

**Agilent G1978B
Multimode Source for
6500 Series Q-TOF
LC/MS**

Set-Up Guide



Agilent Technologies

Notices

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WARNING

A **WARNING** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a **WARNING** notice until the indicated conditions are fully understood and met.

In This Guide

This guide explains how to install, maintain and troubleshoot your multimode ion source.

1 Installation

This chapter tells you how to install the multimode source.

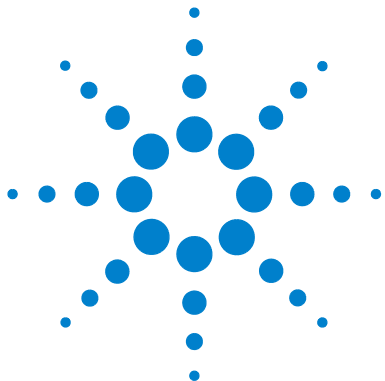
2 Set-Up

This chapter describes basic operation and maintenance for the multimode source.

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This chapter contains instructions to install the multimode source on a 6510 Series Q-TOF LC/MS system, and also to remove and replace the source.



1 Installation

Step 1. Prepare to install

Step 1. Prepare to install

The Multimode Enablement Kit, G1978-60451, is shipped with the multimode source. This kit needs to be installed before the multimode source is used.

Note that the multimode source and its accessories are to be installed by an Agilent Customer Engineer.

1 Check that the Multimode Enablement Kit contains the following parts:

- Multimode Bd HV Cable, p/n G1960-60858
- Multimode HV PCA, p/n G1960-61015
- Multimode Bd Power/Data Cable, p/n G1960-60873



Figure 1 From left to right: G1960-60858, G1960-61015 and G1960-60873

2 Install the APCI Enablement Kit, G1947-60451, which is shipped with the multimode source.

The APCI Enablement kit contains the following parts:

- Fast APCI HV Supply, p/n G1946-80058
- Valve BD-APCI Supply Cable, p/n G1960-60802
- Valve BD-APCI Needle Interlock Cable, p/n G1960-60856

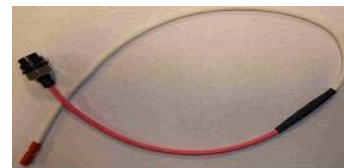


Figure 2 From left to right: G1946-80058, G1960-60802 and G1960-60856

Step 2. Install the HV control PCA and cables

- 1 Turn off the system power and remove the system power cord.

The power cord should be kept intact if the vacuum control switch box is used. The switch box is intended to keep the vacuum on while a service engineer works on the electronics. The switch box is for service engineer use only.

- 2 Remove the CDS cover, top, side, front, and the Aux Module cover.
- 3 Disconnect the ribbon cable that connects the valve PCA to the Vcap/Vchamber power supply. Then disconnect the Vcap and Vchamber cable from the power supply.

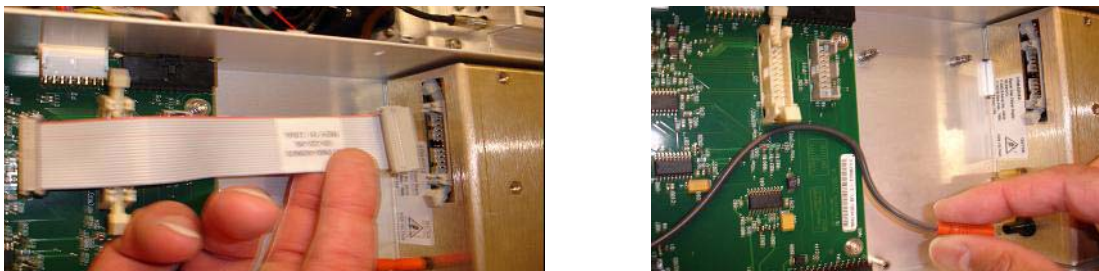


Figure 3 Disconnecting the Vcap/Vchamber power supply from the valve PCA (left) and the Vcap/Vchamber.

- 4 Place the multimode HV power supply PCA in the slot between the valve PCA and the Vcap/Vchamber power supply. Secure the board by pressing it down into its slot and then attach it with two screws.
- 5 Connect the short gray cable from the valve PCA to the multimode HV power supply.



Figure 4 Connecting the valve PCA to the multimode HV power supply.

1 Installation

Step 2. Install the HV control PCA and cables

- 6 Install the APCI HV power supply. The APCI HV power supply is located at the end of the AUX Module.
- 7 Connect ribbon cable between the valve PCA and Vcap/Vchamber power supply.



Figure 5 Connecting the valve PCA to the Vcap/Vchamber power supply.

- 8 Connect the Vcap and Vchamber cables to the Vcap/Vchamber power supply.



Figure 6 Connecting the Vcap and Vchamber cables to the power supply.

- 9 Connect the long ribbon cable, p/n G1960-60802, from the APCI HV power supply to the valve PCA.

Step 2. Install the HV control PCA and cables



Figure 7 Connecting the APCI HV power supply to the valve PCA.

10 Insert one end of the APCI Needle Interlock cable, G1960-60856, through the slot at the front of the system and then plug it to the APCI HV connector. Attach the other end to the chassis with the o-ring and the nut (see [Figure 8](#)).

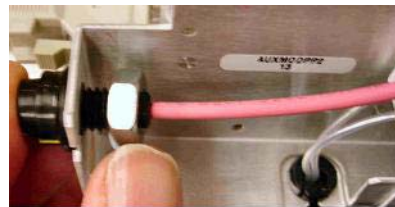


Figure 8 Connecting the APCI HV to the chassis.

11 Insert the cable, G1960-60858, to the top slot and attach it to the chassis. Plug the other two ends into the multimode HV PCA.



Figure 9 Connecting the HV PCA to the chassis.

12 Close the AUX Module cover and reconnect all cables.

13 Install the multimode source onto the system and connect all connectors.

1 Installation

Step 2. Install the HV control PCA and cables

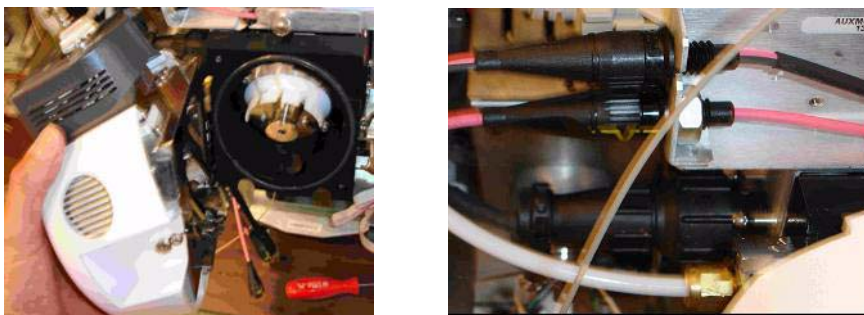


Figure 10 Installing the multimode source (left) and connecting all connectors.

14 Put back the side, top, front and CDS cover.

15 Plug the system power cord back on and turn the front switch on.

The pump down process will start.

16 Start the MassHunter Workstation program and verify that the software recognizes the source.

17 Set the **Context** view to **Tune**, and in **Manual Tune**, verify that the system can generate the proper tune peaks.

To remove the multimode source

Do the following steps to remove the multimode source.

- 1 Turn off the multimode source temperatures and flows:
 - a Change the **Context** view to **Acquisition**.
 - b Click the **MS Q-TOF** tab.
 - c Turn off all voltages and temperatures in the **Source** tab.
 - d Wait approximately 20 minutes for the source to cool down.

WARNING

Do not touch the multimode source or the capillary cap. They may be very hot. Let the parts cool before you handle them.

WARNING

Never touch the source surfaces, especially when you analyze toxic substances or when you use toxic solvents. The source has several sharp pieces which can pierce your skin including the APCI corona needle, vaporizer sensor and counter current electrode.

WARNING

Do not insert fingers or tools through the openings on the multimode chamber. When in use, the capillary and capillary cap are at high voltages up to 4 kV.

