometer in Standby mode. Refer to the Analyst TF software Help.
4. Let the ion source cool for at least 10 minutes.
5. Disconnect the sample tubing from the grounding union.
6. Turn the two source latches upward to release the ion source.
7. Pull the ion source gently away from the vacuum interface.
8. Put the ion source on a clean, secure surface.

Remove the Probe

WARNING! Electrical Shock Hazard: Disconnect the source from the mass spectrometer before starting any maintenance procedures.

1. Remove the ion source from the mass spectrometer. Refer to Remove the Ion Source.
2. Loosen the 1/8-in. sample tubing nut and remove the sample tubing from the probe.
3. Loosen the bronze retaining ring that fastens the probe to the ion source housing.
4. Gently pull the probe straight up out of the tower. Do not let the tip of the probe touch anything during removal or storage.
5. Put the probe on a secure, clean surface.

Clean the Electrode Tube

Clean the electrode tube periodically, or when performance decreases.

This procedure applies to both the TurboIonSpray and APCI probes. Use this procedure to remove the electrode tube for cleaning. If the electrode tube cannot be cleaned, then use this procedure to replace it with a new part.

WARNING! Electrical Shock Hazard: Remove the ion source from the mass spectrometer before starting any maintenance procedures.

1. Remove the ion source from the mass spectrometer. Refer to Remove the Ion Source on page 96.
2. Remove the probe from the ion source. Refer to Remove the Probe on page 96.
3. Remove the electrode adjustment nut. Hold the probe with the tip pointing downwards so the spring remains inside the probe as the electrode tube is withdrawn. Refer to Figure 7-4.

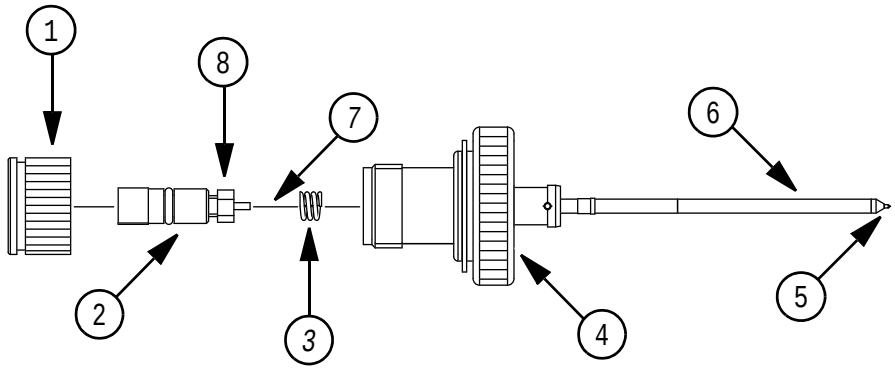


Figure 7-4 Probe - expanded view

Item	Description
1	Electrode adjustment nut
2	PEEK union
3	Spring
4	Bronze retaining ring
5	Electrode tip
6	Sprayer tube
7	Electrode tube
8	1/4-inch retaining nut

4. Pull the PEEK union and the attached electrode tube from the probe. Refer to Figure 7-4.
5. Use the 1/4 inch open-ended wrench to remove the retaining nut that holds the electrode tube in the PEEK union.

6. Remove the electrode tube from the retaining nut.
7. Clean the electrode tube with a 50:50 methanol:water solution, by running the solution through the electrode tube or by soaking the tube in an ultrasonic bath.

Replace the Electrode

1. Insert the electrode tube into the retaining nut and then into the PEEK union fitting.

   Make sure that the electrode tube is inserted as far into the PEEK union fitting as it will go. If there is a gap between the electrode tube and its seat inside the union fitting, a dead sample volume may occur.
2. Align the electrode tube with the narrow opening in the sprayer tube, and then insert the PEEK union fitting and attached electrode tube into the probe. Be careful not to bend the electrode tube.
3. Make sure that the spring is still inside the probe and then tighten the electrode adjustment nut.
4. Insert the probe into the tower, taking care not to allow the tip of the probe to touch any part of the ion source housing.
5. Push down the bronze retaining ring to engage its thread with the thread on the ion source housing and then tighten the ring.
6. Insert the sample tubing into the sample tubing nut, insert the sample tubing nut into the fitting at the top of the probe, and then tighten the sample tubing nut until it is finger-tight.
7. Install the ion source on the mass spectrometer. Refer to Install the Ion Source on page 88.
8. Adjust the electrode tip to specification. Refer to Adjust the Electrode Tip Extension on page 98.

