Agilent G1978A Multimode for 6210/6220 TOF

Set-Up Guide

Agilent Technologies

Notices

Manual Part Number

G1978-90060

Edition

First Edition, December 2008

Printed in USA

Agilent Technologies, Inc.
3501 Stevens Creek Blvd.
Santa Clara, CA 95052 USA

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In This Guide...

This guide contains information to install and maintain the Multimode for 6210/6220 TOF.

1 Installation

This chapter contains information to prepare the TOF instrument for the G1978A multimode source and to replace the existing source with the multimode source.

2 TOF Software and TOF Firmware Upgrade for Multimode

This chapter contains information to update your software and firmware for the multimode source.

3 Installation Verification

This chapter contains information to verify the installation of the multimode source.

Contents

1 Installation

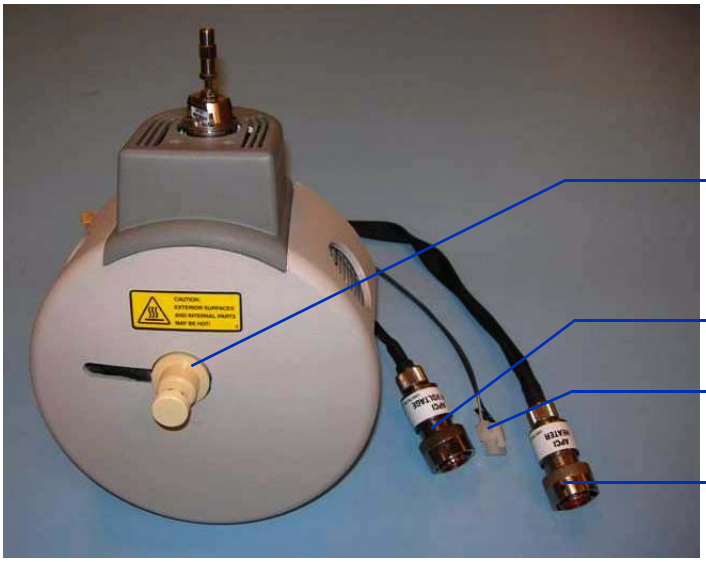
This chapter contains instructions to install the G1978A Multimode Source. You need to make changes to the instrument as part of the installation.

The multimode source is supported with the following software:

- TOF Software A.02.00 or A.02.01 with G1978-10004 patch
- MassHunter Workstation Acquisition for TOF A.02.02
- MassHunter Workstation Acquisition for TOF B.01.03 or higher

To upgrade from A.02.02 to B.01.03 or higher, you must completely remove the Analyst software. To make sure Analyst is completley removed from your system, reimage the computer.

Refer to the *TOF Installation Guide* for software installation instructions.


APCI Corona
HV cable +/- 2kv
APCI High voltage
Vaporizer Heater Cable

Installation

Step 1. Prepare to install

1. Check that you have these parts:
   - Bundled LC/MSD Multimode ESI/APCI Source (p/n G1978A)
   - LC/MSD Multimode ESI/APCI Source (p/n G1978-65239)
   - LCMSD-TOF MM ESI/APCI Enablement Kit (p/n G1978-60251)
   - TOF Software A.02.02 or higher
   - TOF Multimode Installation Guide (p/n G1978-90007)
2. Check that the TOF instrument has serial numbers greater than US50600501 or US54100700.
3. Check that the TOF has Smart Card 4.
4. Check that you have the supported revision of the TOF Software (and any needed patch) or the MassHunter Workstation Software - Acquisition for TOF software. *Do not install the patch that comes with the ESI/APCI Enablement Kit.*
5. Check that you have these tools, supplies and chemicals. The items in this list are not provided with your multimode source.
   - Cloths and gloves, clean, lint-free
   - Water and organics, such as acetone, methanol, acetonitrile or isopropyl alcohol, all HPLC grade.
   - open-end wrench
   - Torx drive T10
6. Verify the current performance of the TOF system:
   - With the dual-ESI source installed, do Positive and Negative mode Autotunes.
   - Examine the tune reports to verify that the TOF system meets tune specifications.
7. In the MS TOF tab, click **Parameters** and select **Positive ion polarity**. Click **Save As** to save the positive tune parameters as **d:\Program Files\Agilent\TOF Software\Tune\PositiveESI.prm**.

8 In the MS TOF tab, click **Parameters** and select **Negative ion polarity**. Click **Save As** to save the negative tune parameters as **d:\Program Files\Agilent\TOF Software\Tune\NegativeESI.prm**.