- 2 Wait approximately 20 minutes or until the source is cool.
- 3 Open the CDS door at the front of the MS to access the cables.
- 4 Disconnect the ESI high voltage charging electrode cable.
- 5 Disconnect the APCI Needle Interlock, and multimode HV cable.
- 6 Unscrew the nebulizer gas line from the nebulizer.
- 7 Unscrew the LC sample tubing from the nebulizer.
- 8 Open the latch on the source and open the source.
- 9 Remove the multimode source from the spray chamber mount.
- 10 Place the source shipping cover on the source.

1 Installation

To convert from multimode to ESI or APCI

To convert from multimode to ESI or APCI

WARNING

Never touch the source surfaces, especially when you analyze toxic substances or when you use toxic solvents. The source has several sharp pieces which can pierce your skin including the APCI corona needle, vaporizer sensor and counter current electrode.

- 1 Unscrew and remove the multimode spray shield with the field shaping electrodes.
- 2 Install the new source and the standard spray shield, making sure that the hole in the spray shield is in the 12 o'clock position.
- 3 For an APCI ion source, connect the vaporizer heater cable and the APCI high voltage cable.
- 4 For all sources, reconnect the nebulizer gas line tubing and the LC/MS sample tubing.

To convert from ESI or APCI to the multimode source

CAUTION

If you are installing this source on this instrument for the first time, follow the steps in “Installation” on page 7.

- 1 Turn off the multimode source temperatures and flows:
 - a Change the **Context** view to **Acquisition**.
 - b Click the **MS Q-TOF** tab.
 - c Turn off all voltages and temperatures in the **Source** tab.
 - d Wait approximately 20 minutes for the source to cool down.
- 2 Wait for the source to cool (until temperatures are at least below 100°C).
- 3 Disconnect the nebulizer gas tubing from the currently installed ion source.
- 4 Disconnect the LC/MS sample inlet tubing.
- 5 If the APCI source is installed, remove the APCI vaporizer heater cable and APCI high voltage cable.
- 6 Remove the currently installed ion source.
- 7 Unscrew and remove the spray shield. See [Figure 11](#).

WARNING

Do not touch the multimode source or the capillary cap. They may be very hot. Let the parts cool before you handle them.

WARNING

Do not insert fingers or tools through the openings on the multimode chamber. When in use, the capillary and capillary cap are at high voltages up to 4 kV.

1 Installation

To convert from ESI or APCI to the multimode source

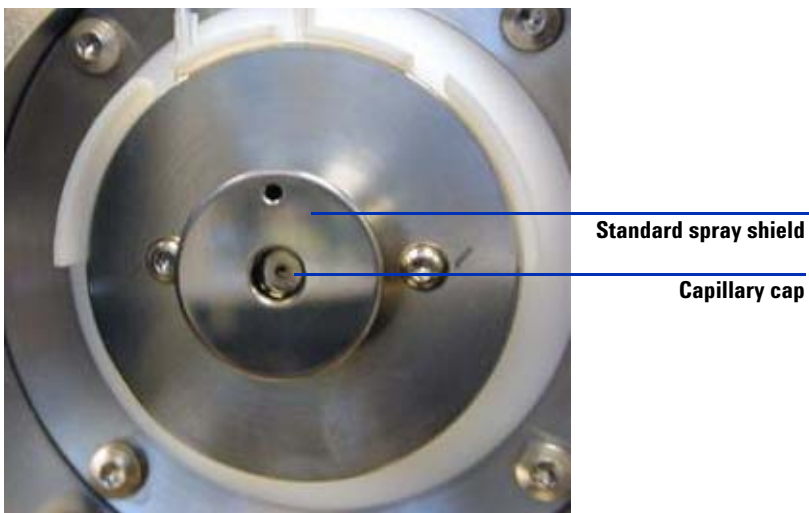


Figure 11 Standard spray shield and capillary cap for ESI or APCI

- 8 Remove the capillary cap. If needed, moisten a clean cloth with isopropyl alcohol and wipe the capillary cap. See [Figure 12](#).

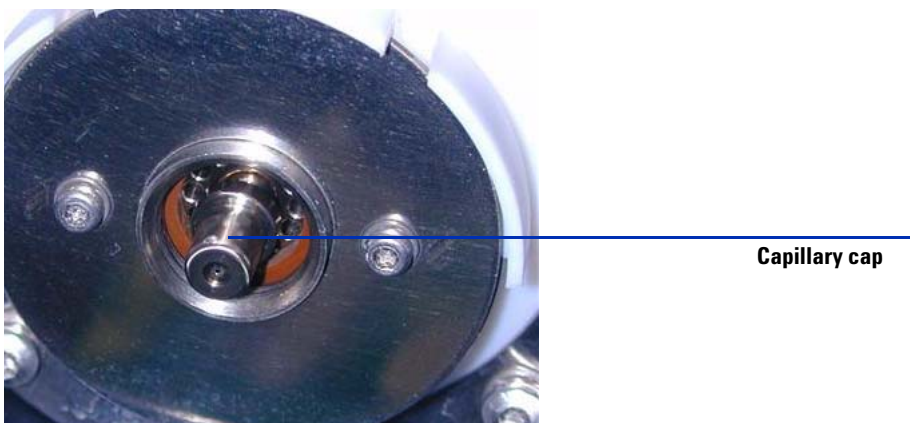


Figure 12 Spray shield removed.

- 9 Place the capillary cap back on the capillary.
- 10 Install the new spray shield with field shaping electrodes. See [Figure 13](#).

To convert from ESI or APCI to the multimode source



Figure 13 Multimode spray shield

11 Screw the multimode spray shield into the holder for the spray shield. See [Figure 14](#).

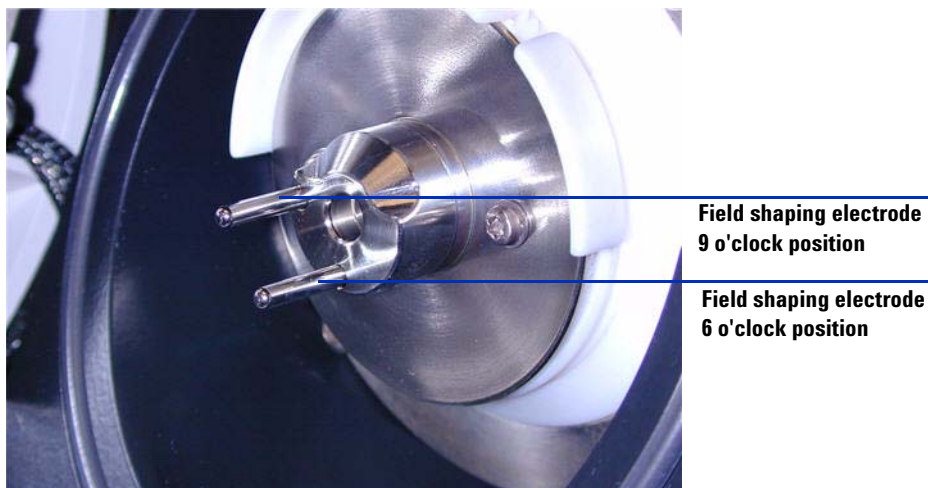


Figure 14 Multimode spray shield installed

NOTE

The field shaping electrodes should be in the nine o'clock and the six o'clock position. Loosen the end plate screws on each side to adjust the field shaping electrodes position.

