AB SCIEX

TripleTOF® 4600 System

System User Guide

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Operational Precautions and Limitations 1

This section contains general safety-related information 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 *Hazard Symbols on page 14* for information about the symbols and conventions used in the laboratory environment, on the system, and in this documentation. Refer to the *Site Planning Guide* for site requirements, including AC mains supply, source exhaust, ventilation, air, nitrogen, and roughing pump requirements.

General Safety Information

To prevent personal injury or system damage, read, understand, and obey all safety precautions, warnings in this document, and labels on the mass spectrometer. These labels are shown with internationally recognized symbols. Failure to heed these warnings could result in serious injury.

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

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 and IEC 61010-2-061

Canada

- **Electromagnetic Interference**—CAN/CSA CISPR11. This ISM device complies with Canadian ICES-001.

- **Safety**—CAN/CSA C22.2 No. 61010-1 and CAN/CSA C22.2 No. 61010-2-061

Europe

- **Electromagnetic Interference**—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 61010-1 and IEC 61010-2-061

International

- **Electromagnetic Compatibility**—IEC 61326-1 and CEI/IEC CISPR 11 Class A

- **Safety**—IEC 61010-1 and IEC 61010-2-061

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

Electrical Precautions

AC 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 and safety standards.**

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

> **CAUTION: Potential System Damage. Do not unpack the mass spectrometer crate or computer boxes. The FSE will unpack and move the mass spectrometer at the time of the installation.**

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

Protective Conductor

The mains supply must include a correctly installed protective earth conductor. The protective earth conductor must be installed or checked by a qualified electrician before the mass spectrometer is connected. Make sure that the mains supply connector is accessible, so that the device can be disconnected.

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

Chemical Precautions

- Determine which chemicals have been used in the system prior to service and regular maintenance. 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 neoprene 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 procedures for 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 storage, handling, and disposal of biohazard, toxic, or radioactive materials.

System Safe Fluids

The following fluids can safely be used with the system. Refer to *Service and Maintenance Information on page 89* for information on safe cleaning solutions.

> **CAUTION: Potential System Damage. Do not use any other fluid until confirmation is received from AB SCIEX that it will not present a hazard. This is not an exhaustive list.**

- **Organic Solvents**

  - MS-grade acetonitrile; up to 100%

  - MS-grade methanol; up to 100%

  - Isopropanol; up to 100%

  - HPLC-grade or higher water; up to 100%

- **Buffers**

  - Ammonium Acetate; less than 1%

  - Ammonium Formate; less than 1%

- **Acids and Bases**

  - Formic Acid; less than 1%

  - Acetic Acid; less than 1%

  - Trifluoroacetic Acid; (TFA) less than 1%

  - Heptafluorobutyric Acid; (HFBA) less than 1%

  - Ammonia/Ammonium Hydroxide; less than 1%

Ventilation Precautions

The venting of fumes and disposal of waste must comply with all federal, state, provincial, and local health and safety regulations. Use the system indoors in a laboratory that complies with the environmental conditions recommended in the *Site Planning Guide* for the system.

The mass spectrometer ion source exhaust system and roughing pump must be vented to an external fume hood or an external exhaust system, as recommended in the *Site Planning Guide*.

WARNING! Toxic Chemical Hazard or Biohazard . Take care to vent exhaust gases to a laboratory fume hood or dedicated exhaust system, and make sure that the vent tubing is secured with clamps. The use of mass spectrometers without adequate ventilation to outside air might constitute a health hazard and might result in serious injury.

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that 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. Some jurisdictions recommend 4 to 12 air changes per hour in laboratories.

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Do not operate the mass spectrometer if the source exhaust drain and roughing pump exhaust hoses are not properly connected to the laboratory ventilation system. Certain procedures required during the operation of the mass spectrometer might cause gases to be discharged into the exhaust stream. Perform a regular check of the exhaust tubing to make sure that there are no leaks.

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of toxic or injurious materials used with the ion source. Discontinue use of the ion source if the window is cracked or damaged and contact an AB SCIEX Field Service Employee. Any toxic or injurious materials introduced into the equipment will be present in the ion source and exhaust output. Dispose of sharps following established laboratory safety procedures.

Environmental Precautions

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

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

> **WARNING! Biohazard. For biohazardous material use, always comply with local regulations for hazard assessment, control, and handling. This mass spectrometer or any part is not intended to act as a biological containment system.**

> **CAUTION: Potential Mass Shift. Maintain a stable ambient temperature. If the temperature changes by more than 2°C, then the resolution and mass calibration will be affected.**

Electromagnetic Environment

> **CAUTION: Potential Wrong Result. Do not use this device in close proximity to sources of strong electromagnetic (EMC) radiation (for example, unshielded intentional RF sources), as EMC radiation might interfere with the proper operation and cause a wrong result.**

Make sure that a compatible electromagnetic environment for the equipment can be maintained so that the device will perform as intended.

In a domestic environment, the device might cause radio interference. If it does, the user might need to take measures to mitigate the interference. Evaluate the electromagnetic environment prior to operation of the device.

Changes or modifications not expressly approved by the manufacturer could void your authority to operate the equipment.

Decommissioning and Disposal (Waste, Electrical, and Electronic Equipment)

Decontaminate the system before decommissioning following local regulations. Follow the AB SCIEX Red Tag process and complete an instrument Decontamination Form for instrument returns.

When removing the system from service, separate and recycle different materials according to national and local environmental regulations. Refer to *Storage and Handling on page 98*.

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 safely dispose of this equipment, contact a local Customer Service office for complimentary equipment pick-up and recycling.

> **Note:** AB SCIEXwill not accept any system returns without a completed Decontamination Form.

Qualified Personnel

Only qualified AB SCIEX personnel shall install and service the equipment. After installing the system, the Field Service Employee (FSE) uses the *Customer Familiarization Checklist* to orient the customer on system operation, cleaning, and basic maintenance.

Only personnel qualified by the manufacturer shall maintain the equipment. A laboratory designate can be familiarized with the Qualified Maintenance Person (QMP) procedures during the installation.

Customer Training and Documentation

Visit the AB SCIEX Web site (www.absciex.com/training) for information on training.

The *Site Planning Guide* is provided to the customer prior to installation. The guides and tutorials for the Analyst® TF software are installed automatically with the software and are available from the Start menu: **All Programs** > **AB SCIEX** > **Analyst TF** . Guides for the mass spectrometer are available on the *Hardware Documentation DVD*. Guides for the ion sources are available on the *Ion Source Customer Reference CD*. A complete list of the available documentation can be found in the Help. To view the **Analyst TF** software Help, press **F1.**

Equipment Use and Modification

Use the system indoors in a laboratory that complies with the environmental conditions recommended in the *Site Planning Guide*.

If the system is used in an environment or in a manner not prescribed by the manufacturer, then the protection provided by the equipment might be impaired.

Unauthorized modification or operation of the system might cause personal injury and equipment damage, and might void the warranty. Erroneous data might be generated if the system is operated either above or below the recommended environmental conditions or operated with unauthorized modifications. Contact an FSE for information on servicing the system.

> ⚠️ **WARNING! Personal Injury Hazard: Use AB SCIEX-recommended parts only. Use of parts not recommended by AB SCIEX or use of parts for any use other than their intended purpose may place the user at risk of harm or negatively impact system performance. The protection provided by the equipment may be impaired if the equipment is used in a manner not specified by AB SCIEX.**

Hazard Symbols 2

This section lists the hazard symbols and conventions used in the laboratory environment, on the system, and in the documentation.

Occupational Health and Safety Symbols

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

Table 2-1 Chemical Hazard Symbols

Safety Symbol	Definition
	Biohazard
	Explosion Hazard
	Toxic Chemical Hazard

Table 2-2 Electrical Hazard Warning Symbols

Safety Symbol	Definition
	Electrical Shock Hazard

Table 2-3 Pressurized Gas Hazard Warning Symbols

Safety Symbol	Definition
	Pressurized Gas Hazard

Table 2-4 Mechanical Hazard Symbols

Safety Symbol	Definition
	Hot Surface Hazard
	Lifting Hazard
	Puncture Hazard
	Ionizing Radiation Hazard

Symbols, Indicators, and Labels: Packaging

Table 2-5 Labels on the Mass Spectrometer Shipping Materials
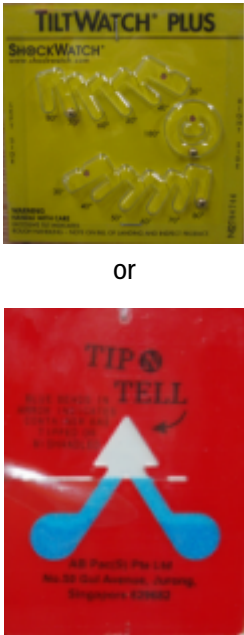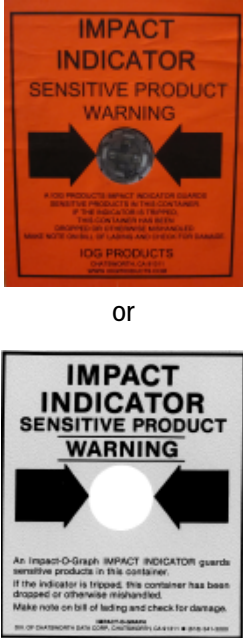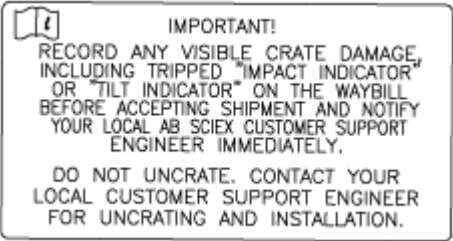
Label/Symbol	Definition
TILTWATCH PLUS or TIP TELL	Tilt Indicator Indicates whether the container was tipped or mishandled. Write on the Bill of Lading and inspect for damage. Any claims for tipping require a notation.

Table 2-5 Labels on the Mass Spectrometer Shipping Materials (continued)

Label/Symbol	Definition
↑↑	Keep upright.
IMPACT INDICATOR SENSITIVE PRODUCT WARNING or IMPACT INDICATOR SENSITIVE PRODUCT WARNING	Impact Indicator If the indicator is tripped, then this container has been dropped or otherwise mishandled. Make a note on bill of lading and check for damage.
IMPORTANT! RECORD ANY VISIBLE CRATE DAMAGE, INCLUDING TRIPPED "IMPACT INDICATOR" OR "TILT INDICATOR" ON THE WAYBILL BEFORE ACCEPTING SHIPMENT AND NOTIFY YOUR LOCAL AB SCIEX CUSTOMER SUPPORT ENGINEER IMMEDIATELY. DO NOT UNCRATE. CONTACT YOUR LOCAL CUSTOMER SUPPORT ENGINEER FOR UNCRATING AND INSTALLATION.	IMPORTANT! RECORD ANY VISIBLE CRATE DAMAGE INCLUDING TRIPPED "IMPACT INDICATOR" OR "TILT INDICATOR" ON THE WAYBILL BEFORE ACCEPTING SHIPMENT AND NOTIFY YOUR LOCAL AB SCIEX CUSTOMER SUPPORT ENGINEER IMMEDIATELY. DO NOT UNCRATE. CONTACT YOUR LOCAL CUSTOMER SUPPORT ENGINEER FOR UNCRATING AND INSTALLATION.
☂	Keep dry.
⚱	Fragile

Symbols, Indicators, and Labels: Mass Spectrometer

Refer to *Panel Symbols on page 23* for more information.

Table 2-6 Labels on the Mass Spectrometer

Label	Definition
WARNING: NO USER SERVICEABLE PARTS INSIDE. REFER SERVICING TO QUALIFIED PERSONNEL.	WARNING: No user serviceable parts inside. Refer servicing to qualified personnel. Consult instructions for use.
	Do not dispose of equipment as unsorted municipal waste (WEEE).
	WARNING: Hot Surface Hazard.
	Consult instructions for use.
	WARNING: High Voltage. Electrical Shock Hazard.
	Protective Earth (ground)
	Alternating Current
A	Amperes (current)
V	Volts (voltage)
VA	Volt Ampere (power)
WARNING: "DO NOT OPERATE WITHOUT FIRST ENSURING BOTTLE CAP IS SECURED"	WARNING: Do not operate without first ensuring bottle cap is secured. This warning appears on the source exhaust waste bottle.

Documentation Symbols and Conventions

The following symbols and conventions are used throughout the guide.

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

WARNING! Warning signifies an action that could cause personal injury if precautions are not followed.

CAUTION: Caution signifies an operation that could cause damage to the system or corruption or loss of data if precautions are not followed.

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

Tip! 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.

Principles of Operation 3

The AB SCIEX TripleTOF® 4600 system is designed for the qualitative and quantitative analysis of chemical species.

System Overview

The system includes the following components:

- An AB SCIEX TripleTOF® 4600 mass spectrometer with a DuoSpray™ ion source and a roughing pump.

- The optional calibrant delivery system (CDS).

- An AB SCIEX-supplied Windows 7 (32-bit) computer and monitor with the Analyst® TF software for instrument optimization, acquisition method development, and data acquisition.

Figure 3-1 Front and Right Side View
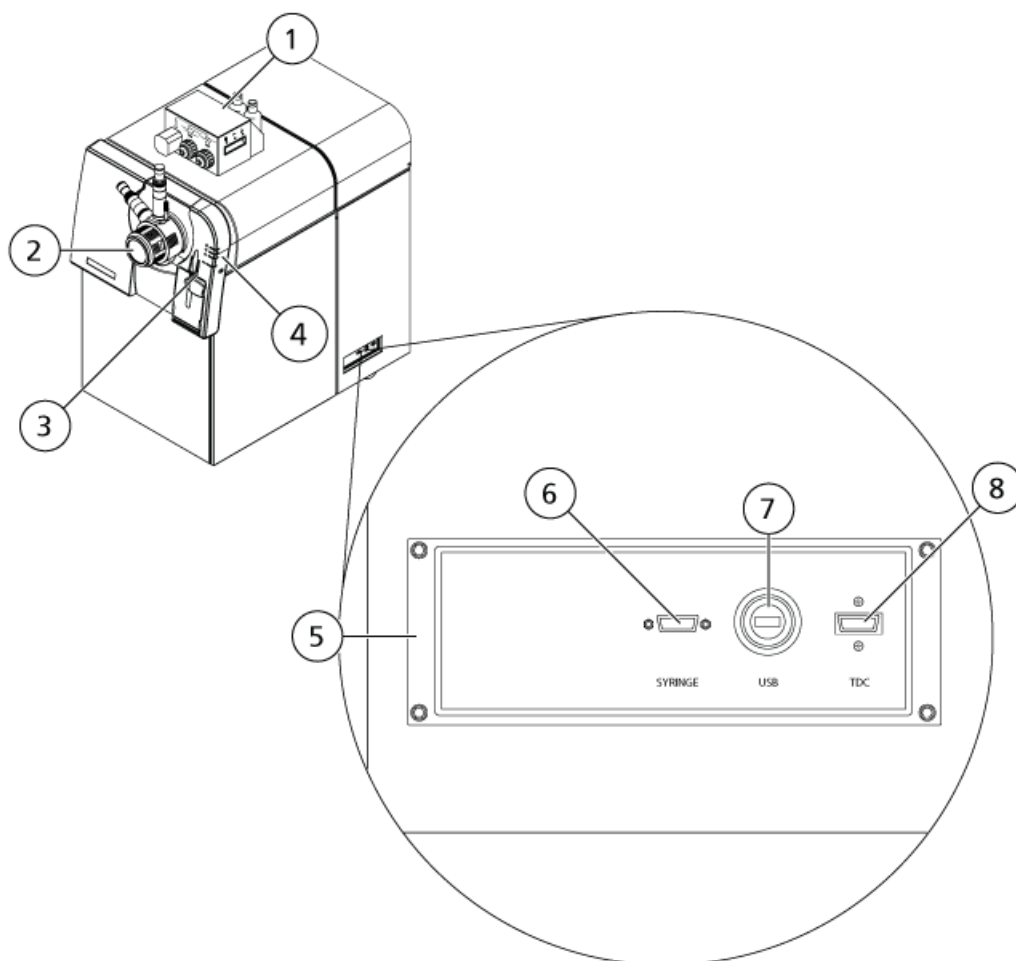
Item	Description	For more information...
1	Optional CDS	Refer to the *CDS Operator Guide*.
2	DuoSpray™ ion source	Refer to the *DuoSpray™ Ion Source for TripleTOF® Systems Operator Guide*.
3	Syringe pump	Refer to *Adjust the Integrated Syringe Pump Position*.
4	Mass spectrometer status LEDs	Refer to *Panel Symbols*.
5	Communications bulkhead	Contact an AB SCIEX Field Service Employee (FSE).
6	Serial (RS-232) cable connection for the syringe pump	Contact an FSE.