Adjust the Electrode Tip Extension

The electrode tip extension should be adjusted for best performance. The optimal setting is compound-dependent. The distance that the electrode tip extends affects the shape of the spray cone, and the cone shape affects mass spectrometer sensitivity.

WARNING! Toxic Chemical Hazard: Make sure that the electrode tip extends past the end of the probe, to prevent the escape of hazardous vapor from the ion source.

- Adjust the black electrode adjustment nut on the top of the probe to extend or retract the electrode tip. The electrode tip should extend between 0.5 mm and 1.0 mm from the end of the probe as shown in Figure 7-5.

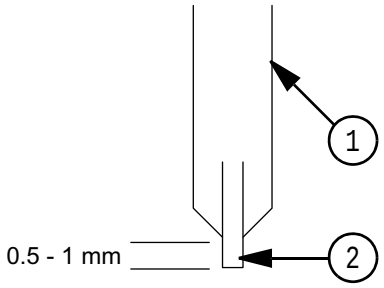


Figure 7-5 Electrode tip extension adjustment

Item	Description
1	Probe
2	Electrode

Remove the Corona Discharge Needle

The corona discharge needle tip may become so corroded that it must be cut off from the corona discharge needle. If this occurs, replace the corona discharge needle.

WARNING! Electrical Shock Hazard: Remove the ion source from the mass spectrometer before starting any maintenance procedures.

WARNING! Piercing Hazard: The tip of the needle is extremely sharp. Take care to handle it safely.

1. Remove the ion source and probe from the mass spectrometer.Refer to Remove the Ion Source on page 96.
2. Rotate the ion source so that the open side is toward you.
3. Press down on the corona discharge needle adjustment knob on the top of the tower. The corona discharge needle extends.
4. Holding the corona discharge needle tip between the thumb and forefinger of one hand and the corona discharge needle with the other hand, rotate the corona discharge needle tip counter-clockwise to loosen and gently remove the tip.

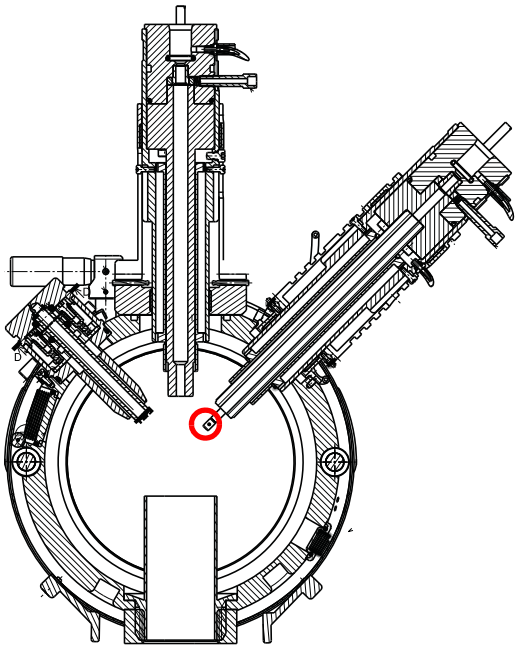


Figure 7-6 Corona discharge needle tip at rear of ion source

5. Turn the corona discharge needle adjustment knob counter-clockwise until it is loose.
6. Gently pull the corona discharge needle adjustment knob to remove the corona discharge needle from the ceramic sleeve, taking care not to break the sleeve.
7. Remove the corona discharge needle adjustment knob from the corona discharge needle.
8. Install the corona discharge needle adjustment knob on a new corona discharge needle and then insert the needle into the sleeve.
9. Tighten the corona discharge needle adjustment knob until the connection is firm.
10. Holding a new tip between the thumb and forefinger of one hand and the corona discharge needle with the other hand, rotate the corona discharge needle tip clockwise to install the tip.
11. Install the ion source on the mass spectrometer. Refer to Install the Ion Source on page 88.