12 Remove the shipping cover from the multimode source spray chamber.

1 Installation

To convert from ESI or APCI to the multimode source



Figure 15 Multimode Spray Chamber

13 Install the spray chamber on the spray chamber mount.

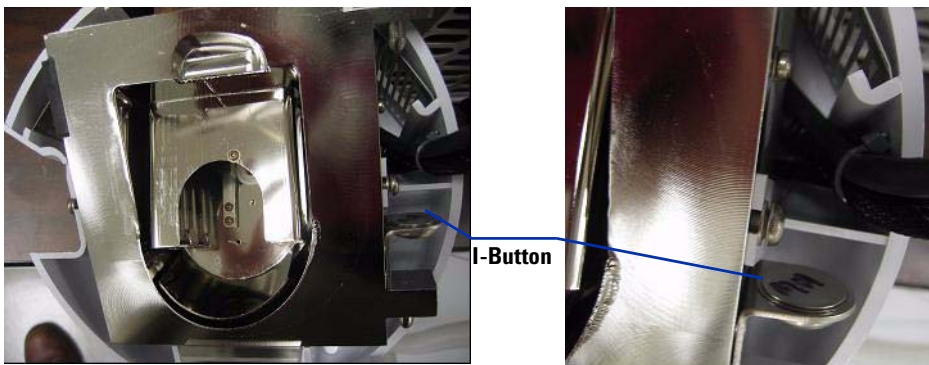


Figure 16 Multimode source with I-Button

14 Install the nebulizer on the multimode source spray chamber.

To convert from ESI or APCI to the multimode source



Figure 17 No nebulizer on top of the multimode source

15 Connect the 1/8-inch nebulizer gas tubing from the LC/MS mainframe to the nebulizer gas fitting. See [Figure 18](#).

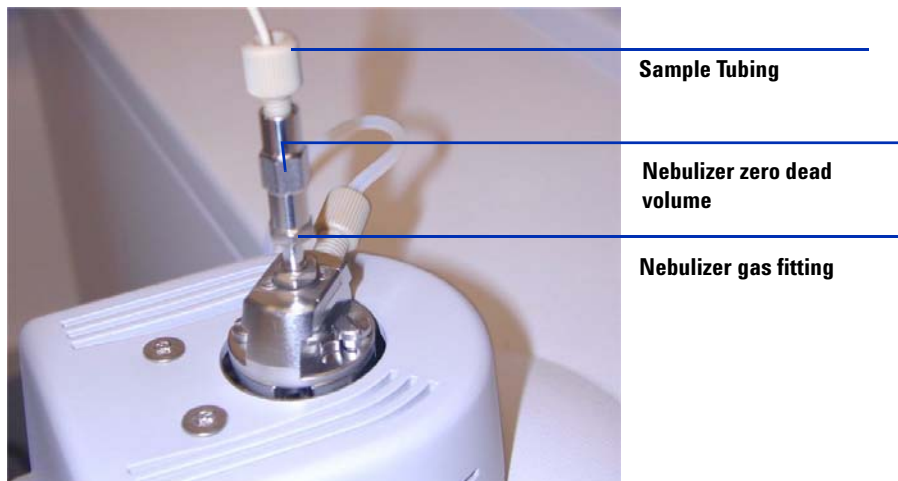


Figure 18 Nebulizer with gas tubing connected

1 Installation

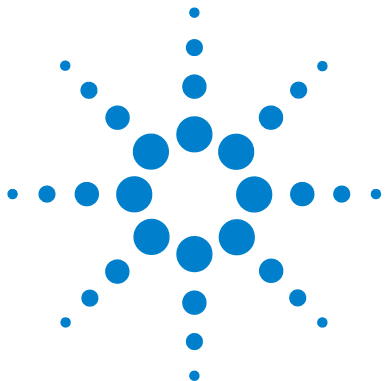
To convert from ESI or APCI to the multimode source

16 Connect the LC/MS sample tubing to the LC/MS diverter valve inlet filter.

WARNING

The LC/MS Liquid Chromatograph diverter valve is an integral part of the G1978B safety system. The LC mobile phase flow must always be connected to the diverter valve inlet filter. Never bypass the diverter valve and connect directly to the nebulizer. If the diverter valve is used in a manner not specified by Agilent Technologies, the protections provided by the diverter valve may be impaired.

17 If you are installing the multimode source for the first time, follow the steps in “[Step 2. Install the HV control PCA and cables](#)” on page 9.



2 Set-Up

To set up a method to use the multimode source [22](#)

To check tuning with the multimode source [25](#)

This chapter describes the tasks that you need to operate and maintain the multimode source.



To set up a method to use the multimode source

WARNING

The LC/MS diverter valve is an integral part of the G1978B safety system. The LC mobile phase flow must always be connected to the diverter valve inlet filter. Never bypass the diverter valve and connect directly to the nebulizer. If the diverter valve is used in a manner not specified by Agilent Technologies, the protections provided by the diverter valve may be impaired and the system may catch fire.

- 1 In the MassHunter software, change the **Context** to **Acquisition**.
- 2 In the MS Q-TOF tab, set **Ion source** to **Multimode** (see [Figure 19](#) on page 23).
- 3 In the **Sources** tab, choose an ionization mode from the **Ion Modes (Seg)** list. You may set the ionization mode to one of the following:
 - ESI
 - APCI
 - Mixed

The Ion Mode selection Mixed will specify a method for simultaneous ESI and APCI operation.

Note that the Ionization Modes selection is only visible if **Ion source** is set to **Multimode**.

- 4 In the **Source** tab, set the desired source conditions. See “Guidelines” in the *Agilent G1978A/B Multimode Source Maintenance Guide* for suggested source conditions for the multimode source for the different ionization modes.
- 5 Make any other changes that are necessary for your method.
- 6 Save the method.

To set up a method to use the multimode source

Multimode (Seg)		MS TOF (Expt)			
Gas Temp	<input type="text" value="325"/> °C	<input type="text" value="324"/> °C	Fragmentor	<input type="text" value="175"/> V	
Vaporizer	<input type="text" value="200"/> °C	<input type="text" value="198"/> °C	Skimmer	<input type="text" value="65"/> V	
Drying Gas	<input type="text" value="5"/> l/min	<input type="text" value="5.0"/> l/min	OCT 1 RF Vpp	<input type="text" value="750"/> V	
Nebulizer	<input type="text" value="30"/> psig	<input type="text" value="30"/> psig			
Multimode (Expt)		Ionization Modes (seg)			
VCap	<input type="text" value="2000"/> V	Capillary	<input type="text" value="0.141"/> uA	<input type="text" value="Mixed"/>	
Corona+	<input type="text" value="4"/> uA	Corona	<input type="text" value="110"/> V		
		Chamber	<input type="text" value="3.61"/> uA	Charging Voltage	<input type="text" value="2000"/> V

Figure 19 Multimode acquisition settings

2 Set-Up

To open the multimode source

To open the multimode source

Open the multimode source to access the end cap and the capillary cap for cleaning and inspection.

WARNING

Do not touch the multimode source or the capillary cap. They may be very hot. Let the parts cool before you handle them.

WARNING

Never touch the source surfaces, especially when you analyze toxic substances or when you use toxic solvents. The source has several sharp pieces which can pierce your skin including the APCI corona needle, vaporizer sensor and counter current electrode.

WARNING

Do not insert fingers or tools through the openings on the multimode chamber. When in use, the capillary and capillary cap are at high voltages up to 4 kV.

- 1 Turn off the multimode source temperatures and flows:
 - a Change the **Context** view to **Acquisition**.
 - b Click the **MS Q-TOF** tab.
 - c Put the instrument in Standby mode.
 - d Wait approximately 20 minutes for the source to cool down.
- 2 Open the spray chamber cover by pulling the latch.

The high voltage automatically turns off when the chamber door is opened so that no high voltages are present within the chamber.
- 3 Check that the vaporizer temperature sensor is straight and extends 15 mm from back of chamber.
- 4 Check that the separator is aligned vertically.
- 5 Check that the APCI corona needle is in and extends approximately 3 mm from the corona guide.
- 6 Check that the source is clean.

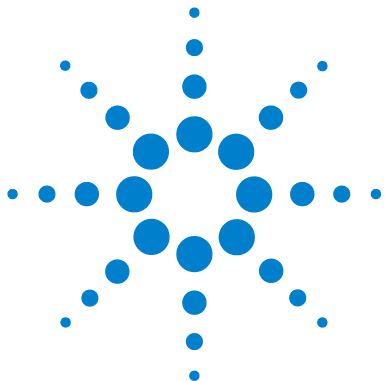
To check tuning with the multimode source

Autotune is currently only available for the G3251B Dual Electrospray source. However, mass calibrations and manual optimization of mass resolution can be done using the G1978B source. To calibrate mass accuracy, do these steps.