Item	Description	For more information...
7	USB cable connection for the USB-GPIB card	Contact an FSE.
8	InfiniBand cable connection for the TDC card	Contact an FSE.

Figure 3-2 Left Side View
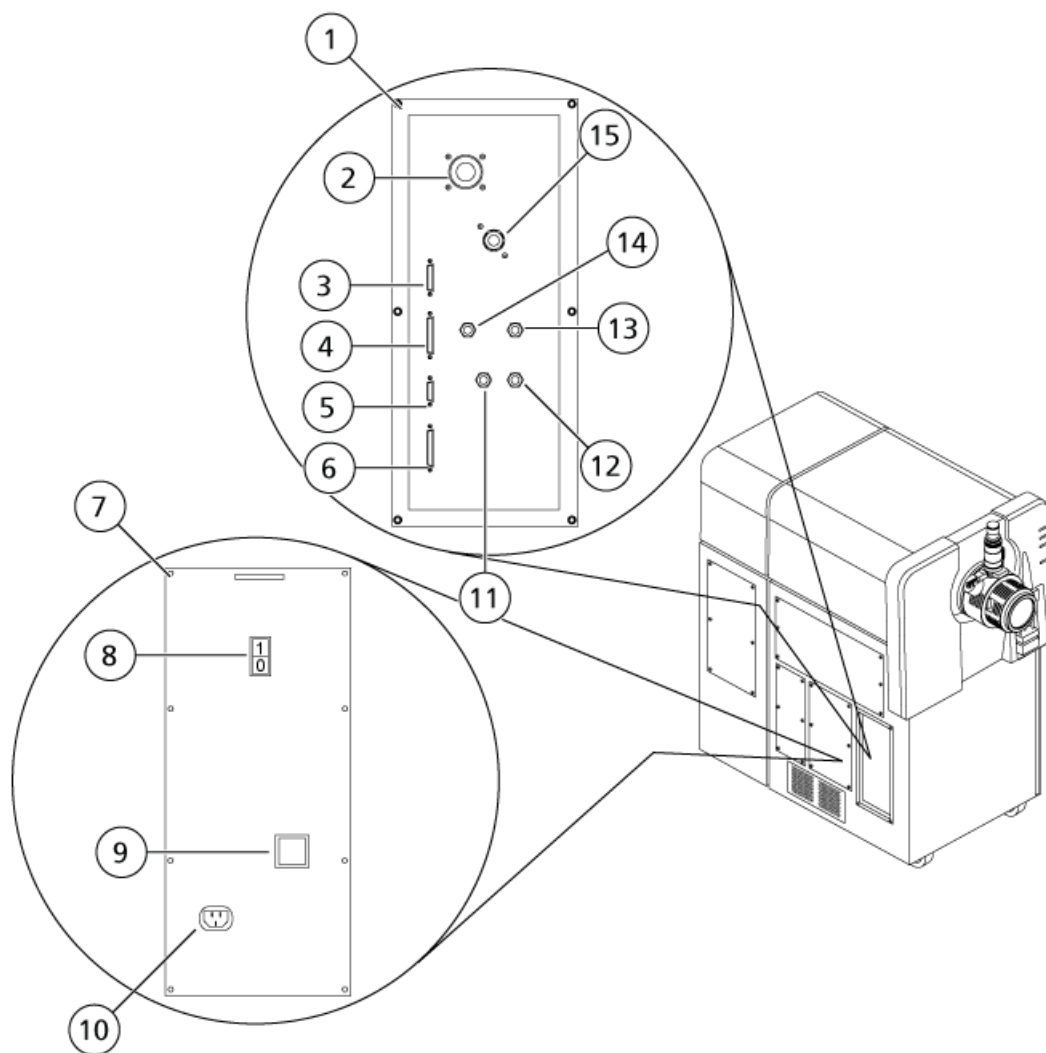
Item	Description	For more information...
1	Gas and vacuum bulkhead	Contact an FSE.
2	Roughing pump vacuum connection	Contact an FSE.
3	Calibrant control connection	Refer to the *CDS Operator Guide*.
4	AUX IO connection. The optional LC system start signal connects to this port.	Contact an FSE.
5	External control connection. This port is intended for future use.	Contact an FSE.
6	Sources connection. Some ion sources connect to this port.	Contact an FSE.
7	AC distribution panel	Contact an FSE.
9	Instrument power switch	Refer to *Start up the System*.
9	Cover over circuit breaker	Refer to *Start up the System*. Use the power switch rather than the circuit breaker to shut down the system.
10	Mains supply connection	Refer to *Start up the System*.
11	Curtain Gas^{TM} (nitrogen) supply connection	Contact an FSE.
12	Gas 1 and Gas 2 (zero) supply connection	Contact an FSE.
13	Source exhaust gas (zero air or nitrogen) supply connection	Contact an FSE.
14	CAD gas (nitrogen) supply connection	Contact an FSE.
15	Source exhaust waste connection	Contact an FSE.

Panel Symbols

Table 3-1 describes the mass spectrometer status LEDs.

Table 3-1 Panel Symbols

LED	Color	Name	Description
⏻	Green	Power	Lit when the system is powered up.
∀	Green	Vacuum	Lit when the correct vacuum has been achieved. Flashing if the vacuum is not at the correct vacuum (during pump down and venting).
✓	Green	Ready	Lit when the system is in the Ready state. The system must be in the Ready state to operate.
⚠	Red	Fault	Lit when the system encounters a system fault.

After the system is turned on, all of the LEDs illuminate. The power LED remains lit. The other four LEDs flash for two seconds and then turn off. The vacuum LED starts flashing. After the correct vacuum has been achieved this LED remains lit.

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 TripleTOF® 4600 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 7 (32-bit) operating system. The computer with the associated system software works with the system controller and associated firmware to control the system and data acquisition. During system operation, the acquired data is sent to the software where it can be shown as either full mass spectra, intensity of single or multiple ions versus time, or total ion current versus time.

Operating Instructions—Hardware   4

Start up the System

Note: Before operating the instrument, read the safety information in the *Operational Precautions and Limitations*.

⚠ **WARNING! Electrical Shock Hazard. Make sure that the mass spectrometer can be disconnected from the AC mains supply outlet in an emergency. Do not block the AC mains supply outlet.**

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 the 4 L drain bottle is connected to the **Exhaust Waste** connection on the rear of the instrument and to the laboratory ventilation system.

2. Make sure that the mains supply cable is plugged in to the mass spectrometer.

3. Make sure that the mass spectrometer and roughing pump mains supply cable are plugged into the 200 V to 240 V mains supply.

4. Make sure that three cables are connected to both the mass spectrometer and the computer: a serial (RS-232) cable, a USB cable, and an InfiniBand cable. Refer to *Figure 3-1*.

5. Turn on the roughing pump.

6. Remove the cover on the circuit breaker switch on the left side of the mass spectrometer, when viewed from the front and then turn on the circuit breaker. Refer to *Figure 3-1*.

7. Replace the cover over the circuit breaker switch and then tighten the screw holding the cover until it is finger tight.

8. Turn on the instrument power switch. Refer to *Figure 3-1*.

9. Turn on the computer, if it was turned off.

10. Start the software.

Shut Down the System

1. Complete or stop any ongoing scans. Refer to *Stop Sample Acquisition*.

> **CAUTION: Potential System Damage. Turn off the sample flow before the system is shut down.**

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. Deactivate the hardware profile, if it is active, and then close the software.

4. Turn off the instrument power switch on the left side of the instrument. Refer to *Figure 3-1*.

5. Turn off the roughing pump.

6. Wait 15 to 20 minutes to fully vent the system.

7. Remove the cover on the circuit breaker switch on the left side of the mass spectrometer and then turn off the circuit breaker. Refer to *Figure 3-1*

8. Replace the cover over the circuit breaker switch and then tighten the screw holding the cover until it is finger tight.

Adjust the Integrated Syringe Pump Position

> ⚠️ **WARNING! Puncture Hazard. Take care when inserting the syringe. The tip of the syringe is extremely sharp.**

1. Press the **Release** button on the right side of the syringe pump to lower the base and then insert the syringe. Refer to *Figure 4-1*.

2. 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 4-1 Lowering the Syringe
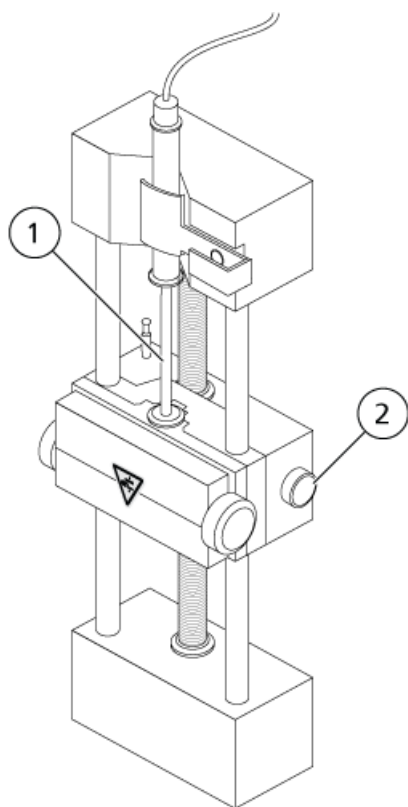
Item	Description
1	Syringe plunger
2	Release button. Press to raise or lower the base.

⚠️ **WARNING! Personal Injury Hazard. Make sure that the syringe is seated properly in the syringe pump and that the automatic syringe pump stop is adjusted properly to avoid damaging or breaking the glass syringe.**

3. Adjust the post so that it triggers the automatic syringe stop before the syringe plunger hits the bottom of the glass syringe. Refer to *Figure 4-2*.

Figure 4-2 Automatic Syringe Stop
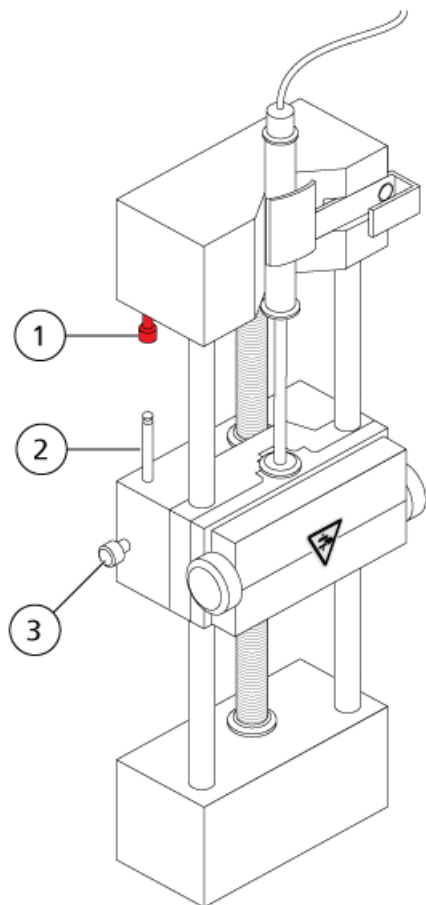
Item	Description
1	Automatic syringe stop. After the post hits the automatic syringe stop, the syringe pump stops.
2	Post. Adjust the height to prevent the syringe plunger from hitting the syringe during sample infusion.
3	Post lock screw. Tighten the screw after the height of the post is adjusted.

4. Turn the side screws as shown in *Figure 4-3* to secure the syringe.

Figure 4-3 Syringe Pump Screws
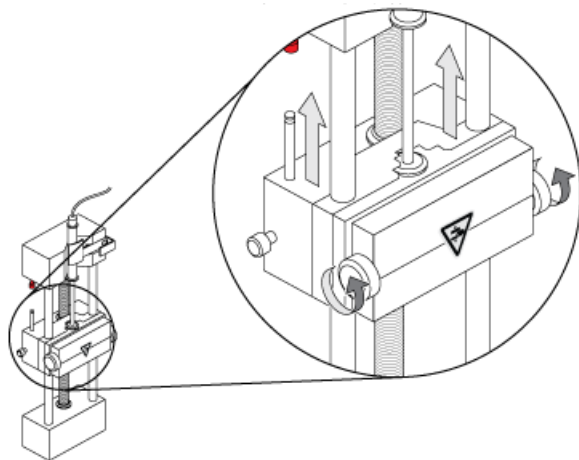
5. In the Analyst® TF software, on the navigation bar, double-click **Manual Tuning**.

6. Click **Start Syringe**.

7. To stop the syringe pump, click **Stop Syringe**.

Reset the Syringe Pump

If the Analyst® TF software stops communicating with the syringe pump, then reset the syringe pump.

• Use a paper clip or similar tool to press the reset button, shown in *Figure 4-4*.