Replace the Sample Tubing

Use the following procedure to replace the sample tubing if it has a blockage.

1. Stop the sample flow and make sure that any remaining gas has been removed through the source exhaust system.
2. Remove the ion source. Refer to Remove the Ion Source on page 96.
3. Disconnect the sample tubing from the probe and the union.
4. Replace the sample tubing with the same length of tubing used previously.

5. Install the ion source. Refer to Install the Ion Source on page 88.
6. Resume the sample flow.

Troubleshooting

Table 7-4 Troubleshooting

Symptom	Possible cause	Solution
The Analyst® TF software reports that the mass spectrometer is in Fault state. (The mass spectrometer icon on the Analyst TF software status bar is red.)	• The probe is not installed. • The probe is not connected securely.	• Install the probe. Refer to Install the Probe in the Ion Source Housing on page 87. • Remove and replace the probe. Tighten the probe connection bronze ring securely. Refer to Remove the Probe on page 96 and Install the Probe in the Ion Source Housing on page 87.
The heater does not work.	The F3 fuse is blown.	Contact your FSE.
The spray does not appear to be uniform.	The electrode is blocked.	Clean or replace the electrode. Refer to Clean the Electrode Tube on page 97.
Sensitivity is poor.	Excess high voltage induces fragmentation before the ions enter the mass filters.	Optimize ISVF or DP. Refer to Optimize the TurboIonSpray Probe on page 90 or Optimize the APCI Probe on page 92.
During testing, the ion source fails to meet specifications.	The mass spectrometer has not passed the installation tests. The test solution was not prepared correctly.	Perform installation tests on the mass spectrometer with the default source. Confirm that the test solutions were prepared correctly. If the problem cannot be resolved, contact an FSE.
Background noise is high.	• Temperature (TEM) is too high. • Gas 2 flow rate (GS2) is too high.	• Optimize TEM. • Optimize GS2.

Table 7-4 Troubleshooting (Continued)

Symptom	Possible cause	Solution
Arcing or sparks occur.	The position of the corona discharge needle is incorrect.	Turn the corona discharge needle toward the curtain plate, and away from the stream of Gas 2. Refer to Adjust the Corona Discharge Needle on page 94.

Consumables

The following tables list the orderable parts for the DuoSpray™ ion source. The parts are available in the Consumables Kit for the mass spectrometer (PN 1026540).

Table 7-5 Orderable Parts for the Ion Source

Part No.	Description	Quantity
016316	PEEK tubing, Red, 1/16 o.d. × 0.005 bore	100 cm
016325	PEEK fitting, Brown, 10-32 × 1/16 inch	5
025388	Electrode, Nebulizer	1
025392	Electrode, TuroIonSpray	1
027471	PEEK Graph-tite fitting, Black, 1/16 inch	2
1005601	PEEK tubing kit to connect to TurboIonSpray® probe, 30 cm	1
1005602	PEEK tubing kit to connect to APCI probe, 45 cm	1
025348	PEEK union in probe	1
026626	Spring for probe	1

Table 7-6 Spares

Part No.	Description	Quantity
1006177	APCI Corona discharge needle tip	1
1006174	APCI Corona discharge needle rod	1
027497	Gold-plated spring for HV connection	1
027013	Spring for corona discharge needle	1

Regularly clean and maintain the instrument for optimal performance. Table 8-1 provides a recommended schedule for cleaning and maintaining the instrument. Contact your Qualified Maintenance Person to order consumable parts.