- 1 Run an Autotune with the G3251B Dual Electrospray source installed.
- 2 Remove the G3251B Dual Electrospray source and install the G1978B multimode source.
- 3 Uninstall the Electrospray Calibrant Bottle B from the instrument. Cap the calibrant bottle with one of the supplied bottle caps (p/n 9300-2575).
- 4 Rinse one of the extra calibrant bottles (p/n 9300-2576) that was supplied as part of the Q-TOF Shipping Kit (p/n G2581-60170) with high purity acetonitrile. Pour the contents of the MMI-L Low Concentration Tuning Mix (p/n G1969-85020) into the rinsed calibrant bottle. Install the calibrant bottle on the Q-TOF mainframe in the bottle B location.
- 5 Set the **Context** view to **Tune** in the MassHunter Workstation program.
 - a Load the most recently used autotune file. Change the source type Multimode.
 - b Click the **Mass TOF Calibration** tab and do a mass calibration.
 - c Adjust the lens voltages and other tune parameters as required to optimize the mass resolution of the instrument. If changes are made to the Mid Mirror, a mass calibration will have to be done again.
 - d Verify that you have sufficient abundance for the tune peaks, that the tune peak at 2122 has greater than 10,000 resolution, and that all mass assignments are with 2 ppm after a mass calibration has been done.
- 6 Save the tune file and close the tune context.

2 **Set-Up**

To check tuning with the multimode source



3 Installation Verification

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In this chapter, you create and run methods to check out the system.



3 Installation Verification

Step 1. Auto tune

Step 1. Auto tune

This step applies to MassHunter Workstation Software - Acquisition for TOF/Q-TOF revision B.01.03 or higher.

- Run autotune with the G1969-85000 ESI-L Low Concentration Tuning Mix. There are no tune specific methods.
 - Tune the 6220 in 2GHz extended dynamic range for both positive and negative.
 - Tune the 6210 in Standard (3200 m/z) mode 1GHz.

Step 2. Set up method names and parameters

- 1 Create six methods from Default.m for the multimode ESI + APCI LC Demo Sample (p/n G1978-85000), using these method names:
 - MMCHECKTOF_EI_POS.m
 - MMCHECKTOF_EI_NEG.m
 - MMCHECKTOF_CI_POS.m
 - MMCHECKTOF_CI_NEG.m
 - MMCHECKTOF_MX_EI_POS_CI_POS.m
 - MMCHECKTOF_MX_EI_NEG_CI_NEG.m
- 2 Use these parameters for each method:

Table 1

Parameter/Tab	Value
Column	Cartridge Hardware, Rapid Resolution, (p/n 820555-901) SB-C18 Rapid Res 3.5um,2.1x30mm, (p/n 873700-902)
Sample Tab	Name: MM Demo Sample Position 1 Run Type: Standard Acquisition only Path D:\PE Sciex Data\Projects\Data
ALS Tab	Standard Injection 1µL Bin Pump Tab: Flow .4mL/min Stop time: 3 min Solvent A 100.0 % (65%MeOH:35%H ₂ O + 0.2%acetic acid) Run time same as pump
Data files (data files for B.01.03 or greater use the suffix .d)	Data File: MM_ESI_POS.wiff Data File: MM_ESI_NEG.wiff Data File: MM_APCI_POS.wiff Data File: MM_APCI_NEG.wiff Data File: MM_ESI_APCI_POS.wiff Data File: MM_ESI_APCI_NEG.wiff

3 Installation Verification

Step 3. Create MMCHECKTOF_EI_POS.m

Step 3. Create MMCHECKTOF_EI_POS.m

The graphics in this topic differ slightly for MassHunter B.01.03 or higher. For B.01.03, access these tabs from the Acquisition view.

- Set the parameters for MMCHECKTOF_EI_POS.m:

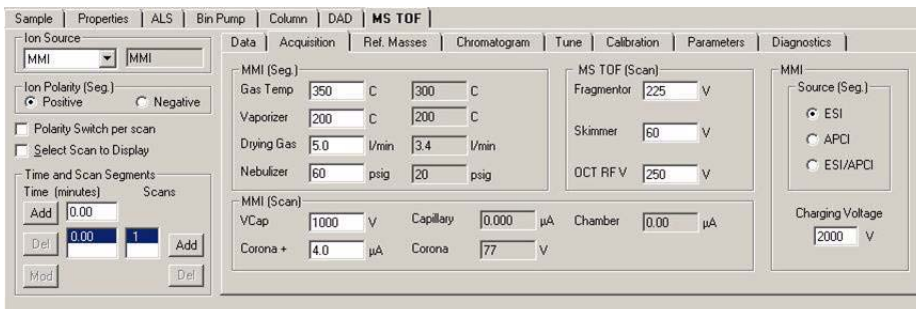


Figure 20 Acquisition parameters

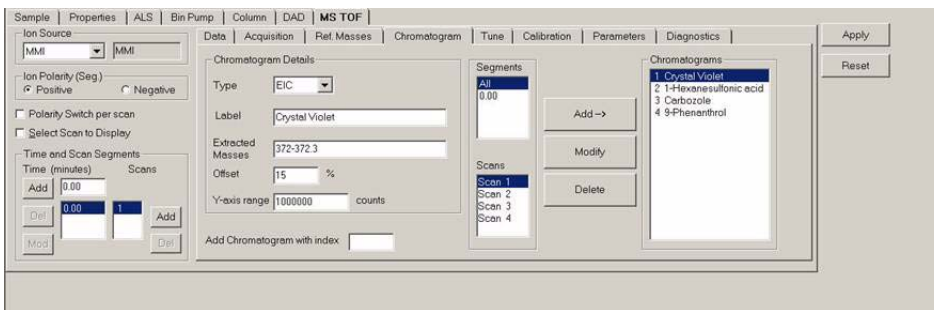


Figure 21 Chromatogram

Ionization Mode	MM-ES	
Polarity	Negative	
1100 Binary Pump 1		
Control		
Column flow	0.400 mL/min	
Stop Time	No Limit	
Post Time	Off	
Solvents		
Solvent A	100.0 % (65%MeOH:35%H ₂ O + 0.2%acetic acid)	
Solvent B	0.0 %	
Pressure Limits		
Minimum Pressure	0 bar	
Maximum Pressure	400 bar	
Spray Chamber		
[MSZones]		
Gas Temp	350 °C	Maximum 350 °C
Vaporizer	200 °C	Maximum 250 °C
Drying Gas	5.0 L/min	Maximum 13.0 L/min
Neb Pres	60 psig	Maximum 60 psig
VCap (Positive)	1000 V	
VCap (Negative)	1000 V	
VCharge (Positive)	2000 V	
VCharge (Negative)	2000 V	
Corona (Positive)	0.0 µA	
Corona (Negative)	0.0 µA	

3 Installation Verification

Step 4. Create MMCHECKTOF_EI_NEG.m

Step 4. Create MMCHECKTOF_EI_NEG.m

- Set the parameters for MMCHECKTOF_EI_NEG.m:

The screenshot shows the MS TOF software interface with the following parameters:

- Ion Source:** MMI
- Ion Polarity (Seg.):** Negative
- Time and Scan Segments:** Time (minutes) = 0.00, Scans = 1
- MMI (Seg.):** Gas Temp = 350 C, Vaporizer = 200 C, Drying Gas = 5.0 l/min, Nebulizer = 60 psig
- MS TOF (Scan):** Fragmentor = 225 V, Skimmer = 60 V, OCT RFV = 250 V
- MMI (Scan):** VCap = 1000 V, Capillary = 0.000 μA, Chamber = 0.00 μA, Corona = 4.0 μA, Corona = 77 V
- Source (Seg.):** ESI
- Charging Voltage:** 2000 V

Figure 22 Acquisition

The screenshot shows the MS TOF software interface with the following details:

- Chromatogram Details:** Type = EIC, Label = 1-Hexanesulfonic acid, Extracted Masses = 165-165.3, Offset = 15 %, Y-axis range = 1000000 counts
- Segments:** All, 0.00
- Scans:** Scan 1, Scan 2, Scan 3, Scan 4
- Chromatograms:** 1 Crystal Violet, 2 1-Hexanesulfonic acid, 3 Carbazole, 4 9-Phenanthrol