Figure 4-4 Reset Button
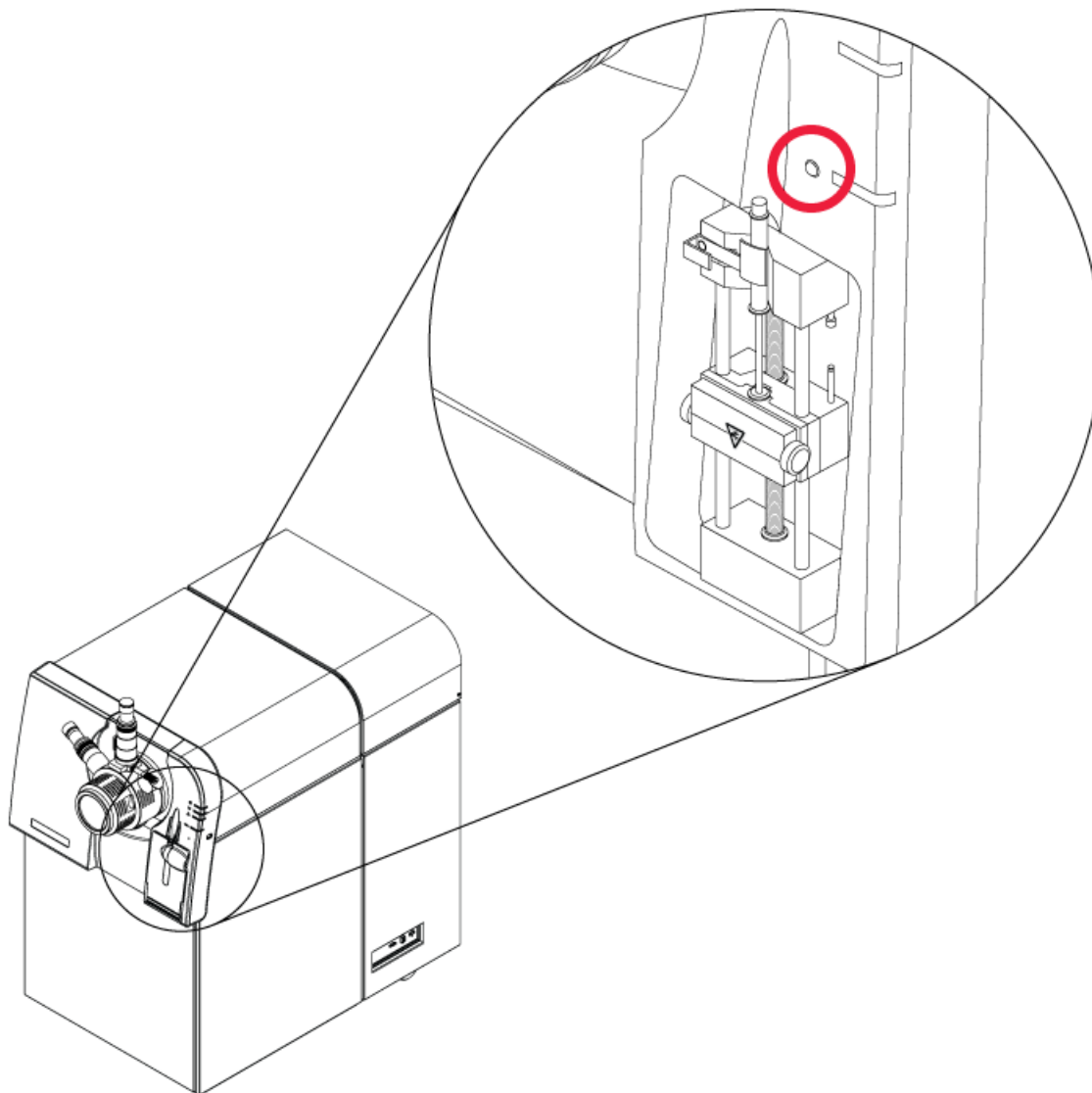
Operating Instructions — Sample Workflows 5

Table 5-1 Instrument Setup

Step	To do this...	Find the information in....	What does it do?
1	Create a hardware profile.	*Create a Hardware Profile*	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*	Before starting an experiment, decide where to store the files related to the experiment. Using projects and subprojects improves data management and makes comparison of results easier.
3	Optimize the mass spectrometer.	*Optimize the Mass Spectrometer*	This is the process of optimizing the resolution and mass spectrometer parameters, and calibrating the mass spectrometer to obtain the best sensitivity and performance from the system.

Table 5-2 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*	Before starting an experiment, decide where to store the files related to the experiment. Using projects and subprojects improves data management and makes comparison of results easier.
2	Create an acquisition method.	*Operating Instructions — Acquisition Methods*	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.
3	Create and submit a batch.	*Add Sets and Samples to a Batch* and *Submit a Sample or Set of Samples*	After creating an acquisition method, run samples by creating an acquisition batch and submitting the batch to the Acquisition Queue.
4	Acquire data.	*Acquire Data*	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 facilitates management of samples and batches in the queue.

Table 5-2 Sample Acquisition Workflow (continued)

Step	To do this...	Find the information in....	What does it do?
5	Analyze data in Explore mode. —OR—	*Operating Instructions — Analyze and Process Data*	In Explore mode, many tools are available for viewing and processing the acquired data. Graphs can be customized with peak labels and captions, contour plots can be displayed, and spectra can be saved in the library.
6	Analyze data and print reports using companion software.	MultiQuant™ software/PeakView® software	Use the MultiQuant software or PeakView software to analyze data. For more information, refer to the documentation that comes with the software.

Table 5-3 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 > Software Guides.**
2	Optimize the mass spectrometer.	Manual Optimization Tutorial located in **Start > Programs > AB SCIEX > Analyst® TF > Software Guides.**

Operating Instructions — Hardware Profiles and Projects   6

Hardware Profiles

A hardware profile tells the software how the mass spectrometer and the devices are configured and connected to the computer.

Each hardware profile must include a mass spectrometer. 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, make sure that the syringe pump is enabled if it will be used during acquisition.

The devices configured in the active hardware profile and selected in the **Add/Remove Device Method** dialog are shown as icons in the **Acquisition method** pane. Only devices included in the active hardware profile can be used to create acquisition methods.

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

Create a Hardware Profile

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

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

Figure 6-1 Hardware Configuration Editor Dialog
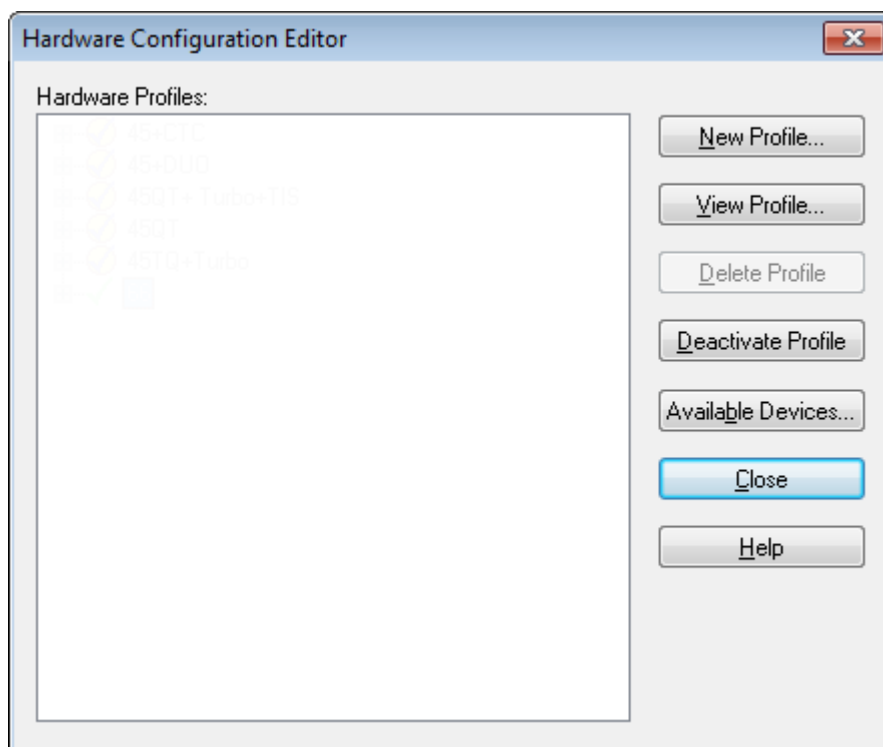
2. Click **New Profile**.

Figure 6-2 Create New Hardware Profile Dialog
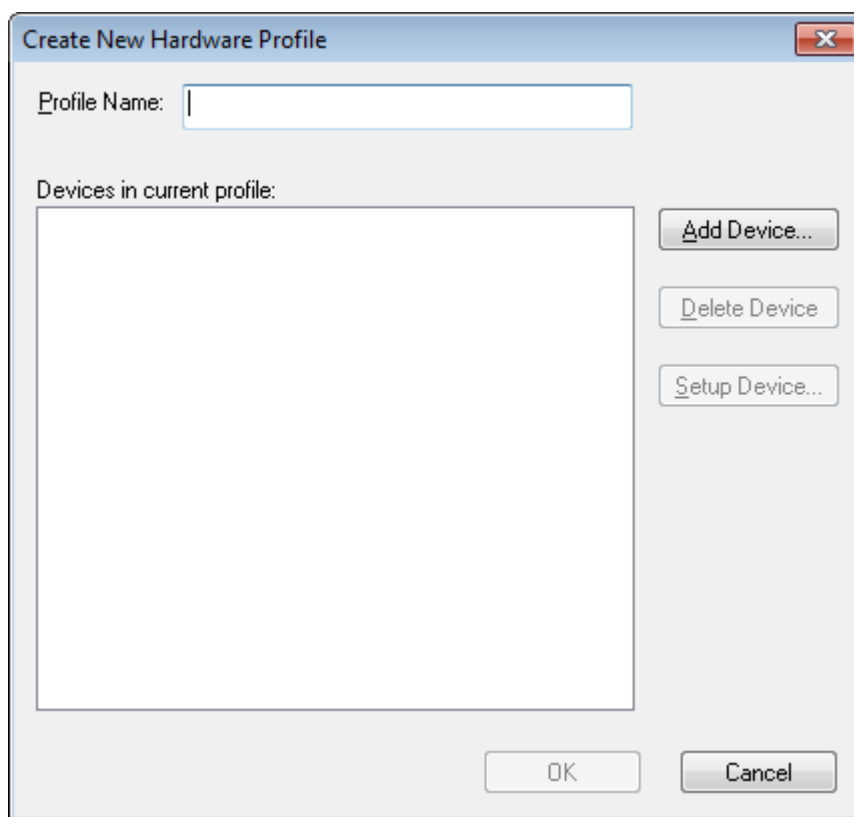
3. Type a name in the **Profile Name** field.

4. Click **Add Device**.

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

5. Select the mass spectrometer from the **Devices** list.

6. Click **OK**.

7. Select the mass spectrometer from the **Devices in current profile** list.

Figure 6-3 Available Devices Dialog
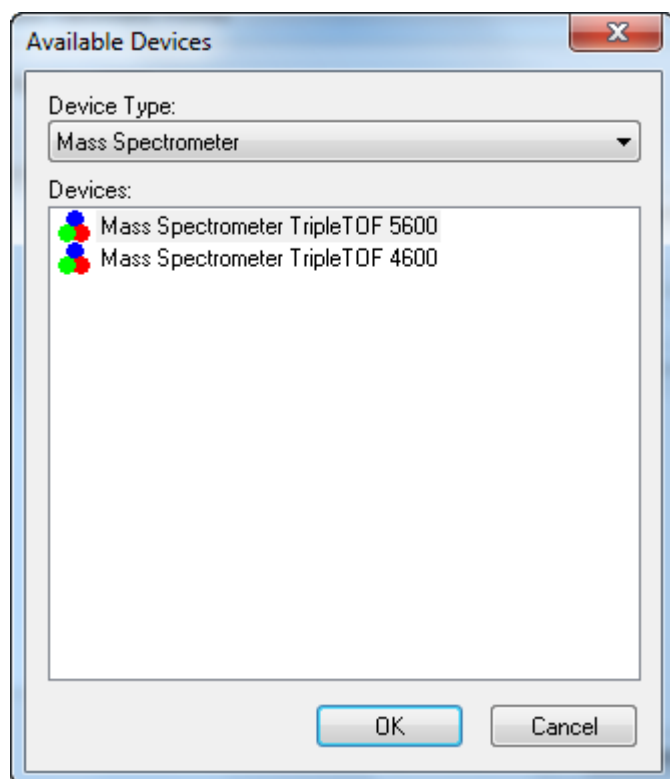
8. Click **Setup Device**.

9. (Optional) To configure the mass spectrometer for the integrated syringe pump, on the **Configuration** tab, select the **Use integrated syringe pump** check box.

> ⚠️ **WARNING! Personal Injury Hazard. Make sure that the syringe is seated properly in the syringe pump and that the automatic syringe pump stop is adjusted properly to avoid damaging or breaking the glass syringe.**

Figure 6-4 Configuration Tab with CDS and Syringe Pump Configured
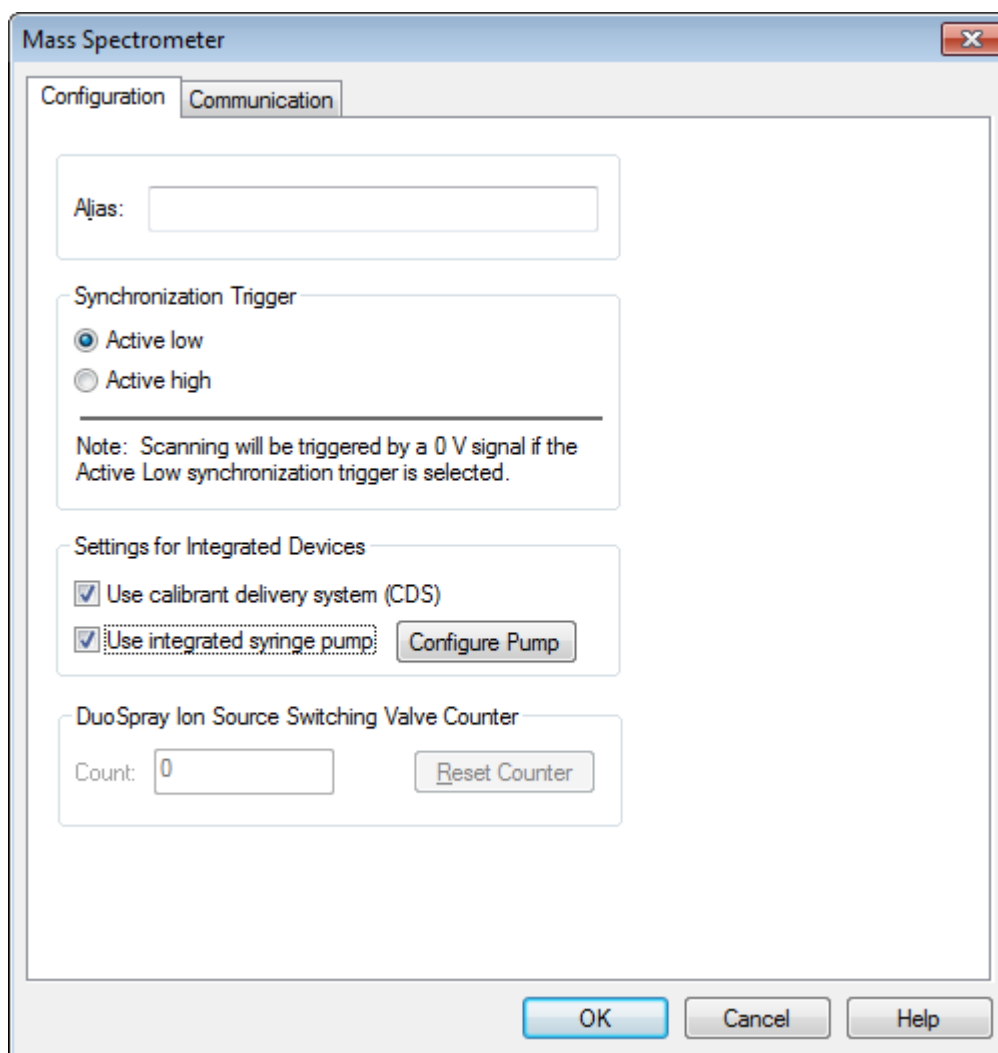
10. Select additional features on the **Configuration** and **Communication** tabs as required.