Table 8-1 System Maintenance Tasks

Component	Frequency	Task	For more information, refer to...
Curtain plate	As needed	Clean	Clean the Curtain Plate
QJet® ion guide	As needed	Clean	Contact an AB SCIEX FSE.
Q0 and IQ1 lens	As needed	Clean	Contact an AB SCIEX FSE.
Instrument cooling fan filter	Every 6 months	Replace	Contact an AB SCIEX FSE.
Instrument surfaces	As needed	Clean	Clean the Surfaces
Drain bottle	As needed	Empty	Empty the Drain Bottle
Roughing pump oil	As needed	Check and fill	Contact an AB SCIEX FSE.
	Every 6 to 12 months	Replace	Contact an AB SCIEX FSE.
Electrode	As needed	Inspect and clean or replace	Clean the Electrode Tube on page 97
Corona discharge needle	As needed	Replace	Remove the Corona Discharge Needle on page 99

For “As needed” tasks, follow these guidelines:

- Clean the curtain plate, orifice plate, QJet ion guide, and Q0 region if system sensitivity degrades.
- Clean the instrument surfaces after a spill, or when they become dirty.
- Empty the drain bottle when it becomes full.

Contact an AB SCIEX FSE for maintenance service and support.

Health and Safety Precautions

- Determine what chemicals may have been used in the instrument prior to service. Refer to Safety Data Sheets for the health and safety precautions that must be followed with chemicals.
- Work in a well-ventilated area.
- Always wear assigned personal protective equipment, including powder-free nitrile gloves, safety glasses, and a laboratory coat.
- Follow required electrical safe work practices.

- Avoid ignition sources when working with flammable materials, such as isopropanol, methanol, and other flammable solvents.
- Take care in the use and disposal of any chemicals. Potential risk of personal injury if proper handling and disposing of chemicals are not followed.
- Avoid skin contact with chemicals during cleaning, and wash hands after use.
- Comply with all local regulations for the handling of biohazard, toxic, or radioactive materials.

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard: Determine whether instrument decontamination is required prior to cleaning. Instrument decontamination should be conducted prior to cleaning if radioactive materials, biological agents, or toxic chemicals have been used with an instrument.

Caution: Potential Instrument Damage: Rinse off any acid-containing cleaning solvents with water. Do not use chlorinated solvents because these may damage the QJet ion guide components

Clean the Surfaces

Clean the external surfaces of the instrument after a spill, or when they become dirty.

- Using warm, soapy water and a soft cloth, wipe the external surfaces.

Empty the Drain Bottle

Empty the drain bottle when it becomes full.

WARNING! Biohazardous Material: Deposit biohazardous material in appropriately labelled containers. Potential risk of personal injury if proper handling and disposing of biohazardous materials are not followed