9 Right-click on the TOF icon in the Status pane and click **Vent**.

10 After the TOF system has completed the vent process, turn off the front switch and the main breaker.

11 Prepare a static-free work surface to store the electronics assemblies that are removed during the upgrade procedure.

Step 2. Remove the TOF E-Tub Electronics

- Remove the following assemblies from the TOF Electronics Tub in this order:
  1 Top Foam piece from the Electronics Tub.
  2 RF Power Amplifier and front and back foam pieces.
  3 Mid Foam piece from the Electronics Tub
  4 Analyzer 3 PCA (G1946-65250)
  5 SmartCard 4+ PCA with PDB cover
  6 Power Distribution Board (G1946-65002)

Step 3. Change the firmware chips on the Analyzer and Power Distribution Boards

The Main PLCC Firmware chip U129 must be changed on the Analyzer 3 PCA for source identification (p/n G1978-80067). Two chips on the power distribution board U6 (p/n G1978-80100) Programmed ROM MM LON and U18 Chip EPROM (p/n G1978-80200) will also be changed.

1 Locate the Firmware Upgrade Kit, MM (part number G1978-60156) in the upgrade kit parts box.

2 Locate the Analyzer board that was removed in "Step 2. Remove the TOF E-Tub Electronics" on page 10. Place the Analyzer Board on a static free surface.

3 On the Analyzer Board, locate the U129 socket. See Figure 1.

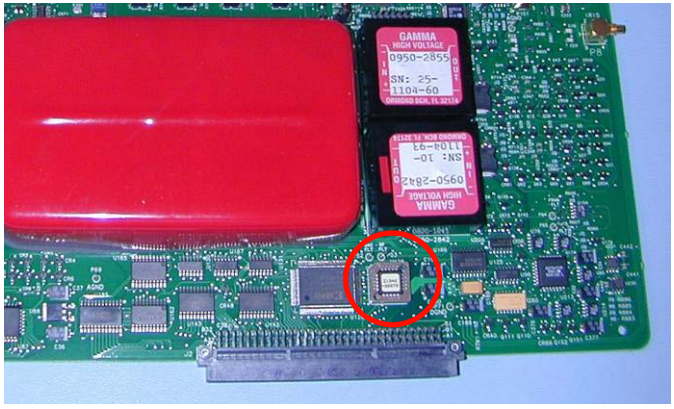


Figure 1 Location of the U129 socket

4 Look at the chip in the socket. Note the orientation of the chip in the socket. Using the chip removal tool, carefully remove the logic chip from the U129 socket. Be very careful when using the tool because you can damage the chip socket.

NOTE You only need to insert the very tip of the tool under the chip. Using more of the tool under the chip to pry or remove the chip will lead to damage of the socket. See Figure 2.

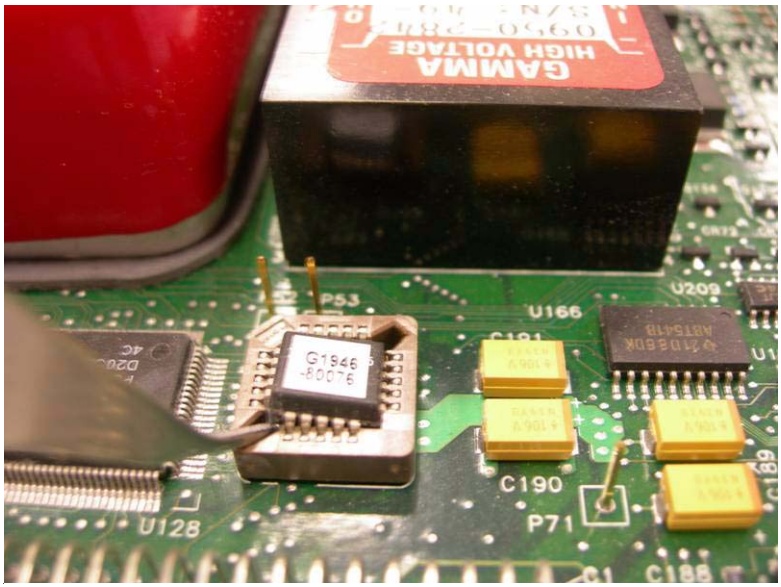


Figure 2 Carefully remove the chip from the socket

5 In the Firmware Upgrade Kit, find the chip with the part number G1978-80067.

6 Find the correct orientation of the chip so that it fits into the socket. Press the chip into the socket.

CAUTION Be sure that the chip is completely in the socket. Otherwise, when the board is energized the chip will be destroyed.