11. Click **OK** to return to the **Create New Hardware Profile** dialog.

12. Add and configure each device that is used with the mass spectrometer.

13. Click **OK** in the **Create New Hardware Profile** dialog.

14. Click the hardware profile in the **Hardware Configuration Editor**.

15. Click **Activate Profile**.

The check mark turns green. If a red x is shown, then there is an issue with the hardware profile activation.

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

16. Click **Close**.

Add Devices to a Hardware Profile

Devices must be configured to enable the software to communicate with them. When the software is installed, the driver required for each device is also installed. After the devices are physically connected to the computer, configure the device.

1. Open the **Hardware Configuration Editor**.

2. In the **Hardware Profiles** list, 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.

Figure 6-5 Available Devices Dialog
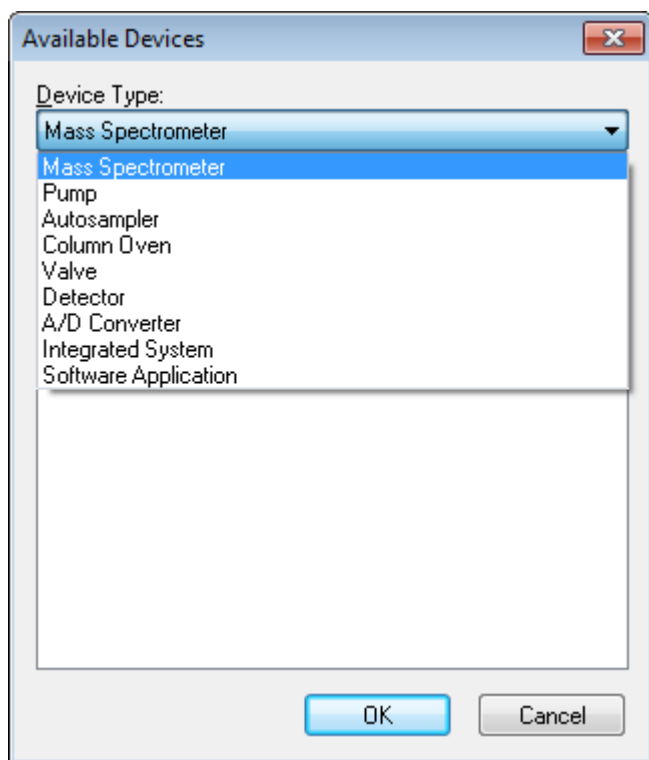
6. Click **OK**.

7. Select the device from the **Devices in current profile** list.

8. Click **Setup Device**.

   A dialog containing configuration values for the device opens.

9. (Optional) On the **Communication** tab, in the **Alias** field, type a name or other identifier.

   > **Note:** For devices using serial communication, make sure that the serial port selected matches the serial port to which the device is physically connected.

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

   - If the device uses a **Serial Port** as a communication interface, then in the **COM Port Number** list, select the COM port to which the device is connected.

   - If the device uses **Ethernet** as a communication interface, then type the **IP Address** assigned to the device by the administrator or use the corresponding **Host Name** for the address.

   - If the device uses **GPIB Board** as a communication interface, then do not change the settings for the GPIB board.

   The rest of the preset values for the device are probably appropriate. Do not change them. 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 configuration, click **OK**.

12. Repeat step *4* to step *11* for each device.

13. Click **OK** in the **Create New Hardware Profile** dialog.

14. To activate the hardware profile, in the **Hardware Configuration Editor**, click the hardware profile.

15. Click **Activate Profile**.

    The check mark turns green. If a red x is shown, then there is an issue with the hardware profile activation. For more information, refer to *Troubleshoot Hardware Profile Activation on page 41*.

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

16. Click **Close**.

Troubleshoot Hardware Profile Activation

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

1. Read the error message generated. Depending on the message, there might be an issue with a device or how the communication is set up.

2. 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 device (for example, dip switch settings) are set correctly and match the settings on the **Communication** tab.

5. Turn off the device.

6. Wait 10 seconds.

7. Turn on the device.

   Wait until all device power-up activities are complete before trying to activate the hardware profile again. Some devices might require 30 seconds or more to complete the power-up activities.

8. Activate the hardware profile.

9. If the issue persists, then delete the failing profile and create a new one.

10. If the issue persists, then contact technical support.

Projects and Subprojects

Create Projects and Subprojects

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

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

Figure 6-6 Create New Project/Subproject Dialog
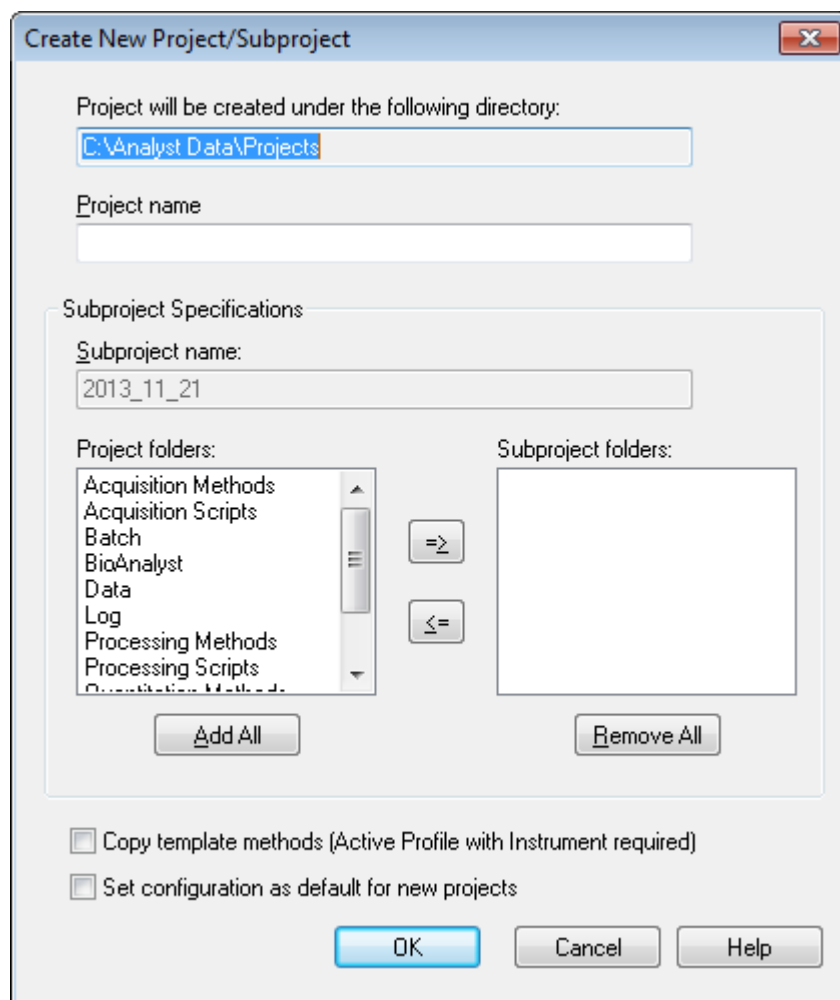
2. Type a project name in the **Project name** field.

3. (Optional) To use subprojects, select the required folders and then use the arrow buttons to move them to the **Subproject folders** list.

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 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 are created with this folder configuration.

6. Click **OK**.

Create Subprojects

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

1. On the **Project** tool bar, from the **Project** list, select the project.

2. Click **Tools > Project Create Subproject.**

3. In the **Subproject name** box, type a name for the subproject or use the existing date.

4. Click **OK**.

Copy Subprojects

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

1. Click **Tools > Project Copy Subproject.**

2. Click **Browse** to navigate to the subproject source in the **Copy Subproject** dialog.

3. Click **OK**.

4. Select the subproject from the **Source Subproject** list.

5. Click **Browse** to navigate to the subproject destination

6. Type the name in the **Target Subproject** field.

7. Click **OK**.

8. Do one of the following:

    • To copy all folders and files from the **Subproject Source** into the **Subproject Destination**, select the **Copy Contents** check box.

    • To copy only the folders in the same structure into the **Subproject Destination**, make sure that the **Copy Contents** check box is cleared.

9. Click **Copy**.

Switch Between Projects and Subprojects

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

Figure 6-7 Project List
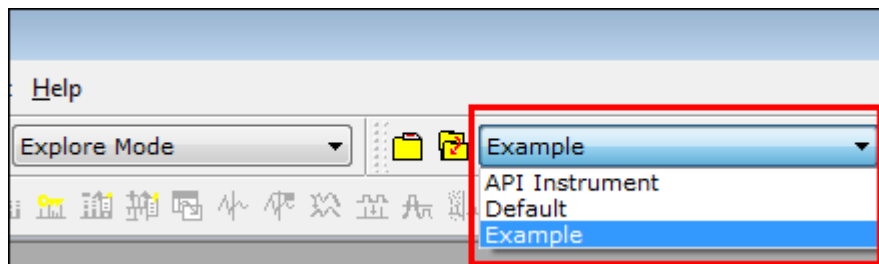
The project list in this figure shows the **API Instrument**, **Default**, and **Example** folders.

Installed Project Folders

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

API Instrument Folder

The **API Instrument** folder is unique and very important to the correct functioning of the mass spectrometer. The **API Instrument** folder contains the information required for tuning and calibrating the mass spectrometer. This information includes parameter settings files, reference files, instrument data files that contain calibration and resolution information, and the acquisition methods used during automatic tuning. The **API Instrument** folder also contains data files for manual tuning runs that were performed using the **Start** button rather than the **Acquire** button. These data files are saved automatically in the **API Instrument** folder in the **Tuning Cache** folder and named with the date and time they were created. The **Tuning Cache** folder is automatically cleared periodically.

Default Folder

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

Example Folder

The **Example** folder contains sample methods and data files. Users can practice working with the **Explore** mode using the example data files

Back Up the API Instrument Folder

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

• Copy the **API Instrument** folder, paste it to a different location, preferably to another computer, and then rename the folder. Use the date and a mass spectrometer reference if there is more than one mass spectrometer

when the folder is named. To recover the folder, rename the current **API Instrument** folder, copy the backup folder into the **Projects** folder, and then change the name of the backup folder to **API Instrument**.

Recover the API Instrument Folder

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

1. Rename the current **API Instrument** folder.

2. Copy the backup folder into the **Projects** folder.

3. Change the name of the backup folder to **API Instrument**.

Operating Instructions — Tune and Calibrate 7

Required Materials
• Tuning solutions that are supplied in the Standards Chemical Kit shipped with the system. If required, a new kit can be ordered from AB SCIEX.
• gas-tight syringe (1.0 mL recommended)
• Red PEEK sample tubing.

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

Optimize the Mass Spectrometer

The following procedure describes how to verify the performance of the mass spectrometer. For more information about using the other instrument performance options, refer to the Help.

1. On 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. On the navigation bar, under **Tune and Calibrate**, double-click **Instrument Optimization**.

   The Instrument Optimization dialog opens.

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 or Adjusting Performance** screen opens. After the process has completed, the **Results Summary** opens. For more information, refer to the Help.

About the Verifying or Adjusting Performance Dialog

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

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

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

Results Summary

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

Figure 7-1 Results Summary
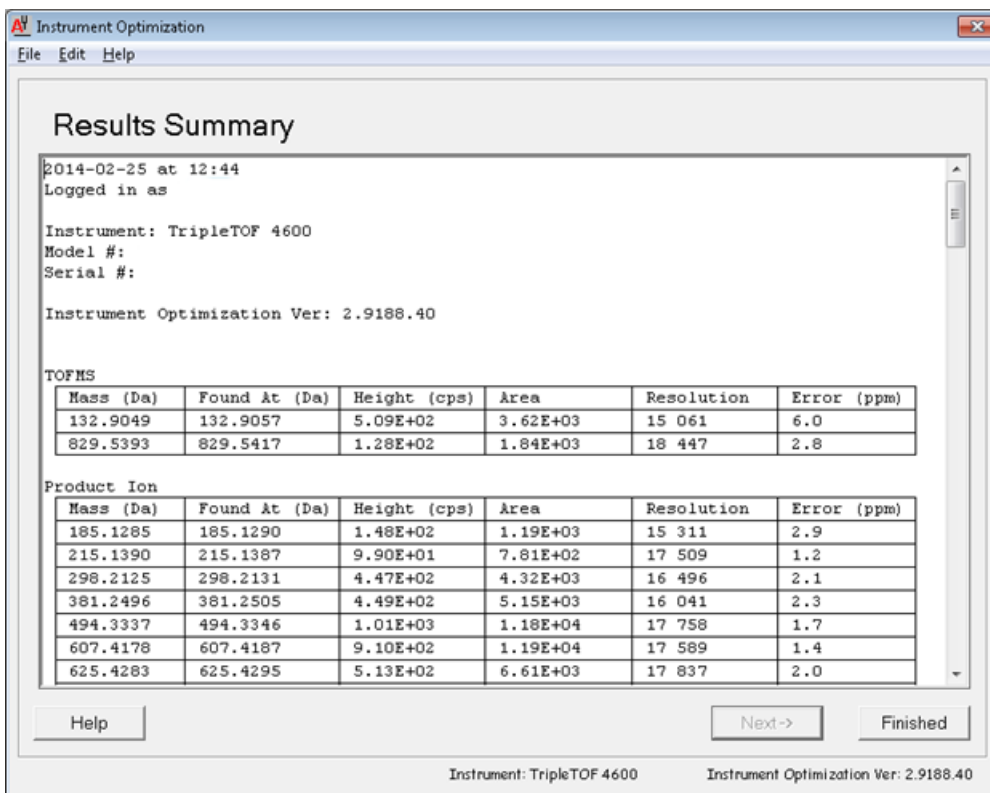
The **Results Summary** is saved as a document in the following folder: **\Analyst Data\Projects\API Instrument\Data\Instrument Optimization**. Users can print the **Results Summary** or open a previously saved **Results Summary**.

Operating Instructions — Acquisition Methods 8

Use the SWATH™ acquisition feature, available in both the **Method Wizard** and the **Acquisition Method Editor**, to create SWATH acquisition methods. Also, SWATH Variable width window methods can be created using the **Method Wizard** or **Acquisition Method Editor**. For more information, refer to the *Advanced User Guide*, Analyst® TF Help, and **Method Wizard** Help.

It is recommended that only users who are proficient in method development create or modify acquisition and quantitation methods. Refer to the About People and Roles section in the *Laboratory Director's Guide* for more information about roles and security.