1. Shut Down the System on page 21.
2. Disconnect the tubes from the top of the drain bottle.

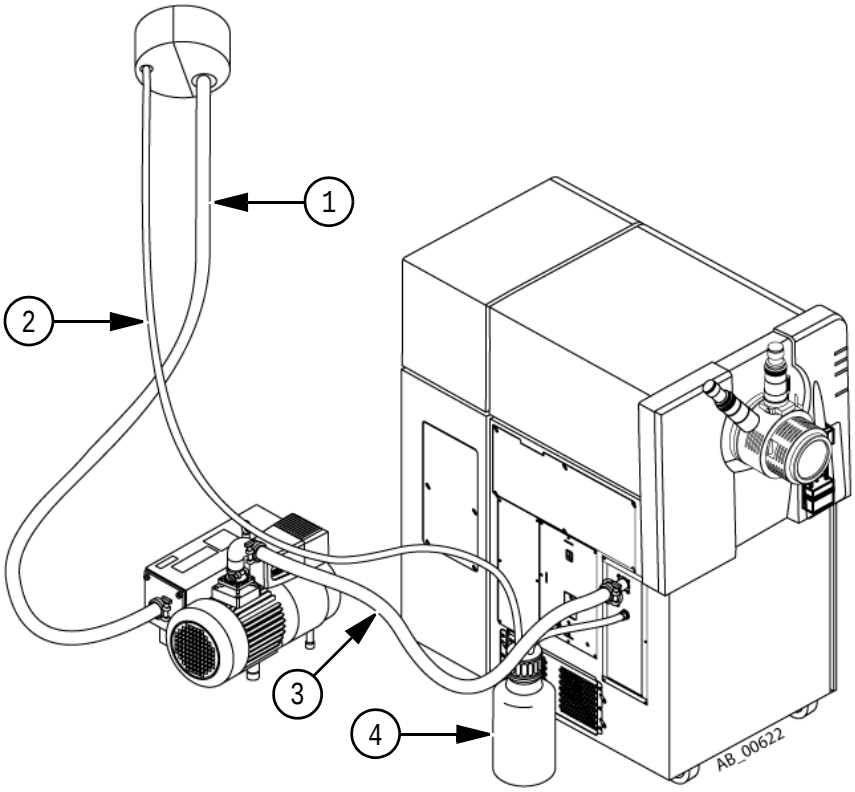


Figure 8-1 Vent connections

Item	Description
1	Roughing pump exhaust connection to vent
2	Source exhaust output connection to vent
3	Vacuum hose
4	Source exhaust drain bottle

3. Unscrew the cap and dispose of the waste.
4. Replace the cap and connect the tubes.

Front-End Cleaning

Clean the instrument front-end using the routine cleaning method, to:

- Minimize unscheduled instrument downtime.
- Maintain optimum sensitivity.
- Avoid more extensive cleaning that requires a service visit.

Symptoms of contamination: Significant loss in sensitivity and increased background noise.

When contamination occurs, perform an initial routine cleaning. Clean up to and including the front of the orifice plate. If routine cleaning does not resolve issues with sensitivity, a full cleaning may be necessary.

This section provides instructions for performing routine cleaning without breaking vacuum and full cleaning under atmospheric pressure, after venting the instrument.

Note: Follow all applicable local regulations. For health and safety guidelines, refer to Health and Safety Precautions for more information.

Required tools and materials

- Powder free gloves (nitrile recommended)
- Safety glasses
- Laboratory coat
- Fresh, high quality water (at least 18 Mohm de-ionized water [DI water] or ultra-pure HPLC-grade water). Old water can contain contaminants which can further contaminate the mass spectrometer.
- HPLC- or LCMS-grade methanol, isopropanol (2-propanol), or acetonitrile
- Cleaning solution. Use one of:
  - 100% methanol
  - 100% isopropanol
  - 50:50 acetonitrile:water solution (freshly prepared)
  - 50:50 acetonitrile:water with 0.1% acetic acid solution (freshly prepared)

Caution: Potential Instrument Damage: Do not use chlorinated solvents.

Note: For consumables ordering information and inquiries, call 877-740-2129 (U.S. only), or visit www.absciex.com.

Table 8-2 Tools and Supplies Available from AB SCIEX

Description	P/N
Small polyester swab (thermally bonded)	1017396
Small lint-free wipe (11 cm x 21 cm); available in Consumables kits	WC018027

Best Practices

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard: Determine whether instrument decontamination is required prior to cleaning. Instrument decontamination should be conducted prior to cleaning if radioactive materials, biological agents, or toxic chemicals have been used with an instrument.

- Always wear clean, powder-free gloves for the cleaning procedures.
- After cleaning the instrument components and before reassembling them, put on a clean pair of gloves.
- Do not use cleaning supplies other than those specified in this procedure.
- If possible, prepare cleaning solutions just before beginning.

- Prepare and store all organic solutions and organic-containing solutions in very clean glassware only. Never use plastic squirt bottles. Contaminants can leach from these bottles and further contaminate the mass spectrometer.
- Allow only the center area of the wipe to contact the instrument surface. Cut edges can leave fibers behind.

Tip! Wrap the wipe around a thermally-bonded polyester swab.