Figure 23 Chromatogram

Ionization Mode	MM-ES	
Polarity	Negative	
1100 Binary Pump 1		
Control		
Column flow	0.400 mL/min	
Stop Time	No Limit	
Post Time	Off	
Solvents		
Solvent A	100.0 % (65%MeOH:35%H ₂ O + 0.2%acetic acid)	
Solvent B	0.0 %	
Pressure Limits		
Minimum Pressure	0 bar	
Maximum Pressure	400 bar	
Spray Chamber		
[MSZones]		
Gas Temp	350 °C	Maximum 350 °C
Vaporizer	200 °C	Maximum 250 °C
Drying Gas	5.0 L/min	Maximum 13.0 L/min
Neb Pres	60 psig	Maximum 60 psig
VCap (Positive)	1000 V	
VCap (Negative)	1000 V	
VCharge (Positive)	2000 V	
VCharge (Negative)	2000 V	
Corona (Positive)	0.0 µA	
Corona (Negative)	0.0 µA	

3 Installation Verification

Step 5. Create MMCHECKTOF_CI_POS.m

Step 5. Create MMCHECKTOF_CI_POS.m

- Set the parameters for MMCHECKTOF_CI_POS.m:

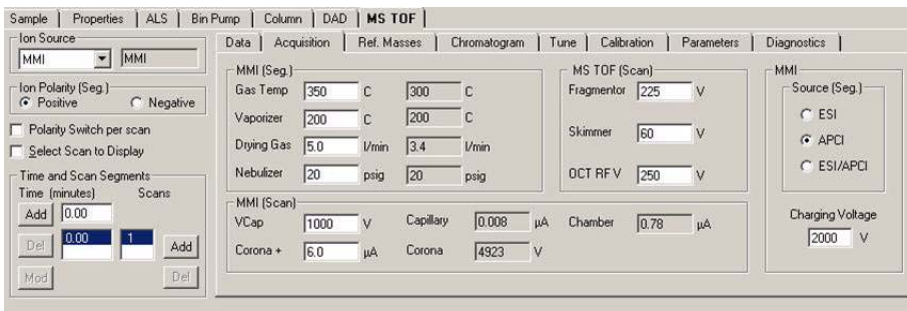


Figure 24 Acquisition

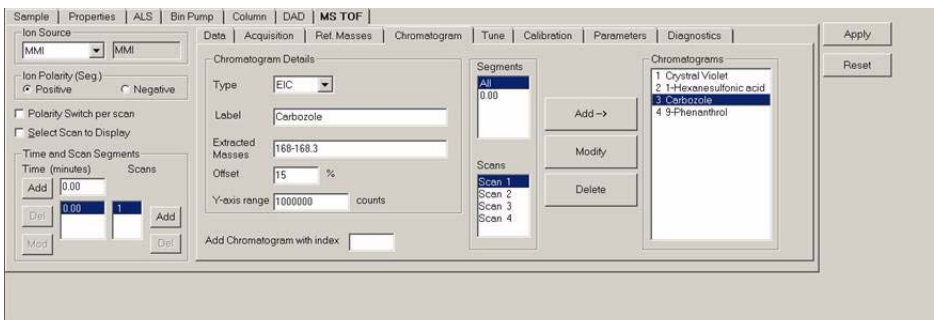


Figure 25 Chromatogram

Step 5. Create MMCHECKTOF_CI_POS.m

Ionization Mode	MM-APCI	
Polarity	Positive	
1100 Binary Pump 1		
Control		
Column flow	0.400 mL/min	
Stop Time	No Limit	
Post Time	Off	
Solvents		
Solvent A	100.0 % (65%MeOH:35%H ₂ O + 0.2%acetic acid)	
Solvent B	0.0 %	
Pressure Limits		
Minimum Pressure	0 bar	
Maximum Pressure	400 bar	
Spray Chamber		
[MSZones]		
Gas Temp	350 °C	Maximum 350 °C
Vaporizer	200 °C	Maximum 250 °C
Drying Gas	5.0 L/min	Maximum 13.0 L/min
Neb Pres	20 psig	Maximum 60 psig
VCap (Positive)	1000 V	
VCap (Negative)	1000 V	
VCharge (Positive)	2000 V	
VCharge (Negative)	2000 V	
Corona (Positive)	6.0 µA	
Corona (Negative)	6.0 µA	

3 Installation Verification

Step 6. Create MMCHECKTOF_CI_NEG.m

Step 6. Create MMCHECKTOF_CI_NEG.m

- Set the parameters for MMCHECKTOF_CI_NEG.m:

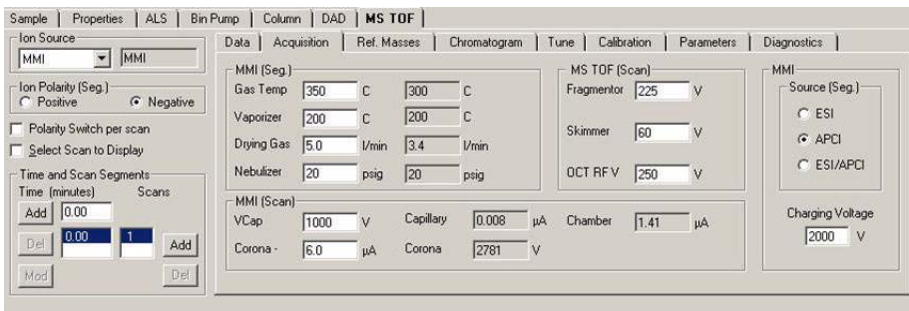


Figure 26 Acquisition

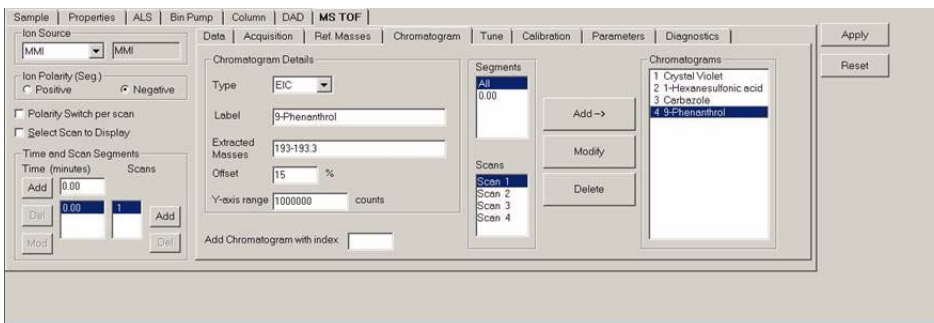


Figure 27 Chromatogram

Step 6. Create MMCHECKTOF_CI_NEG.m

Ionization Mode	MM-APCI	
Polarity	Negative	
1100 Binary Pump 1		
Control		
Column flow	0.400 mL/min	
Stop Time	No Limit	
Post Time	Off	
Solvents		
Solvent A	100.0 % (65%MeOH:35%H ₂ O + 0.2%acetic acid)	
Solvent B	0.0 %	
Pressure Limits		
Minimum Pressure	0 bar	
Maximum Pressure	400 bar	
Spray Chamber		
[MSZones]		
Gas Temp	350 °C	Maximum 350 °C
Vaporizer	200 °C	Maximum 250 °C
Drying Gas	5.0 L/min	Maximum 13.0 L/min
Neb Pres	20 psig	Maximum 60 psig
VCap (Positive)	1000 V	
VCap (Negative)	1000 V	
VCharge (Positive)	2000 V	
VCharge (Negative)	2000 V	
Corona (Positive)	6.0 µA	
Corona (Negative)	6.0 µA	

3 Installation Verification

Step 7. Create MMCHECKTOF_MX_EI POS_CI POS.m

Step 7. Create MMCHECKTOF_MX_EI POS_CI POS.m

- Set the parameters for MMCHECKTOF_MX_EI POS_CI POS.m.