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** opens.

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

   ---

4. Select **TOF MS (+)** from the **Choose MS Method** list.

5. Select the LC method that was created for the hardware profile from the **Choose LC Method** list.

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**.

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

Create an Acquisition Method Using the Acquisition Method Editor

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

Only devices configured in the active hardware profile appear in the **Acquisition method** 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. On the Navigation bar, under **Acquire**, double-click **Build Acquisition Method**.

3. Select a **Synchronization Mode** on the **Acquisition Method Properties** tab.

4. (Optional) Select the **Auto-Equilibration** check box and then type the required equilibration time, in minutes.

5. Click the **Mass Spec** icon in the **Acquisition method** pane.

6. Select a **Scan type** on the **MS** tab.

7. Type values in the fields as required. Refer to *Parameters on page 54*.

8. On the **Advanced MS** tab, type values in the fields as required.

9. On the **MS** tab, click **Edit Parameters**.

10. On the **Source/Gas** tab, specify values in the fields as required.

11. On the **Compound** tab, specify values in the fields as required and then click **OK**.

12. Click a device icon and then select the parameters for the device.

13. Add any additional periods and experiments. Refer to *Add an Experiment on page 52* and *Add a Period on page 52*.

14. Click **File > Save.**

Add an Experiment

1. Right-click the period and then click **Add experiment**.

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

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

2. Select the appropriate device or instrument parameters in the **Acquisition Method Editor** pane.

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

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

1. Open a multi-period method.
2. In the **Acquisition method** pane, press **Ctrl**, and then drag the experiment to the period.

   The experiment is copied below the last experiment in the period.

Copy an Experiment within a Period

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

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

A copy of the experiment is added below the last experiment created. 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
- of tandem mass spectrometry (MS/MS):
  - Product 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.

About Spectral Data Acquisition

Spectral data can be acquired in one of the modes described in *Table 8-1*.

Table 8-1 Spectral Data

| Mode	Description
Profile	The preset value is 0.1 Da. Profile data is the data generated by the mass spectrometer and corresponds to the intensity recorded at a series of evenly spaced discrete mass values.For example, for 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 (for example, 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 (fewer data steps are made) but with the loss of peak shape information.

Parameters

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

- Source and gas parameters: (Ion source-dependent) These parameters can change depending on the ion source used.

- Compound 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.

Figure 8-1 shows the location of the parameters on the ion optics path.

Figure 8-1 Ion Optics Path and Parameters
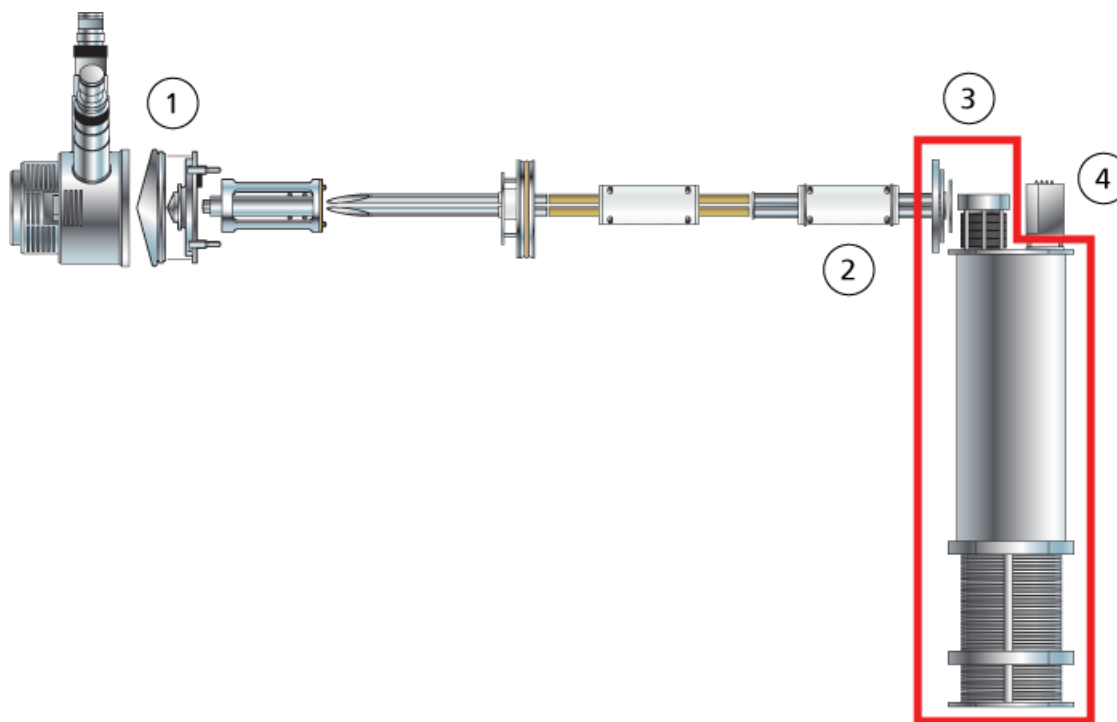
Item	Parameter	Parameter Type	Use	Scan Type
1	IonSpray Voltage Floating (ISVF)	Source and gas	The ISVF parameter affects the stability of the spray and hence the signal sensitivity. This is the voltage applied to the needle that sprays the sample.	All
1	Nebulizer Current (NC)	Source and gas	The NC parameter controls the current applied to the corona discharge needle in the atmospheric pressure chemical ionization (APCI) probe. The discharge ionizes solvent molecules, which in turn ionize the sample molecules.	All

Item	Parameter	Parameter Type	Use	Scan Type
1	Interface Heater Temperature (IHT)	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°C to 180°C range. The maximum heater temperature that can be set is 250°C, but this is too high for most applications.	All
1	Ion Source Gas 1 (GS 1)	Source and gas	For the Turbo V™ ion source , the GS1 parameter controls the nebulizer gas for both the TurboIonSpray® and APCI probes. For the DuoSpray™ ion source, the GS1 parameter controls the nebulizer gas for the TurboIonSpray probe.	All
1	Ion Source Gas 2 (GS 2)	Source and gas	For the Turbo V™ ion source , the GS2 parameter controls the heater gas for the TurboIonSpray® probe. For the DuoSpray™ ion source, the GS2 parameter controls the heater gas for the TurboIonSpray probe and the nebulizer gas for the APCI probe.	All
1	Temperature (TEM)	Source and gas	The TEM parameter controls the temperature of the heater gas for the TurboIonSpray probe or the temperature of the APCI probe.	All
1	Curtain Gas (CUR)	Source and gas	The CUR parameter controls the gas flow of the Curtain Gas™ interface. The Curtain Gas interface is located between the curtain plate and the orifice. It prevents the contamination of the ion optics.	All

Item	Parameter	Parameter Type	Use	Scan Type
1	Declustering Potential (DP)	Compound	The DP parameter controls the voltage on the orifice, which controls the ability to decluster ions between the orifice and the 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.	All
2	CAD Gas	Source and gas	The CAD parameter controls the pressure of CAD 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 scan types, the CAD gas helps to fragment the precursor ions. When the precursor ions collide with the collision gas, they dissociate to form product ions. Use the preset value and optimize for the compound.	All
2	Collision Energy (CE)	Compound	The CE parameter controls the potential difference between the Q0 region and the Q2 collision cell. It is used only in MS/MS scan types. This parameter is the amount of energy that the precursor ions receive as they are accelerated into the Q2 collision cell, where they collide with gas molecules and fragment. Use the preset value and optimize for the compound.	TOF MS, TOF MS/MS

Item	Parameter	Parameter Type	Use	Scan Type
2	Collision Energy Spread (CES)	Compound	The CES parameter, in conjunction with the CE parameter, determines which three discreet collision energies are applied to the precursor mass in an Product Ion scan when CES is used. 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.	TOF MS/MS
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** wizard 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 the **Instrument Optimization** wizard 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

Operating Instructions — Batches   9

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*.

Set Queue Options

The queue goes one-by-one through the list, acquiring each sample with the selected acquisition method. After all of the samples have been acquired, the queue stops and the mass spectrometer goes into **Standby** mode. In **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 the Analyst® TF software puts the mass spectrometer into **Standby** mode. For information about the other fields in the **Queue Options** dialog, refer to the Help.

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

Figure 9-1 Queue Options Dialog
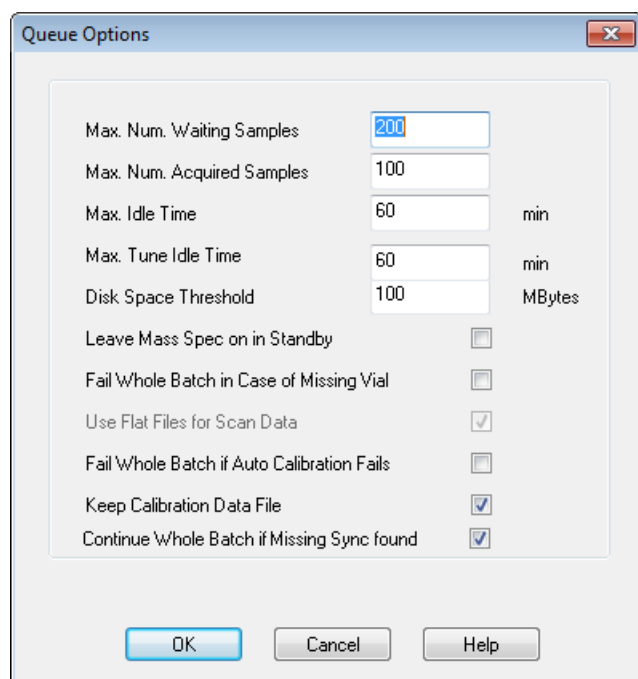
3. In the **Max. Num. Waiting Samples** field, set the maximum number of samples to a value that is greater than the number of samples that will be submitted to the queue

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

   If an LC method is used, then before the run is started, make sure that there is enough solvent in the reservoirs for all of the sample runs at the primary flow rate and the maximum idle time.

5. Select the **Leave Mass Spec on in Standby** check box to keep the mass spectrometer running after analysis has been completed. This feature allows the heaters and gases to continue running, even after devices have entered **Idle** state, so that the ion source and entrance to the mass spectrometer are kept free of contaminants.

6. Select the **Fail Whole Batch in Case of Missing Vial** check box to fail the entire batch when a missing vial is encountered. If this option is not selected, then only the current sample will fail and the queue will continue to the next sample.

7. Select the **Fail Whole Batch if Auto Calibration Fails** check box to stop the batch if auto calibration fails.

8. Select the **Keep Calibration Data File** check box to keep the calibration data file in a subfolder in the Data folder of the project from which samples are being submitted.

9. Select the **Continue Whole Batch if Missing Sync found** check box to continue acquiring the whole batch when a missing sync signal is encountered. If this check box is not selected, then the current sample fails and the queue does 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.

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

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

Figure 9-2 Batch Editor Dialog
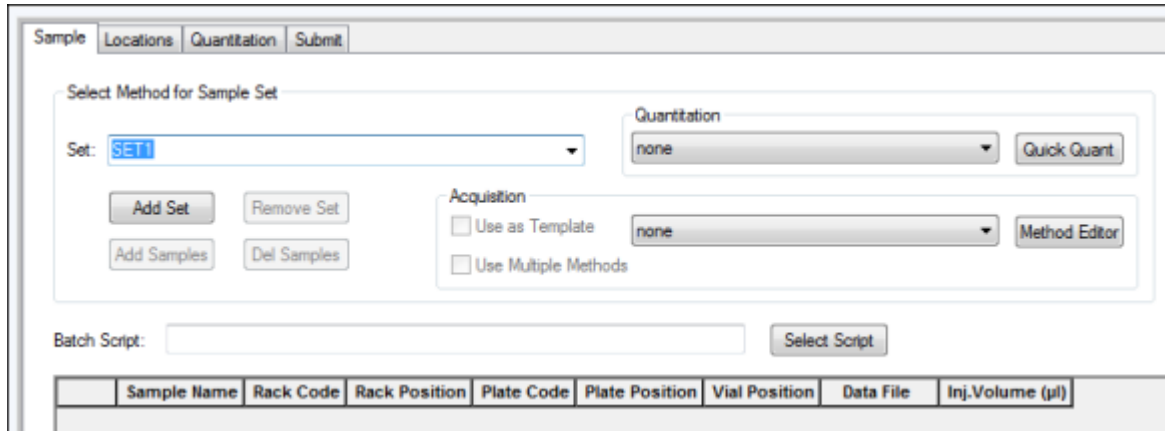
2. In the **Sample** tab, in the **Set** list, type a name.

3. Click **Add Set**.

4. Click **Add Samples** to add samples to the new set.

Figure 9-3 Add Sample Dialog
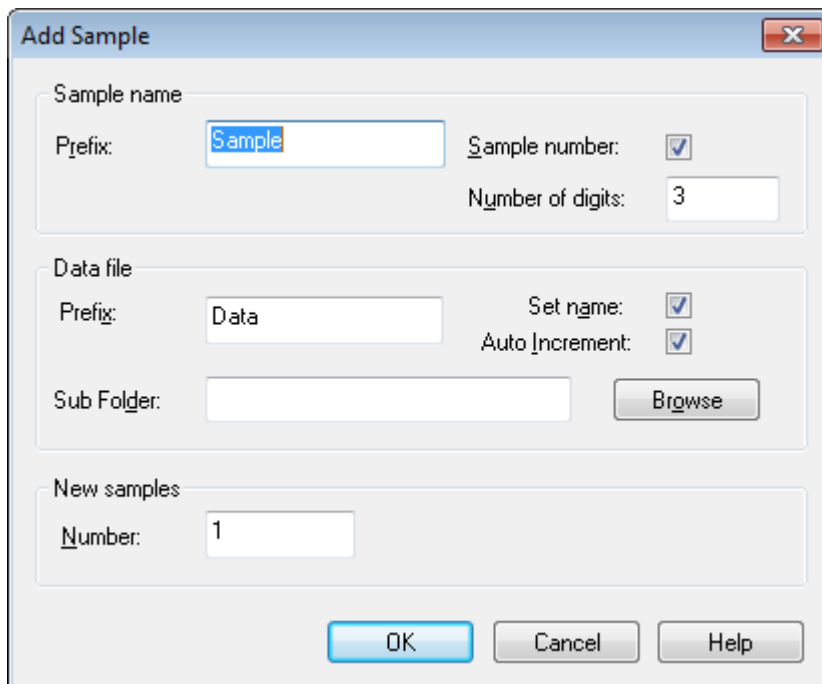
5. In the **Sample name** section, in the **Prefix** field, type a name for the samples in this set.

6. To add incremental numbering to the end of the sample name, select the **Sample number** check box.

7. If the **Sample number** check box is selected, then in the **Number of digits** field, type the number of digits to include in the sample name.

   For example, if 3 is typed, then the sample names would be samplename001, samplename002, and samplename003.

8. In the **Data file** section, in the **Prefix** field, type a name for the data file that will store the sample information.