Figure 8-2 Example: Folding the wipe

- Allow the wipe or swab to contact the surface once, and then discard it, to avoid cross-contamination.
- Larger parts of the vacuum interface, such as the curtain plate, may require several cleanings, using multiple wipes.
- To avoid contaminating the solution, pour the solution on the wipe or swab.
- Only moisten the wipe or swab slightly when applying water or cleaning solution. Water, more so than organic solvents, may cause the wipe to deteriorate, leaving residue on the instrument.

Prepare for Routine Cleaning

In routine cleaning, clean the curtain plate and the front of the orifice plate. Routine cleaning can be performed while the instrument remains under vacuum.

Note: Instruments with a NanoSpray® ion source may require a full cleaning for best results. Contact an AB SCIEX FSE.

1. Deactivate the hardware profile.

WARNING! Hot Surface Hazard: Surfaces of the ion source become hot during operation. Let the ion source cool for at least 10 minutes before starting any cleaning procedures.

2. Remove the ion source. Be sure to place the ion source in a safe location.
3. Wait at least 20 minutes for the curtain plate and orifice plate to cool.
4. Cover the source drain with the exhaust cover plate (if available), or a similar cover.

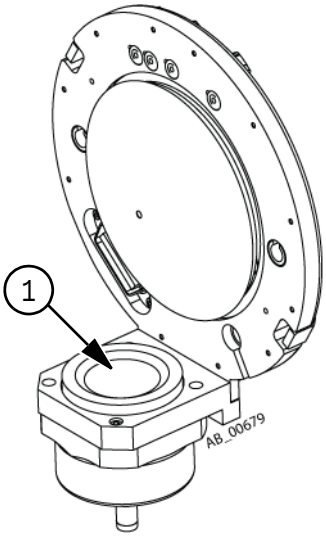


Figure 8-3 Source drain on the vacuum interface

Item	Description
1	Source drain

Clean the Curtain Plate

Caution: Potential Instrument Damage: Do not rest the curtain plate on the orifice. Make sure that the conical side faces up.

1. Remove the curtain plate and then place it, conical side up, on a clean, stable surface.

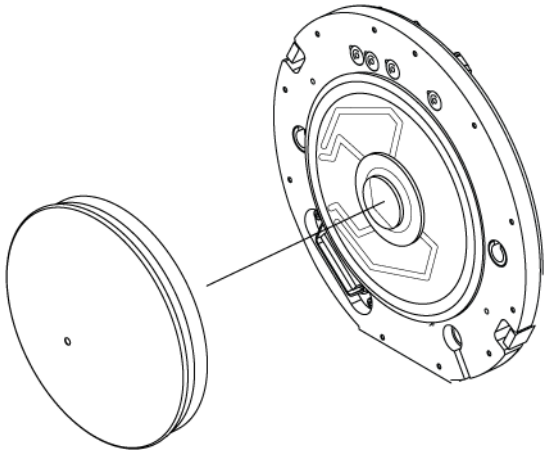


Figure 8-4 Interface with curtain plate removed

2. Using wipes and water, clean both sides of the curtain plate.
3. Repeat step 2 using the cleaning solution.
4. Using a dampened wipe or small poly swab, clean the aperture.
5. Wait until the curtain plate is dry.

6. Inspect the curtain plate for solvent stains or lint, removing any residue with a clean, slightly damp lint-free wipe.

Note: Persistent spotting or filming is an indicator of contaminated solvent.

Clean the Front of the Orifice Plate

Note: If the standard orifice plate has a removable interface heater, do not remove the heater during cleaning.

1. When cleaning a NanoSpray orifice plate, remove the interface heater and clean it:
   i. Wipe the heater with a lint-free wipe dampened with water.
   ii. Wipe the heater with a lint-free wipe dampened with cleaning solution.
2. Moisten the lint-free wipe with water and then wipe the front of the orifice plate.

Caution: Potential Instrument Damage: Do not insert a wire or metal brush into the orifice, to avoid damaging the aperture.

3. Repeat step 2 using the cleaning solution.
4. Wait until the orifice plate is dry.
5. Inspect the orifice plate for solvent stains or lint, removing any residue with a clean, slightly damp lint-free wipe.