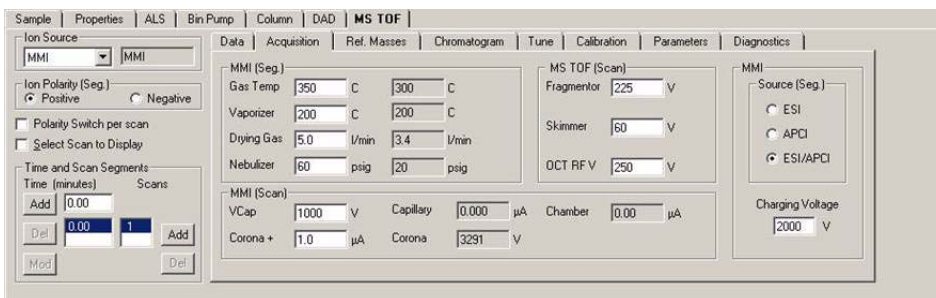


Figure 28 Acquisition

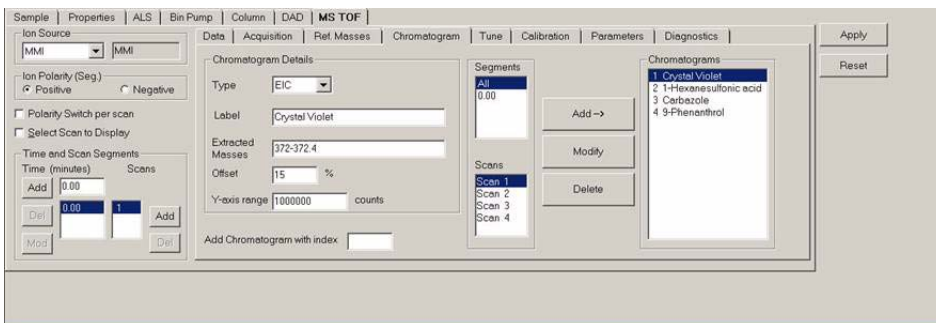


Figure 29 Chromatogram

Step 7. Create MMCHECKTOF_MX_EI POS_CI POS.m

Ionization Mode	MM-ES+APCI	
Polarity	Positive	
1100 Binary Pump 1		
Control		
Column flow	0.400 mL/min	
Stop Time	No Limit	
Post Time	Off	
Solvents		
Solvent A	100.0 % (65%MeOH:35%H ₂ O + 0.2% acetic acid)	
Solvent B	0.0 %	
Pressure Limits		
Minimum Pressure	0 bar	
Maximum Pressure	400 bar	
Spray Chamber		
[MSZones]		
Gas Temp	350 °C	Maximum 350 °C
Vaporizer	200 °C	Maximum 250 °C
Drying Gas	5.0 L/min	Maximum 13.0 L/min
Neb Pres	60 psig	Maximum 60 psig
VCap (Positive)	1000 V	
VCap (Negative)	1000 V	
VCharge (Positive)	2000 V	
VCharge (Negative)	2000 V	
Corona (Positive)	1.0 µA	
Corona (Negative)	1.0 µA	

3 Installation Verification

Step 8. Create MMCHECKTOF_MX_EI NEG_CI NEG.m

Step 8. Create MMCHECKTOF_MX_EI NEG_CI NEG.m

- Set the parameters for MMCHECKTOF_MX_EI NEG_CI NEG.m:

The screenshot shows the MS TOF software interface with the Acquisition tab selected. The Ion Source is set to MMI. Ion Polarity is set to Negative. Parameters for Gas Temp, Vaporizer, Drying Gas, and Nebulizer are visible. MS TOF (Scan) parameters include Fragmentor, Skimmer, and OCT RF V. Charging Voltage is set to 2000 V.

Figure 30 Acquisition

The screenshot shows the MS TOF software interface with the Chromatogram tab selected. Chromatogram Details include Type (EIC), Label (1-Hexanesulfonic acid), Extracted Masses (165-165.3), and Y-axis range (1000000 counts). A list of Chromatograms shows 1 Crystal Violet, 2 1-Hexanesulfonic acid, 3 Carbazole, and 4 9-Phenanthrol. Scans 1, 2, 3, and 4 are listed.

Figure 31 Chromatogram

Ionization Mode	MM-ES+APCI	
Polarity	Negative	
1100 Binary Pump 1		
Control		
Column flow	0.400 mL/min	
Stop Time	No Limit	
Post Time	Off	
Solvents		
Solvent A	100.0 % (65%MeOH:35%H ₂ O + 0.2% acetic acid))	
Solvent B	0.0 %	
Pressure Limits		
Minimum Pressure	0 bar	
Maximum Pressure	400 bar	
Spray Chamber		
[MSZones]		
Gas Temp	350 °C	Maximum 350 °C
Vaporizer	200 °C	Maximum 250 °C
Drying Gas	5.0 L/min	Maximum 13.0 L/min
Neb Pres	60 psig	Maximum 60 psig
VCap (Positive)	1000 V	
VCap (Negative)	1000 V	
VCharge (Positive)	2000 V	
VCharge (Negative)	2000 V	
Corona (Positive)	1.0 µA	
Corona (Negative)	1.0 µA	

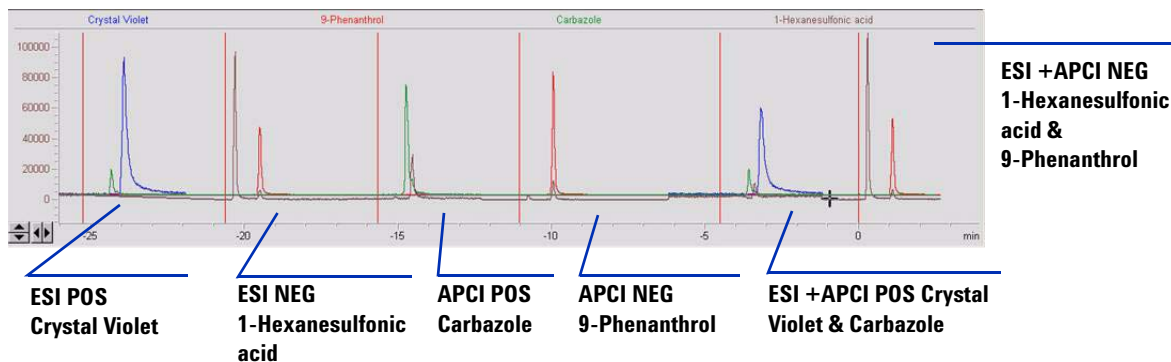
3 Installation Verification

Step 9. Run each of the methods created

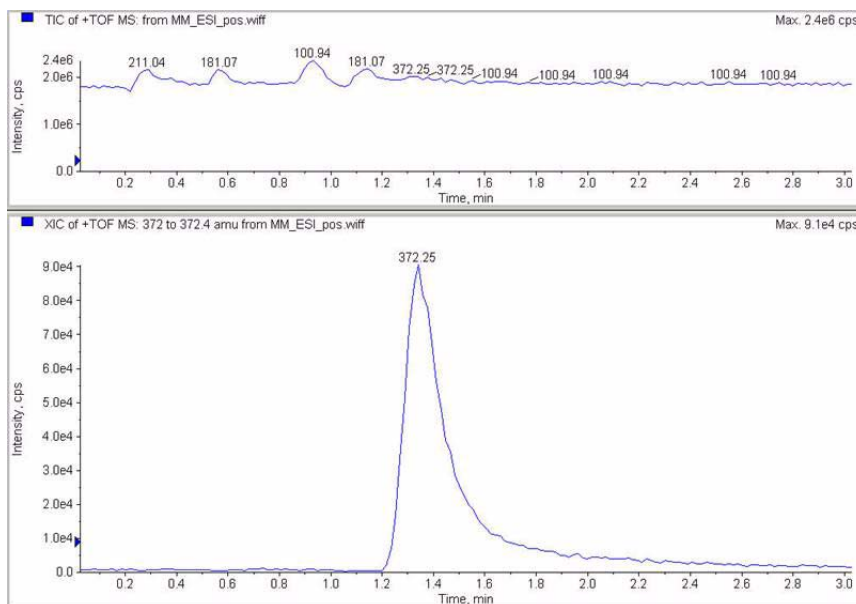
Step 9. Run each of the methods created

- 1 Run each of the methods that you just created.

The real time plot below shows the six runs.