9. Select the **Set name** check box to use the set name as part of the data file name.

10. Select the **Auto Increment** check box to increment the data file names automatically.

11. Type a name in the **Sub Folder** field.

   The folder is stored in the **Data** folder for the current project. If the **Sub Folder** field is left blank, then the data file is stored in the **Data** folder and a subfolder is not created.

12. In the **New samples** section, in the **Number** field, type the number of new samples.

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.

   Depending on how the system is set up, specific information for the autosampler must be entered. Even if the injection volume is set in the method, the user can change the injection volume for one or more samples by changing the value in the injection volume column.

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

15. To change the injection volumes from the volumes listed in the method, in the **Inj. Volume (µL)** column, type the injection volume for each sample.

16. Indicate the positions of the vials in the **Vial Position** column.

   > **Note:** To automatically fill in the samples from the **Locations** tab, click on the first and last vial within a set while pressing the **Shift** key. These vials appear as red circles. On the **Locations** tab, multiple injections from the same vial can be done by pressing the **Ctrl** key while clicking the vial location. The red circle turns green.

17. (Optional) Use the procedures in *Table 9-1* as required.

Table 9-1 Batch Editor 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	select the method and then click **Method Editor** from the list. To create a new acquisition method, select **None** from the list and then click **Method Editor**. Only experienced users should use this feature. Do not use this feature if the **Use Multiple Methods** option is selected.
To apply a previously created quantitation method	select the method from the **Quantitation** list.
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.

18. To set sample locations, do one of the following:

    - *Set Sample Locations in the Batch Editor on page 66*
    - *Select Vial Positions Using the Locations Tab (Optional) on page 66*

19. Click the **Submit** tab.

20. If the **Submit Status** section contains a message about the status of the batch, then do one of the following:

    - If the message indicates that the batch is ready for submission, then proceed to step 21.
    - If the message indicates that the batch is not ready for submission, then make the changes as indicated by the message.

21. Click **Submit**.

    The **Acquisition** dialog opens.

22. Save the file.

Submit a Sample or Set of Samples

1. Click the **Submit** tab in the **Batch Editor**.

2. If the **Submit Status** section contains a message about the status of the batch, then do one of the following:

   - If the message indicates that the batch is ready for submission, then proceed to step *3*.

   - If the message indicates that the batch is not ready for submission, then make the changes as indicated by the message.

3. Click **Submit**.

4. Save the file.

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. Make sure 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 AnalystCal_ plus the acquisition method name (for example, AnalystCal_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 along with the calibration report 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. The calibration report is named with Cal plus the time stamp, calibration sample index, and the word report (for example, Cal20130822154447030_report.txt). The report displays the peak finding criteria, the parameters, and the masses used for calibration. It informs the users whether the calibration succeeded. The report also summarizes the parameters used for calibration.

Change Sample Order

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

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

Acquire Data

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

1. On the navigation bar, click **Acquire**.

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

    The **Queue Manager** opens with all submitted samples.

    Figure 9-4 Queue Manager
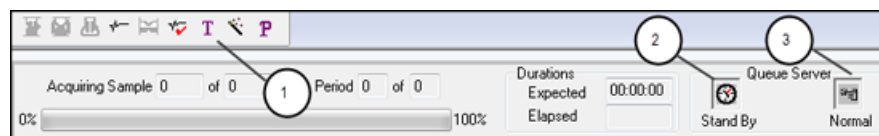
Item	Description
1	The **Reserve Instrument for Tuning** icon should not be pressed in.
2	Queue status should be **Stand By** mode.
3	Queue Server should be in **Normal** mode. Refer to *Queue States on page 68*.

3. Click **Acquire > Start Sample.**

Note: The manufacturer recommends that the sample be run again if an abnormal termination occurs during sample acquisition.

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 60*.

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

1. In the **Sample** tab, from the **Set** list, select the set.

2. For each sample in the set, do the following if applicable:

   - In the **Rack Code** column, select the rack type.

   - In the **Rack Position** column, select the position of the rack in the autosampler.

   - In the **Plate Code** column, select the plate type.

   - In the **Plate Position** column, select the position of the plate on the rack.

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

3. Save the file.

Select Vial Positions Using the Locations Tab (Optional)

1. Click the **Locations** tab in the **Batch Editor**.

2. Select the set from the **Set** list.

3. Select the autosampler from the **Autosampler** list.

   The appropriate number of rack spaces for the autosampler is shown in the graphic rack view.

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.

   The circles depicting the wells or vials for the plate or tray are shown.

Figure 9-5 Locations Tab
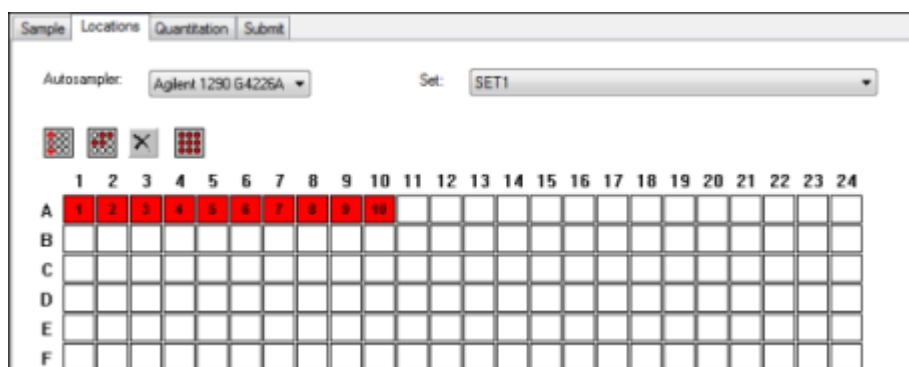
6. To select whether samples are marked by row or column, click the **Row/Column selection** selector button.

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

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

Stop Sample Acquisition

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. On the navigation bar, click **Acquire**.

3. Click **Acquire > Stop Sample.**

   The queue stops after the current scan in the selected sample is complete. The sample status in the **Queue Manager (Local)** window changes to **Terminated**, and all other samples following in the queue are **Waiting**.

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

Batch Editor Right-click Menu

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

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.
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	Copies the same data into the selected cells.
AutoIncrement	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 9-6 Queue Server Indicator Showing Normal Mode
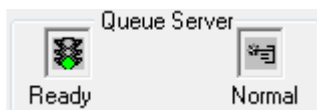
Figure 9-7 Queue Server Indicator Showing Tune Mode

The first icon indicates the queue state. The second icon indicates whether the queue is in **Tune** mode (for tuning) or **Normal** mode (for running samples). *Table 9-2* describes the icons and queue states.

Table 9-2 Queue States

Icons	State	Definition
	Not Ready	The hardware profile is deactivated and the queue is not accepting any sample submissions.
	Stand By	The hardware profile has been activated, but all devices are idle. Pumps are not running and gases are turned off.
	Warming Up	The mass spectrometer and devices are equilibrating, columns are being conditioned, the autosampler needle is being washed, and column ovens are reaching temperature. The duration of equilibration is selected by the operator. From this state, the system can go to the **Ready** state.
	Ready	The system is ready to start running samples and the devices have been equilibrated and are ready to run. In this state, the queue can receive samples and will run after samples are submitted.
	Waiting	The system will automatically begin acquisition when the next sample is submitted.
	PreRun	The method is being downloaded to each device and device equilibration is occurring. This state occurs before the acquisition of each sample in a batch.

Table 9-2 Queue States (continued)

Icons	State	Definition
	Acquiring	The method is running and data acquisition is occuring.
	Paused	The system has been paused during acquisition.

View Instrument and Device Status Icons

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

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

• On the status bar, double-click the icon for the device or mass spectrometer.

The **Instrument Status** dialog opens.

Table 9-3 Instrument and Device Status Icons

Status	Icon	Background Color	Description
Idle		Green or yellow	The device is not running. If the background color is yellow, then the device should be equilibrated before it is ready to run. If the background color is green, the device is ready to run.
Equilibrating		Green or yellow	The device is equilibrating.
Waiting		Green	The device is waiting for a command from the software or another device, or for some action by the operator.
Running		Green	The device is running a batch.

Table 9-3 Instrument and Device Status Icons (continued)

Status	Icon	Background Color	Description
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.

Queue Right-click Menu

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

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 preselected column.
Column Settings	Changes the column settings.

Operating Instructions — Analyze and Process Data **10**

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*.

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

Open Data Files

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

1. On the navigation bar, under **Explore**, double-click **Open Data File**.

2. In the **Data Files** list, navigate to the data file to open, select a sample, and click **OK**.

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

   Tip! To see an example data file, make sure that the **Example** project is selected. Open the TOF folder, and then open the **TOFMS PPGs3000.wiff** file. In the Sample list, select **TOFMS**.

Navigate Between Samples in a Data File

Note: shows the navigation icons used in this procedure. If samples were saved in separate data files, then open each file individually.

- Open a data file and then do one of the following:

  - Click the icon with the arrow pointing to the right to skip to the next sample in the data file.

  - Click the icon with the arrow curving to the right to skip to a non-sequential sample.

  - In the **Select Sample** dialog, from the **Sample** list, select the sample.

  - Click the icon with the arrow pointing to the left to go to the previous sample in the data file.

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 the 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 10-1* shows the software functionality available when the user views the file information.

- 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 10-1 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 as an .rtf file.
Font	Changes the font.
Save Acquisition Method	Saves the acquisition method as a .dam file.

Table 10-1 Right-click Menu for Show File Information Pane (continued)

Menu	Function
Save Acquisition Method to CompoundDB	Opens the **Specify Compound Information** dialog. Select the **IDs** and molecular weights to be saved in the compound database.
Delete Pane	Deletes the selected pane.

Show Data in Tables

1. Open a data file.

2. Click **Explore > Show > Show List Data.**

   The data is shown in a pane below the graph.

Figure 10-1 Peak List Tab
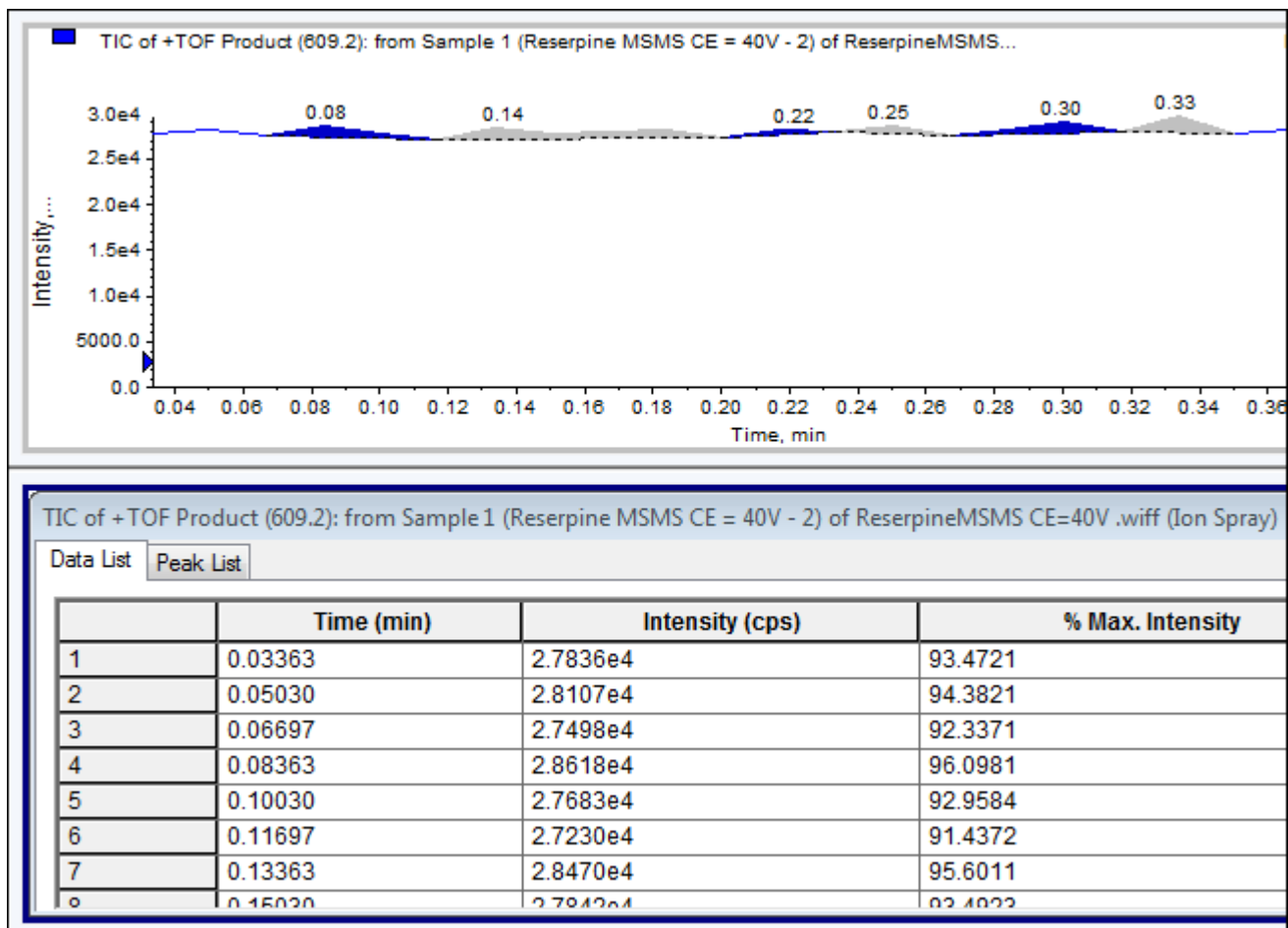
Table 10-2 Right-click Menu for Spectral Peak List Tab

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

Table 10-3 Right-click Menu for Chromatographic Peak List Tab

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

Show ADC Data

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

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

    The **Select ADC Channel** dialog opens.

    Figure 10-2 Select ADC Channel Dialog
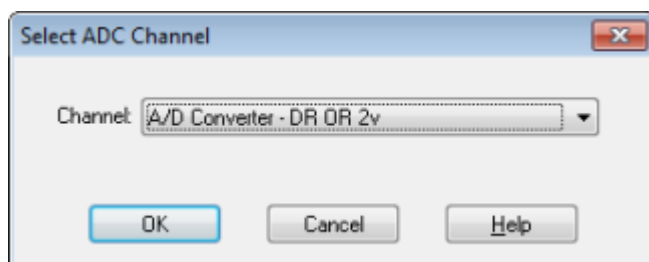
3. From the **Channel** list, select a channel.
4. Click **OK**.

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

Show Basic Quantitative Data

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

3. In the **Peak List** tab, right-click and then select **Show Peaks in Graph**.

   Peaks are shown in two colors.

4. To change the peak finding algorithm settings, right-click and then select either **Analyst Classic Parameters** or **Intelliquan Parameters**, whichever is active.

5. (Optional) To remove the colored peaks, right-click in the **Peak List** tab and then clear **Show Peaks in Graph**.

Chromatograms

Refer to *Table 10-8 on page 87* for more information about using the available icons.