Note: Persistent spotting or filming is an indicator of contaminated solvent.

Put the Instrument Back into Service

1. Install the curtain plate on the front end of the instrument.
2. Remove the protection from the ion source drain.
3. Install the ion source on the mass spectrometer.
4. Tighten the ion source by turning the ion source release latches down into the locking position. (Refer to the ion source Operator Guide.)
5. Activate the hardware profile.

Basic System Troubleshooting

9

This appendix contains basic information for troubleshooting basic system issues. Certain activities may be carried out by the AB SCIEX trained Qualified Maintenance Person in the laboratory. For advanced troubleshooting, contact an AB SCIEX Field Service Employee (FSE).

Table 9-1 System Issues

Issue	Possible cause	Corrective action
Sensitivity loss	Instrument or ion source requires tuning and optimizing	For more information, refer to: • Instrument Tuning and Calibrating • DuoSpray™ Ion Source User Reference on page 83 appendix • Analyst® software Help system
	Dirty curtain plate	Refer to Clean the Curtain Plate on page 108 for more information.
	Dirty orifice plate	Contact an AB SCIEX FSE or your local AB SCIEX trained Qualified Maintenance Person.
	Dirty QJet® ion guide, Q0 or IQ0	Contact an AB SCIEX FSE or your local AB SCIEX trained Qualified Maintenance Person.
Frequent or extreme contamination of the QJet ion guide	Curtain Gas™ flow rate is too low.	Verify, and if applicable, increase the Curtain Gas™ flow rate.
Low vacuum level	Low roughing pump oil level.	Check the roughing pump oil level, and add oil if necessary. Contact an AB SCIEX FSE or your local AB SCIEX trained Qualified Maintenance Person.

For sales, technical assistance or service, contact an AB SCIEX FSE or visit the AB SCIEX Web site at www.absciex.com for contact information.

Recommended Calibration Ions

A

The following tables list the standards recommended by AB SCIEX for calibrating the AB SCIEX TripleTOF® 5600/5600+ Instruments. For information about tuning solutions, refer to Chapter 3: Instrument Tuning and Calibrating.

Table A-1 Q1 PPG Positive Calibration Ions

Masses					
59.04914	175.13286	442.3374	674.50484	906.67228	1196.88158

Table A-2 Q1 PPG Negative Calibration Ions

Masses				
44.99819	411.25991	585.38549	933.63665	1165.80409

Table A-3 APCI Positive Calibration Solution: TOF MS

TOF MS	Masses
aminoheptanoic acid	146.11756
amino-dPEG 4-acid	266.15981
clomipramine	315.16225
amino-dPEG 6-acid	354.21224
amino-dPEG 8-acid	442.26467
reserpine	609.28066
amino-dPEG 12-acid	618.36953
Hexakis(2,2,3,3-tetrafluoropropoxy) phosphazine	922.0098
Hexakis(1H,1H,5H-octafluoroheptoxy) phosphazene	1521.97148

Table A-4 APCI Positive Calibration Solution: MSMS (Clomipramine)

MSMS (Clomipramine)	Masses
C3H8N	58.0651
C5H12N	86.0964
C16H14N	220.1121
C14H10NCl	227.0496
C17H17N	235.1356
C15H13NCl	242.0731
C17H17ClN	270.1044
C19H23ClN2	315.16225

Table A-5 APCI Negative Calibration Solution: TOF MS

TOF MS	Masses
7-aminoheptanoic acid	144.103
amino-dPEG 4-acid	264.14526
sulfinpyrazone fragment	277.09825
amino-dPEG 6-acid	352.19769
sulfinpyrazone	403.11219
amino-dPEG 8-acid	440.25012
amino-dPEG 12-acid	616.35498
amino-dPEG 16-acid	792.45984

Table A-6 APCI Negative Calibration Solution: MSMS (Sulfinpyrazone)