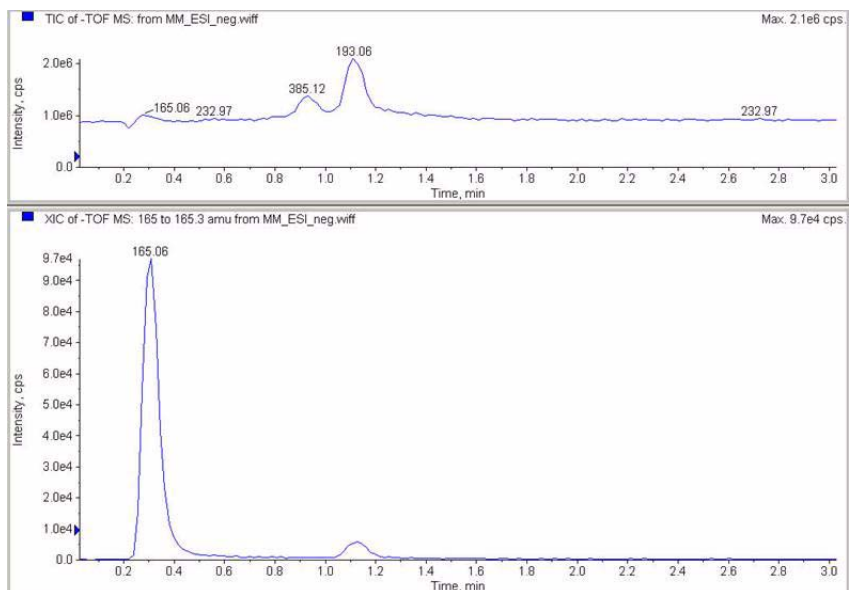


- 2 View the data from Analyst for MM_ESI_pos.wif. Extract Ion 372- 372.4. Record peak height Example: 91,000.



Step 9. Run each of the methods created

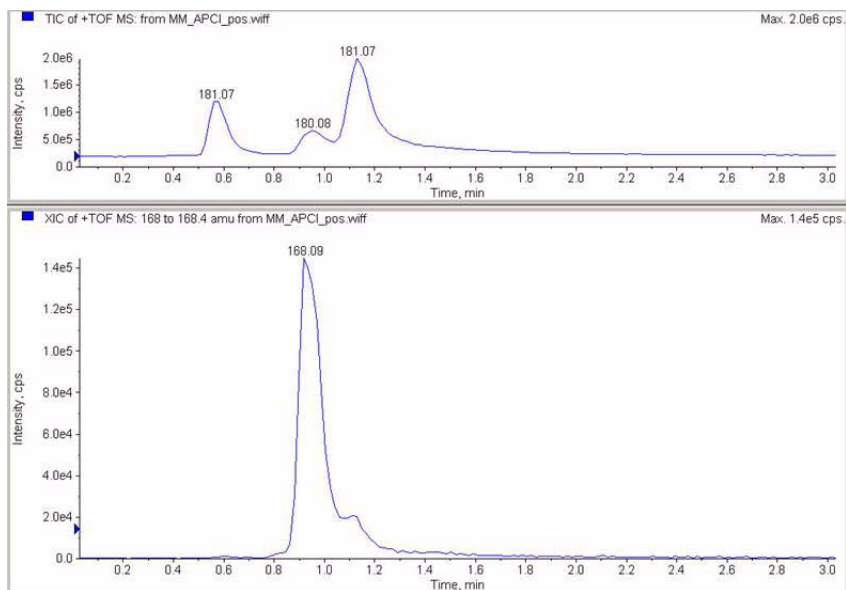
- 3 View the data in the data analysis program for MM_ESI_Neg. Extract Ion 165-165.4. Record the peak height Example 97,000.



3 Installation Verification

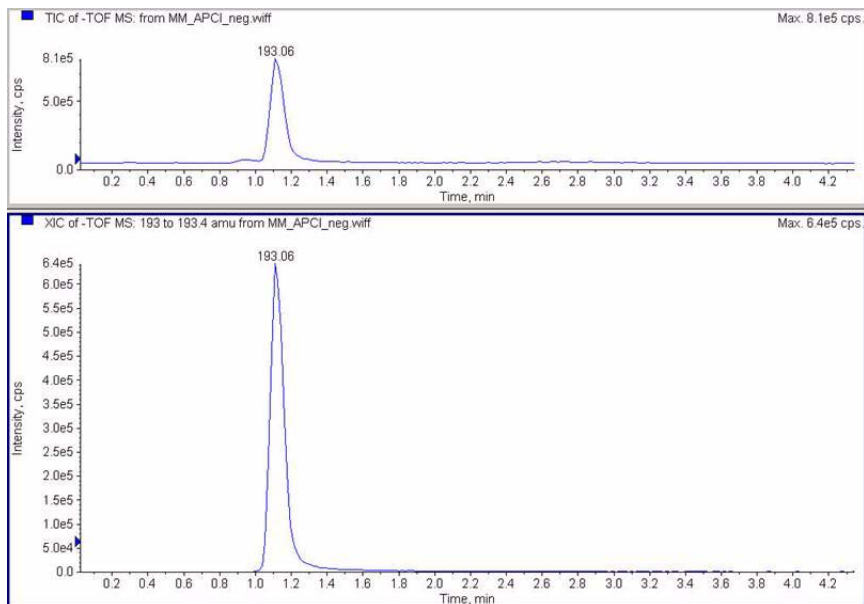
Step 9. Run each of the methods created

- 4 View the data in the data analysis program for MM_APCI_POS. Extract Ion 168-168.4. Record the peak height. Example 140,000.



Step 9. Run each of the methods created

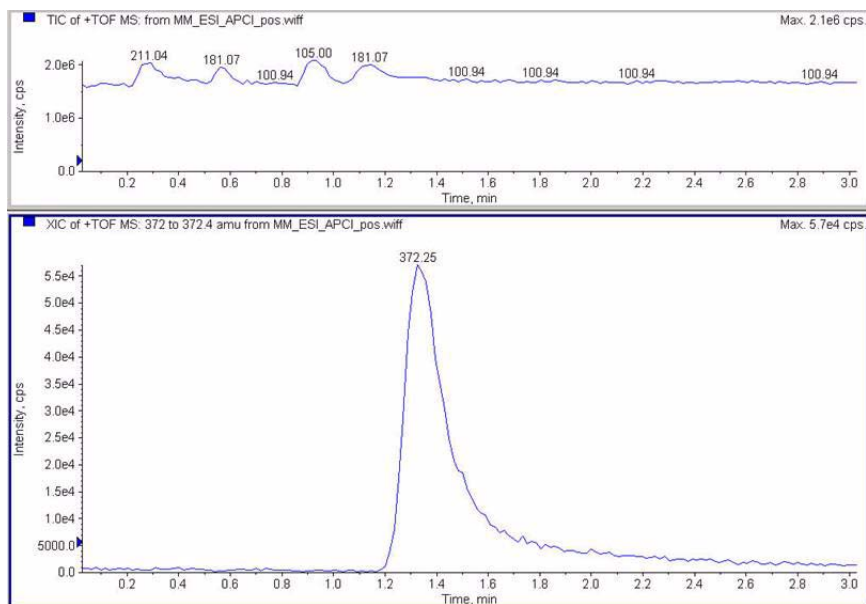
- 5 View the data in the data analysis program for MM_APCI_NEG. Extract Ion 193-193.4. Record the peak height. Example 640,000.