Table 10-4 Types of Chromatograms

Types of Chromatograms	Purpose
TIC (Total Ion Chromatogram)	A chromatographic view generated by plotting the intensity of all ions in a scan against time or scan number. When a data file is opened, it is preset to open as a TIC. If the experiment contains only one scan, then it is shown as a spectrum. If the **MCA** check box is selected during acquisition of the data file, then the data file opens to the mass spectrum. If the **MCA** check box is not selected, then the data file opens as the TIC.
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.
BPC (Base Peak Chromatogram)	A 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 view 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

- 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.

About Generating XICs

XICs can be generated only from single-period, single experiment chromatograms or spectra. To obtain an XIC from multi-period or multi-experiment data, split the data into separate panes by clicking the triangle under the x-axis. Refer to *Table 10-8 on page 87* for more information about using the available icons.

Several methods are available for extracting ions to generate an XIC, depending on whether chromatographic or spectral data is used. *Table 10-5* contains a summary of methods that can be used with chromatograms and spectra.

Table 10-5 Summary of XIC Generation Methods

Method	Use with Chromatogram	Use with Spectrum	Extraction
Selected range	No	Yes	Extracts ions from a selected area in a spectrum.
Maximum	No	Yes	Extracts ions from a selected area in a spectrum using the most intense peak in the selected area. This option creates an XIC using the maximum mass from the selected spectral range.

Table 10-5 Summary of XIC Generation Methods (continued)

Method	Use with Chromatogram	Use with Spectrum	Extraction
Base peak masses	Yes	Yes	Can be used only with Base Peak Chromatograms (BPCs). 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, then the resulting XIC will have an equal number of colored traces representing each mass.
Specified masses	Yes	Yes	Extracts ions from any type of spectrum or chromatogram. Select up to ten start and stop masses for which to generate XICs.

Generate an XIC Using a Selected Range

1. Open a data file containing spectra.

2. Select a range by pressing the left mouse button at the start of the range, dragging the cursor to the stop point, and then releasing the left mouse button.

   The selection is indicated in blue.

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

   An XIC of the selection opens in a pane below the spectrum pane. The experiment information at the top of the pane contains the mass range and the maximum intensity in counts per second.

Generate an XIC Using the Maximum Peak

1. Open a data file containing spectra.

2. Select a range.

   The selection is indicated in blue.

3. Click **Explore > Extract Ions > Use Maximum.**

   An XIC of the maximum peak specified selection opens below the spectrum pane. The experiment information at the top of the pane contains the mass range and the maximum intensity in counts per second.

Generate an XIC Using Base Peak Masses

1. Open a data file containing spectra.

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

   The selection is indicated in blue.

3. Click **Explore > Extract Ions > Use Base Peak Masses.**

   An XIC of the specified selection opens below the spectrum pane. The experiment information at the top of the pane shows the mass range and the maximum intensity in counts per second.

Extract Ion by Selecting Masses

1. Open a spectrum or chromatogram.

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

   Figure 10-3 Extract Ions Dialog
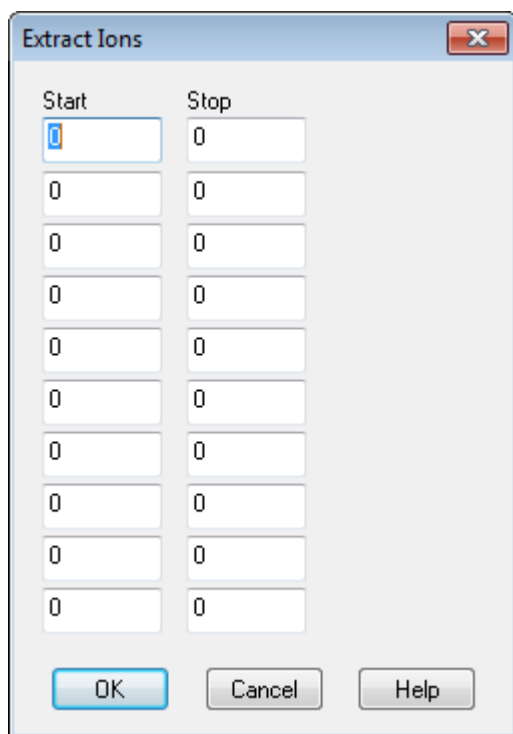
3. Type the values for each XIC to be created. If a stop value is not typed, then the range is defined by the start value.

- In the **Start** field, type the start value (lower value) for the mass range.

- In the **Stop** field, type the stop value (higher value) for the mass range.

4. Click **OK**.

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

Generate BPCs

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

1. Open a data file.

2. Select an area within a TIC.

   The selection is indicated in blue.

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

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

   Figure 10-4 Base Peak Chromatogram Options

4. In the **Mass Tolerance** field, type the value to indicate the mass range used to find a peak. The software finds the peak using a value twice the typed range (± the mass value).

5. Type the intensity below which peaks are ignored by the algorithm in the **Minimum Intensity** field.

6. Type the mass that determines the beginning of the scan range in the **Minimum Mass** field.

7. Type the mass that determines the end of the scan range in the **Maximum Mass** field.

8. To set the start and end times, select the **Use Limited Range** check box and do the following:

   - In the **Start Time** field, type the time that determines the start of the experiment.

   - In the **End Time** field, type the time that determines the end of the experiment.

9. Click **OK**.

   The BPC is generated in a new pane.

Generate XWCs

Up to three ranges can be extracted from a DAD spectrum to generate the XWC. Refer to *Table 10-8 on page 87* for more information about using the available icons.

1. Open a data file that contains a DAD spectrum

2. Right-click anywhere in the pane and then click **Extract Wavelengths**.

Figure 10-5 Extract Wavelengths Dialog
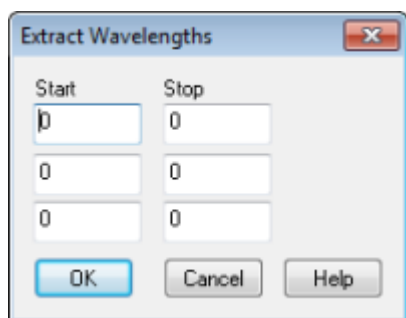
3. Type **Start** and **Stop** values.

4. Click **OK**.

   The XWC opens in a pane below the DAD spectrum.

Generate DAD Data

Like mass spectrometer data, DAD data can be viewed in chromatogram or spectrum form.

1. Open a data file containing data acquired with a DAD.

   The TWC, which is analogous to a TIC, opens in a pane below the TIC.

2. In the **TWC** pane, click a point to select a single point in time, or highlight an area of the spectrum to select a range of time.

3. Click **Explore > Show > Show DAD Spectrum.**

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

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

Generate TWCs

A TWC shows total absorbance (mAU) on the y-axis plotted against time on the x-axis. Refer to *Table 10-8 on page 87* for more information about using the available icons.

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. Do one of the following:

   • 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 and then click **OK**.

- Click **Explore > Threshold.**

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

Chromatogram Panes

Table 10-6 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 containing the spectrum.
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 a chromatogram for the specific ions.
Show Base Peak Chromatogram	Generates a new pane containing a base peak chromatogram.
Show ADC Data	Generates a new pane containing the UV data trace, if acquired.
Show UV Detector Data	Generates a new pane containing the UV data trace, if acquired.
Spectral Arithmetic Wizard	Opens the Spectral Arithmetic Wizard.
Save to Text File	Generates a text file of the pane, which can be opened in Microsoft Excel or other programs.
Save Explore History	Saves information about changes to processing parameters, also called **Processing Options**, that were made when a .wiff file was processed in **Explore** mode. The processing history is stored in a file with an .EPH (Explore Processing History) extension.
Add Caption	Adds a caption at the cursor point in the pane.
Add User Text	Adds a text box at 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.

Table 10-6 Right-click Menu for Chromatogram Panes (continued)

Menu	Function
Subtract Range Locked	Locks or unlocks the subtract ranges. If the subtract ranges are not locked, then each subtract range can be moved independently. The subtract ranges are preset to locked.
Delete Pane	Deletes the selected pane.

Spectra Panes

Table 10-7 Right-click Menu for Spectra Panes

Menu	Function
List Data	Lists the data points and integrates chromatograms.
Show TIC	Generates a new pane containing the TIC.
Extract Ions (Use Range)	Extracts a specific ion or set of ions from a selected pane and then generates a new pane containing a chromatogram for the specific ions.
Extract Ions (Use Maximum)	Extracts ions using the most intense peak in a selected area.
Save to Text File	Generates a text file of the pane, which can be opened in Excel or other programs.
Save Explore History	Saves information about changes to processing parameters, also called **Processing Options**, that were made when a .wiff file was processed in **Explore** mode. The processing history is stored in a file with an .EPH (Explore Processing History) extension.
Add Caption	Adds a caption at the cursor 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	Adds records and compound-related data, including spectra, to the library. An active spectrum is required to perform this task.

Table 10-7 Right-click Menu for Spectra Panes (continued)

Menu	Function
Search Library	Searches the library without constraints or with previously saved constraints.
Set Search Constraints	Searches the library using the criteria typed in **Search Constraints** dialog.

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.

It is recommended that users do not use the Subsetting features included within the software.

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 might be of a variable or fixed size. Panes are automatically tiled within the window and are arranged into column and row format. If the size of a window is changed, then the panes within the window change in size to accommodate the new size. A window cannot be sized to the point where any of the panes become smaller than 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.

Manage Data

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

Table 10-8 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.**	
Move a pane	• Select the graph. Click **Window > Move Pane.** • Select the pane or window and then drag it to the new position. This position can be inside the same window or within another window. A four-headed arrow is shown when the cursor is on the boundary of the active window or pane. • If the pane is at the top or bottom of the target pane, then the pane moves above or below that pane, respectively. • If the pane is at the left or right of the target pane, then the pane moves to the left or right of that pane, respectively. • If the pane is at any other position, then the pane moves to the target row. The drop shadow of the pane as the pane is moved around indicates its new position.	
Link panes	a. With the two graphs open, click one to make that pane active. b. Click **Explore > Link** and then click the other pane.	
Remove linking	Close one of the panes. Click **Explore > Remove Link.**	
Delete a pane	Select the graph. Click **Window > Delete Pane.**	
Lock a pane	Select the graph. Click **Window > Lock Panes.**	
Hide a pane	Select the graph. Click **Window > Hide Pane.**	

Table 10-8 Graph Options (continued)

To do this...	use this menu option...	...or click this icon
Maximize a pane	Select the graph. Click **Window > Maximize Pane.**	
Tile panes	Select the graph. Click **Window > Tile all Panes.**	

Zoom In on the Y-axis

1. Move the pointer to the left of the y-axis to either side of the area to be expanded and then drag away from the starting point in a vertical direction while holding the left mouse button.

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

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

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

Zoom In on the X-axis

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

1. Move the pointer under the x-axis to either side of the area to be expanded and then drag away from the starting point in a horizontal direction while holding the left mouse button.

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

Service and Maintenance Information

11

Regularly clean and maintain the system for optimal performance. Refer to *Table 11-1* for information on tuning frequency.

> **WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Determine whether mass spectrometer decontamination is required prior to cleaning or maintenance. Decontamination should be performed prior to cleaning if radioactive materials, biological agents, or toxic chemicals have been used with a mass spectrometer.**

Recommended Cleaning and Maintenance Schedule

Table 11-1 Maintenance Tasks

Component	Frequency	Task	For more information...
Curtain plate	Daily	Clean	Refer to *Clean the Curtain Plate on page 94*.
Orifice plate (front)	Daily	Clean	Refer to *Clean the Front of the Orifice Plate on page 95*.
Orifice plate (front and rear)	As needed	Clean	Contact the local QMP or AB SCIEX Field Service Employee (FSE).
QJet® ion guide and IQ0 lens	As needed	Clean	Contact the local QMP or FSE.
Q0 and IQ1 lens	As needed	Clean	Contact the local QMP or FSE.
Instrument surfaces	As needed	Clean	Refer to *Clean the Surfaces on page 90*.
Drain bottle	As needed	Empty	Refer to *Empty the Source Exhaust Drain Bottle on page 96*.
Roughing pump oil	As needed	Check and fill	Contact the local QMP or FSE.
Instrument air filter	Every 6 months	Inspect and clean or replace	Contact the local QMP or FSE.

Table 11-1 Maintenance Tasks (continued)

Component	Frequency	Task	For more information...
TurboIonSpray® and APCI Electrodes	As needed	Inspect and clean or replace	
Corona discharge needle	As needed	Replace	

For "As needed" tasks, follow these guidelines:

• Clean the QJet ion guide and Q0 region if system sensitivity degrades.

> **Tip!** Clean the Q0 region regularly to minimize the impact of charging (a significant loss of sensitivity of the ions of interest over a short period of time) on the quadrupoles and lenses. Contact a QMP or AB SCIEX FSE.

• Clean the mass spectrometer surfaces after a spill or when they become dirty.

• Empty the drain bottle before it becomes full.

Clean the Surfaces

Clean the external surfaces of the mass spectrometer after a spill or when they become dirty.

> **WARNING! Biohazard, Toxic Chemical Hazard. Take all appropriate safety precautions, and follow all local regulations and guidelines when handling and disposing of the roughing pump oil. Be careful to avoid spills, and if a spill occurs, follow established spill control procedures.**

1. Wipe the external surfaces with a soft cloth dampened with warm, soapy water.

2. Wipe the external surfaces with a soft cloth moistened with water to remove any soap residue.

Clean the Front-End

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

• Minimize unscheduled system downtime.

• Maintain optimum sensitivity.

• Avoid more extensive cleaning that requires a service visit.

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 mass spectrometer.

Note: Follow all applicable local regulations. For health and safety guidelines, refer to *Chemical Precautions on page 8*.

Symptoms of Contamination

The system might be contaminated if any one of the following is observed:

- Significant loss in sensitivity

- Increased background noise

- Additional peaks that are not part of the sample appear in full scan or survey scan methods

If you observe any of these issues, then clean the mass spectrometer front-end.

Required Materials

Note: U.S. customers can call 877-740-2129 for ordering information and inquiries. International customers can visit www.absciex.com/contact-us.

- Powder-free gloves (nitrile or neoprene recommended)

- Safety glasses

- Laboratory coat

- Fresh, high-quality (pure) water (at least 18 MΩ de-ionized [DI] water or ultra-pure HPLC-grade water). Old water can contain contaminants that can further contaminate the mass spectrometer.

- MS-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)

- Clean 1 L or 500 mL glass beaker to prepare cleaning solutions

- 1 L beaker to catch used solvent

- Organic waste container

- Lint-free wipes. Refer to *Tools and Supplies Available from the Manufacturer on page 92*.

- (Optional) Poly swabs

Tools and Supplies Available from the Manufacturer

Description	Part Number
Small poly swab (thermally bonded). Available in the Cleaning kit.	1017396
Lint-free wipe (11 cm x 21 cm, 4.3 inches x 8.3 inches). Available in the Cleaning kit.	018027
Q0 cleaning tool for cleaning the Q0 rod set. Available in the Cleaning kit.	1028234
Custom QJet® ion guide cleaning brush (tapered). Available in the Cleaning kit.	5020895
Alconox packets. Available in the Cleaning kit.	5020893
Cleaning kit. Contains the small poly swab, lint-free wipes, Q0 cleaning tool, tapered QJet ion guide cleaning brush, and alconox packets.	5020763

Best Practices

WARNING! Toxic Chemical Hazard. Follow all safety guidelines when handling, storing, and disposing of chemicals.