MSMS (Sulfinpyrazone)	Masses
C6H5O	93.0344
C6H5OS	125.0067
C10H8NO	158.06114
C17H13N2O2	277.0983
C23H20N2OS3	403.11219

Table A-7 APCI Negative Calibration Solution: MSMS (Sulfinpyrazone fragment)

MSMS (Sulfinpyrazone fragment)	Masses
C6H5	77.03967
C8H6N	116.0506
C9H8N	130.0662
C10H8NO	158.0611
C11H8N2O2	200.0591
C15H9N2	217.0771
C16H13N2O	249.1033
C17H13N2O2	277.09825

PPG

Table B-1 contains the exact monoisotopic masses and charged species (positive and negative) observed with the PPG (polypropylene glycol) calibration solutions. The masses and ions were calculated using the formula M = $H[OC_3H_6]_nOH$, while the positive ion MSMS fragments used the formula, $[OC_3H_6]_n(H^+)$. In all calculations, H = 1.007825, O = 15.99491, C = 12.00000, and N = 14.00307.

Note: When performing calibrations with the PPG solutions, use the correct isotope peak.

Table B-1 PPG Exact Masses

n	Exact Mass (M)	$(M + NH_4)^+$	MSMS fragments	$(M + NH_4)^{2+}$	$(M + COOH)^-$
1	76.05242	94.08624	59.04914	56.06003	121.05061
2	134.09428	152.12810	117.09100	85.08096	179.09247
3	192.13614	210.16996	175.13286	114.10189	237.13433
4	250.17800	268.21182	233.17472	143.12282	295.17619
5	308.21986	326.25368	291.21658	172.14375	353.21805
6	366.26172	384.29554	349.25844	201.16468	411.25991
7	424.30358	442.33740	407.30030	230.18561	469.30177
8	482.34544	500.37926	465.34216	259.20654	527.34363
9	540.38730	558.42112	523.38402	288.22747	585.38549
10	598.42916	616.46298	581.42588	317.24840	643.42735
11	656.47102	674.50484	639.46774	346.26933	701.46921
12	714.51288	732.54670	697.50960	375.29026	759.51107
13	772.55474	790.58856	755.55146	404.31119	817.55293
14	830.59660	848.63042	813.59332	433.33212	875.59479
15	888.63846	906.67228	871.63518	462.35305	933.63665
16	946.68032	964.71414	929.67704	491.37398	991.67851
17	1004.72218	1022.75600	987.71890	520.39491	1049.72037
18	1062.76404	1080.79786	1045.76076	549.41584	1107.76223
19	1120.80590	1138.83972	1103.80262	578.43677	1165.80409
20	1178.84776	1196.88158	1161.84448	607.45770	1223.84595
21	1236.88962	1254.92344	1219.88634	636.47863	1281.88781
22	1294.93148	1312.96530	1277.92820	665.49956	1339.92967

Reserpine ($C_{33}H_{40}N_2O_9$)

Table B-2 Reserpine Exact Masses

Description	Mass
Molecular Ion $C_{33}H_{41}N_2O_9$	609.28066
Fragment $C_{23}H_{30}NO_8$	448.19659
Fragment $C_{23}H_{29}N_2O_4$	397.21218
Fragment $C_{22}H_{25}N_2O_3$	365.18597
Fragment $C_{13}H_{18}NO_3$	236.12812
Fragment $C_{10}H_{11}O_4$	195.06519
Fragment $C_{11}H_{12}NO$	174.09134

Taurocholic Acid ($C_{26}H_{45}NO_7S$)

Table B-3 Taurocholic Acid Exact Masses

Description	Mass
Molecular Ion $C_{26}H_{44}NO_7S$	514.28440
Fragment $C_2H_3O_3S$	106.98084
Fragment $C_2H_6NO_3S$	124.00739
Fragment SO_3	79.95736

TOF Calibration Solution

Table B-4 TOF Calibration Solution Exact Masses

Description	Mass
Molecular Ion Cs^+	132.90488
Molecular Ion Peptide ALILTLVS	829.53933