3 Installation Verification

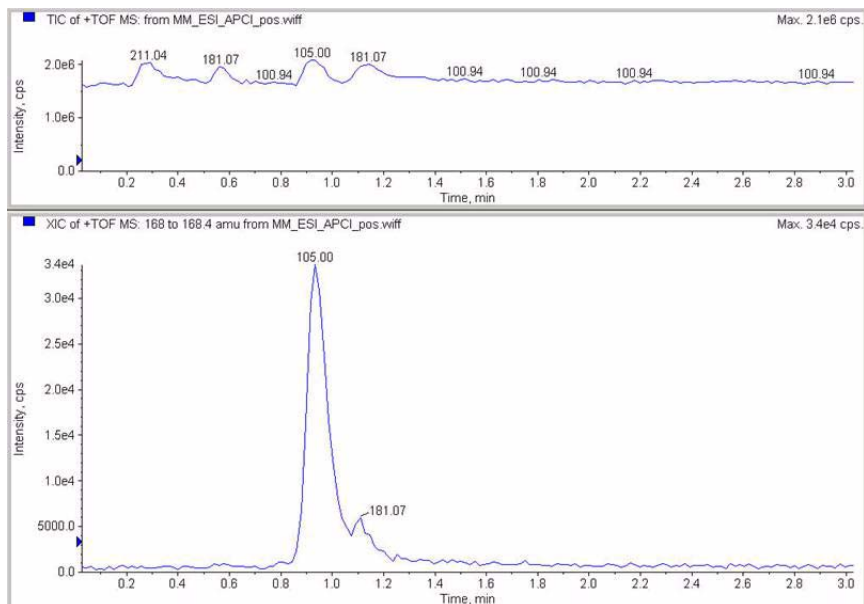
Step 9. Run each of the methods created

- 6 View the data in the data analysis program for MM_ESI_APCI_POS. Extract Ion 372-372.4. Record the peak height. Example: 57,000.



Step 9. Run each of the methods created

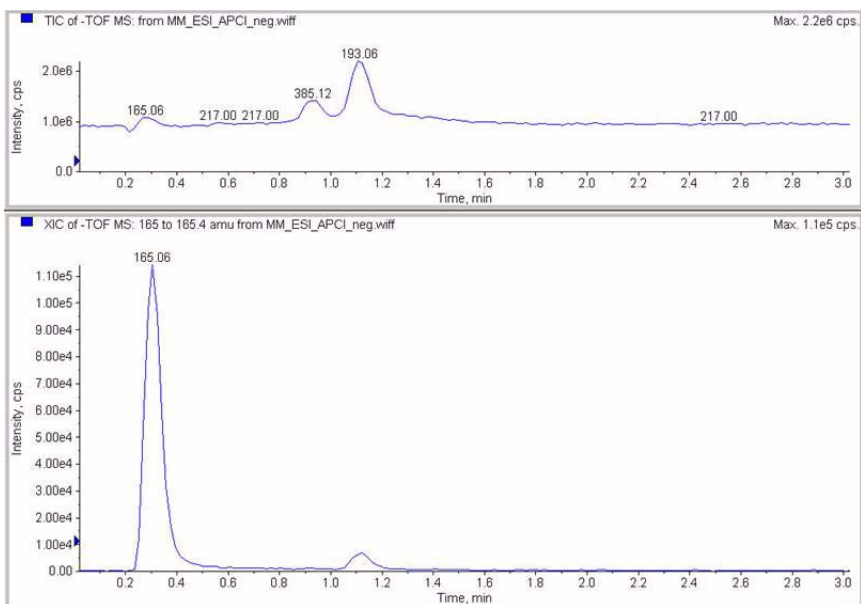
- 7 View the data in the data analysis program for MM_ESI_APCI_POS. Extract Ion 168-168.4. Record the peak height. Example: 34,000.



3 Installation Verification

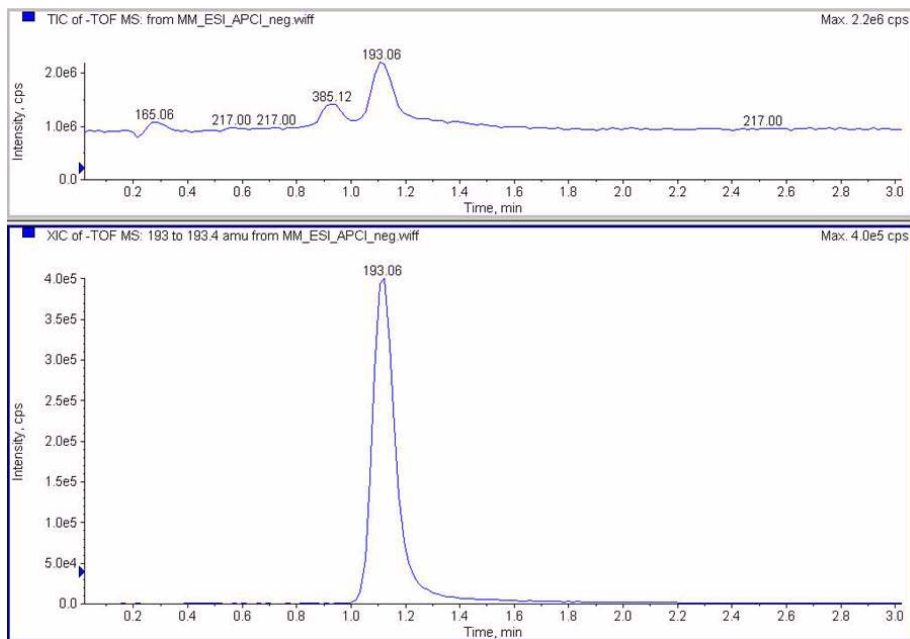
Step 9. Run each of the methods created

- 8 View the data in the data analysis program for MM_ESI_APCI_NEG. Extract Ion 165-165.4. Record the peak height. Example: 110,000.



Step 9. Run each of the methods created

- 9 View the data in the data analysis program for MM_ESI_APCI_NEG. Extract Ion 193-193.4. Record the peak height. Example: 400,000.



3 Installation Verification

Step 10. Calculate the response of Multimode Demo

Step 10. Calculate the response of Multimode Demo

1 Manually fill in the values in the Multimode Ion Source report.

The values in the example report below have been manually entered from the data collected in the runs from the previous steps. This is an example of how to enter the values from the instrument being installed and verified. The blank report is on the next page for installed instruments data.

Multimode Ion Source Report

MSD type: TOF Instrument name: Operator name:

Acquisition date: 23-Feb-2006

Datafiles:

- MM_ESI_pos.wif
- MM_ESI_Neg.wif
- MM_APCI_POS.wif
- MM_APCI_NEG.wif
- MM_ESI_APCI_POS.wif
- MM_ESI_APCI_NEG.wif

ESI Compound Results						
Compound	m/z	Polarity	ESI mode	Mixed mode	Mixed:ESI ratio	Result
Crystal violet	372.2	Positive	91k	57k	63%	Pass
1-Hexanesulfonic acid	165.1	Negative	97k	110k	113%	Pass

APCI Compound Results						
Compound	m/z	Polarity	APCI mode	Mixed mode	Mixed:APCI ratio	Result
Carbazole	168.1	Positive	140k	34k	24%	Pass
9-Phenanthrol	193.1	Negative	640k	400k	63%	Pass

Passing criteria: Mixed mode response 20% or greater of single-mode response.

2 Run all methods and get the peak heights. Calculate the amount of signal.

Step 11. Fill out Multimode Report for calculation of peak heights

Step 11. Fill out Multimode Report for calculation of peak heights

- Use the graphic below to fill out the multimode report for calculation of peak heights.

Multimode Ion Source Report

MSD type: TOF Instrument name: Operator name:

Acquisition date: 23-Feb-2006

Datafiles:
 MM_ESI_pos.wif
 MM_ESI_Neg.wif
 MM_APCI_POS.wif
 MM_APCI_NEG.wif
 MM_ESI_APCI_POS.wif
 MM_ESI_APCI_NEG.wif

ESI Compound Results						
Compound	m/z	Polarity	ESI mode	Mixed mode	Mixed:ESI ratio	Result
Crystal violet	372.2	Positive				
1-Hexanesulfonic acid	165.1	Negative				

APCI Compound Results						
Compound	m/z	Polarity	APCI mode	Mixed mode	Mixed:APCI ratio	Result
Carbazole	168.1	Positive				
9-Phenanthrol	193.1	Negative				

Passing criteria: Mixed mode response 20% or greater of single-mode response.

3 Installation Verification

Step 11. Fill out Multimode Report for calculation of peak heights

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In This Book

This book contains installation, operation, maintenance and troubleshooting instruction for the Multimode Source for 6500 Series Q-TOF LC/MS.

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