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Determine whether mass spectrometer decontamination is required prior to cleaning or maintenance. Decontamination should be performed prior to cleaning if radioactive materials, biological agents, or toxic chemicals have been used with a mass spectrometer.

WARNING! Environmental Hazard. Do not dispose of system components in municipal waste. Follow established procedures when disposing of components.

- Always wear clean, powder-free gloves for the cleaning procedures.

- After cleaning the mass spectrometer components, and before reassembling them, put on a new, clean pair of gloves.

- Do not use cleaning supplies other than those specified in this procedure.

- If possible, prepare cleaning solutions just before you begin cleaning.

- Prepare and store all organic solutions and organic-containing solutions in very clean glassware only. Never use plastic bottles. Contaminants can leach from these bottles and further contaminate the mass spectrometer.

- Allow only the center area of the wipe to contact the mass spectrometer surface. Cut edges can leave fibers behind.

> **Tip!** Wrap the wipe around a thermally-bonded polyester swab (poly swab).

Figure 11-1 Example: Folding the Wipe

- To avoid cross-contamination, discard the wipe or swab after it has touched the surface once.

- Larger parts of the vacuum interface, such as the curtain plate, might require several cleanings, using multiple wipes.

- To avoid contaminating the cleaning solution, pour the solution on the wipe or swab.

- Only dampen the wipe or swab slightly when applying water or cleaning solution. Water, more often than organic solvents, might cause the wipe to deteriorate, leaving residue on the mass spectrometer.

- Do not rub the wipe across the aperture. Wipe around the aperture to prevent fibers from the wipes from entering the mass spectrometer.

- Do not insert the brush into the aperture on the curtain plate or orifice plate.

Prepare the Mass Spectrometer

The following warning applies to all procedures in this section:

> ⚠️ **WARNING! Hot Surface Hazard. Let the ion source cool for at least 30 minutes before starting any maintenance procedures. Surfaces of the ion source and the vacuum interface components become hot during operation.**

> **Note:** Mass spectrometers with a NanoSpray® ion source might require a full cleaning for best results. Contact an FSE.

1. Deactivate the hardware profile. Refer to the *System User Guide*.

2. Remove the ion source. Refer to the ion source *Operator Guide*.

CAUTION: Potential System Damage. Do not drop anything into the source drain when the ion source is removed.

When the ion source is not in use, store it to protect it from damage and to maintain operating integrity.

Figure 11-2 Source Drain on the Vacuum Interface
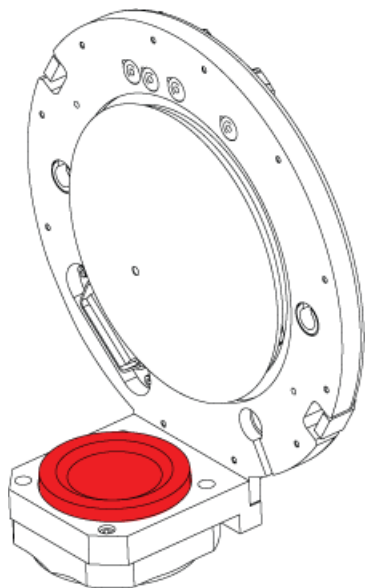
Clean the Curtain Plate

CAUTION: Potential System Damage. Do not rest the curtain plate or orifice plate on the aperture tip. Make sure that the conical side of the curtain plate faces up.

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

Figure 11-3 Curtain Plate Removal
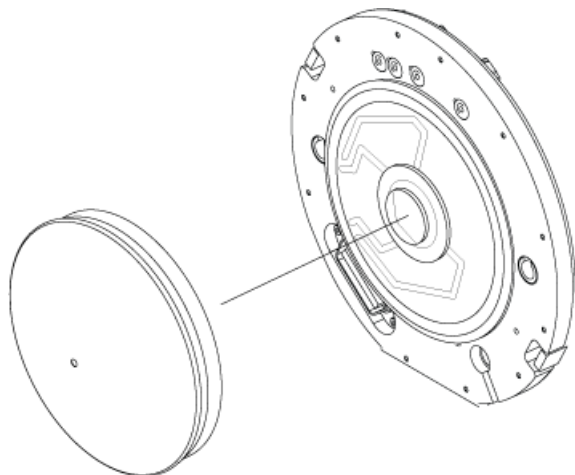
CAUTION: Potential System Damage. Do not insert a wire or metal brush into the aperture on the curtain plate, orifice plate, or interface heater to avoid damaging the aperture.

2. Dampen a lint-free wipe with pure water and then clean both sides of the curtain plate. Use multiple wipes, as required.

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

When cleaning the standard orifice plate with the removable interface heater, do not remove the interface heater. Surface cleaning of the interface heater is adequate for routine cleaning.

CAUTION: Potential System Damage. Do not insert a wire or metal brush into the aperture on the curtain plate, orifice plate, or interface heater to avoid damaging the aperture.

Put the Mass Spectrometer Back in Service

1. Install the curtain plate on the mass spectrometer.

2. Install the ion source on the mass spectrometer. Remember to tighten the ion source by turning the source latches down into the locking position.

3. Activate the hardware profile.

Empty the Source Exhaust Drain Bottle

Empty the source exhaust drain bottle before it becomes full.

> **WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Deposit hazardous materials in appropriately labeled waste containers. Potential risk of personal injury if proper procedures for handling and disposing of hazardous materials are not followed.**

1. Loosen the clamps connecting the hoses to the cap of the source exhaust drain bottle.

2. Disconnect the hoses from the cap.

3. If applicable, lift the drain bottle out of the holder.

4. Remove the drain bottle from the cap.

5. Empty the drain bottle and then dispose of the waste.

6. Install the cap on the bottle and put the bottle in the holder.

7. Attach the hoses to the cap and secure them tightly with clamps.

Figure 11-4 Source Exhaust Drain Bottle
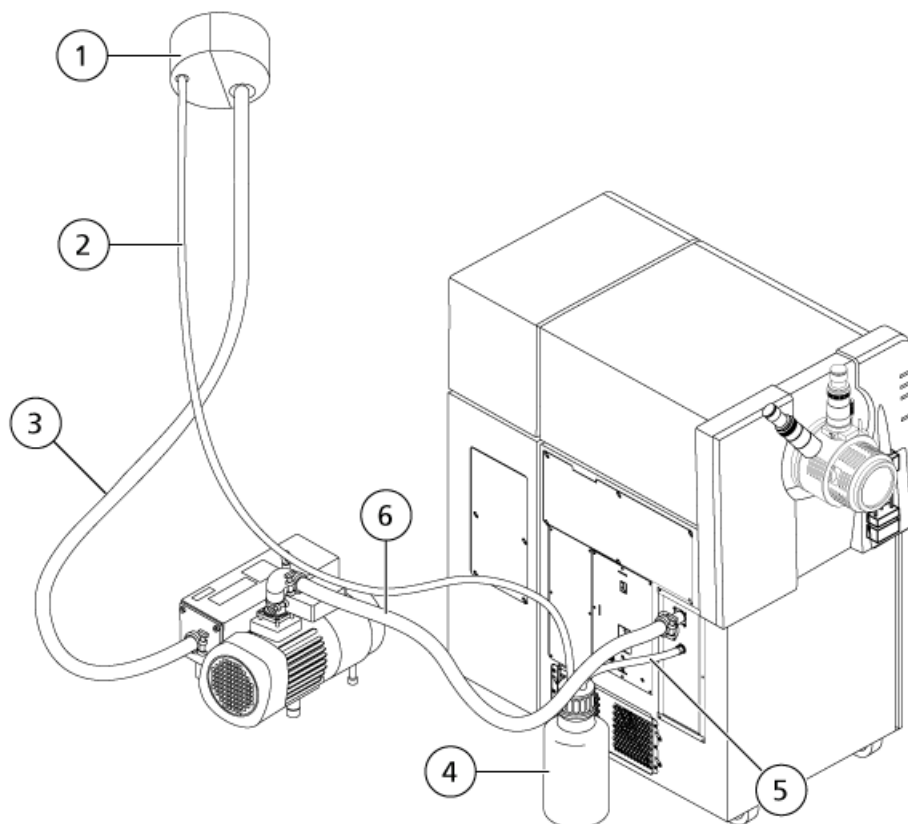
Item	Description
1	Connection to vent
2	Source exhaust drain tubing: 2.5 cm (1.0 inch) inside diameter (i.d.)
3	Roughing pump exhaust hose: 3.2 cm (1.25 inch) i.d.
4	Source exhaust drain bottle (In this drawing, the capped drain bottle is shown at the back of the mass spectrometer to make connection points visible. The drain bottle may be located at the side of the mass spectrometer in the drain bottle holder. Make sure that the bottle is secured to prevent spillage.)
5	Connection to mass spectrometer: 1.6 cm (0.625 inch) i.d.
6	Roughing pump vacuum inlet hose

Storage and Handling

WARNING! Environmental Hazard. Do not dispose of system components in municipal waste. Follow established procedures when disposing of components.

If the mass spectrometer needs to be stored for a long time or prepared for shipping, then contact an AB SCIEX FSE for decommissioning information. To disconnect power from the mass spectrometer, remove the mains supply connector from the AC mains supply.

Note: The system must be transported and stored between −30°C to +60°C (-22°F to 140°F). Store the system below 2000 m (6562 ft) above sea level.

Troubleshooting 12

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

Table 12-1 System Issues

Symptom	Possible Cause	Corrective Action
Sensitivity loss	Instrument or ion source requires tuning and optimizing	Refer to *Operating Instructions — Tune and Calibrate on page 47*. Analyst® TF software Help system
	Dirty curtain plate	Refer to *Clean the Curtain Plate on page 94*.
	Dirty orifice plate	Refer to *Clean the Front of the Orifice Plate on page 95*.
	Dirty QJet® ion guide, skimmer, Q0 or IQ0	Contact an FSE or the local QMP.
Frequent or extreme contamination of the QJet ion guide	Curtain Gas™ flow rate (CUR) is too low.	Verify the setting for the CUR parameter, and increase it, if applicable.
Low vacuum pressure	Low roughing pump oil level.	Check the roughing pump oil level, and add oil if required. Contact an FSE or the local QMP.

For sales, technical assistance or service, contact an 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® 4600 system. For information about tuning solutions, refer to *Operating Instructions — Tune and Calibrate on page 47*.

Table A-1 Q1 PPG Positive Calibration Ions

Masses					
59.04914	233.17472	442.33740	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 and ESI 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-octafluoropentoxy) phosphazine	1521.97148

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

MSMS (Clomipramine)	Masses
C_3H_8N	58.0651
$C_5H_{12}N$	86.0964
$C_{16}H_{14}N$	220.1121
$C_{14}H_{10}NCl$	227.0496
$C_{17}H_{17}N$	235.1356
$C_{15}H_{13}NCl$	242.0731
$C_{17}H_{17}ClN$	270.1044
$C_{19}H_{23}ClN_2$	315.16225

Table A-5 APCI Negative Calibration Solution and ESI 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 and ESI Negative Calibration Solution: MSMS (Sulfinpyrazone)

MSMS (Sulfinpyrazone)	Masses
C_6H_5O	93.0344
C_6H_5OS	125.0067
$C_{10}H_8NO$	158.06114

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

MSMS (Sulfinpyrazone)	Masses
$C_{17}H_{13}N_2O_2$	277.0983
$C_{23}H_2ON_2OS_3$	403.11219

Table A-7 APCI Negative Calibration Solution and ESI Negative Calibration Solution: MSMS (Sulfinpyrazone Fragment)

MSMS (Sulfinpyrazone Fragment)	Masses
C_6H_5	77.03967
C_8H_6N	116.0506
C_9H_8N	130.0662
$C_{10}H_8NO$	158.0611
$C_{11}H_8N_2O_2$	200.0591
$C_{15}H_9N_2$	217.0771
$C_{16}H_{13}N_2O$	249.1033
$C_{17}H_{13}N_2O_2$	277.09825

Exact Masses and Chemical Formulas

B

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

Table B-1 PPG Exact Masses (continued)

n	Exact Mass (M)	$(M + NH_4)^+$	MSMS Fragments	$(M + NH_4)^{2+}$	$(M + COOH)^-$
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

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

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

Toolbar Icons C

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

Table C-1 Tool Bar Icons

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

Table C-2 Acquisition Method Editor Icons

Icon	Name	Description
	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.
	Syringe Pump	Opens the **Syringe Pump Properties** tab.
	Column Oven	Opens the **Column Oven Properties** tab.
	Valve	Opens the **Valve Properties** tab.
	DAD	Opens the **DAD Method Editor**. Refer to *Generate DAD Data on page 83*.
	ADC	Opens the **ADC Properties** tab. Refer to *Show ADC Data on page 76*.

Table C-3 Acquire Mode Icons

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

Table C-3 Acquire Mode Icons (continued)

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

Table C-4 Tune and Calibrate Mode Icons

Icon	Name	Description
	Calibrate from spectrum	Opens the **Mass Calibration Option** dialog and use the active spectrum to calibrate the mass spectrometer.
	Manual Tune	Opens the **Manual Tune Editor**.
	Instrument Optimization	Verifies the instrument performance, adjusts the mass calibration, or adjusts mass spectrometer settings.
	View Queue	Views the sample queue.
	Instrument Queue	Views a remote instrument.
	Status for Remote Instrument	Views the status of a remote instrument.
	Reserve Instrument for Tuning	Reserves the instrument for tuning and calibrating.
	Purge Modifier	Click to purge or clear modifier from the modifier pump.

Table C-5 Explore Quick Reference: Chromatograms and Spectrum

Icon	Name	Description
	Open Data File	Opens files.
	Show Next Sample	Goes to the next sample.
	Show Previous Sample	Goes to the previous sample.
	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.
	Show Base Peak Chromatogram	Generates a BPC.
	Show Spectrum	Generates a spectrum from a TIC.
	Copy Graph to new Window	Copies the active graph to a new window.
	Baseline Subtract	Opens the **Baseline Subtract** dialog.
	Threshold	Adjusts the threshold.
	Noise Filter	Shows the **Noise Filter Options** dialog, which can be used define the minimum width of a peak. Signals below this minimum width are regarded as noise.
	Show ADC	Shows ADC data.
	Show File Info	Shows the experimental conditions used to collect the data.
	Add arrows	Adds arrows to the x-axis of the active graph.

Table C-5 Explore Quick Reference: Chromatograms and Spectrum (continued)

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

Table C-6 Results Table Icons

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

Revision History

Document Number	Reason for Change	Date
D5033332 A	First release of document.	November 2013
RUO-IDV-05-1192-A	Applied new template. Updated for Analyst$^®$ TF 1.7. Updated screen shots for Windows 7. Added support for the SWATH^{TM} acquisition feature.	July 2014

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