7 Locate the Power Distribution Board (PDB) that was removed in "Step 2. Remove the TOF E-Tub Electronics" on page 10. Place the PDB on a static free surface.

8 Using the same technique that was used to remove the chip on the Analyzer Board, remove the chips from the U6 and U18 sockets. See Figure 3.

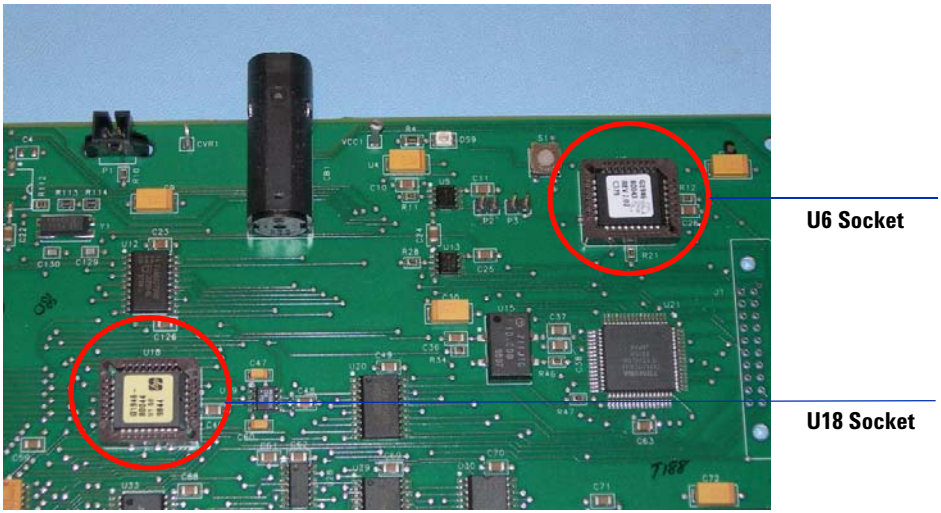


Figure 3 Remove the U6 and U18 chips from their sockets

9 Locate the chip with the part number G1978-80200. Find the correct orientation of the chip so that it fits into the socket. Press the G1978-80200 chip into the U18 socket.

CAUTION Be sure that the chip is completely in the socket. Otherwise, when the board is energized the chip will be destroyed.

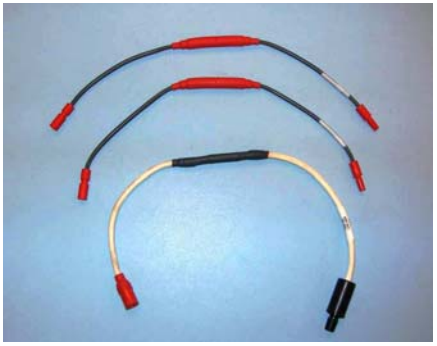
10 Locate the chip with part number G1978-80100. Find the correct orientation of the chip so that it fits into the socket. Press the G1978-80100 chip into the U6 socket.

CAUTION Be sure that the chip is completely in the socket. Otherwise, when the board is energized the chip will be destroyed.

11 After upgrading the chips on the PDB, reinstall the PDB in the E-tub. Leave the analyzer 3 board out until Step 4 has been completed.

Step 4. Install the three 10MΩ cables

1 While the instrument is vented and the analyzer board is out, install the cables in series with the output cable for the Vcap/Vchamber and APCI power supplies. The cables can be installed with the analyzer board installed. It is easier with the analyzer board out.



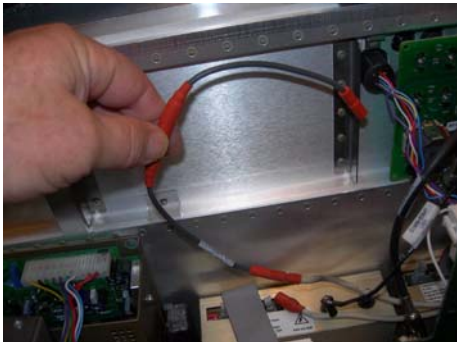


Figure 4 Left: Two M-F 10 MΩ ballast MIDGI cables (p/n G1978-60806) and one M-F 10MΩ ballast SCID cable (p/n G1978-60805). Right: APCI cable connected in series with ouput

2 Connect one of the M-F 10MΩ ballast MIDGI cable (p/n G1978-60806) in series with the existing cable and plug it back into to APCI power supply.

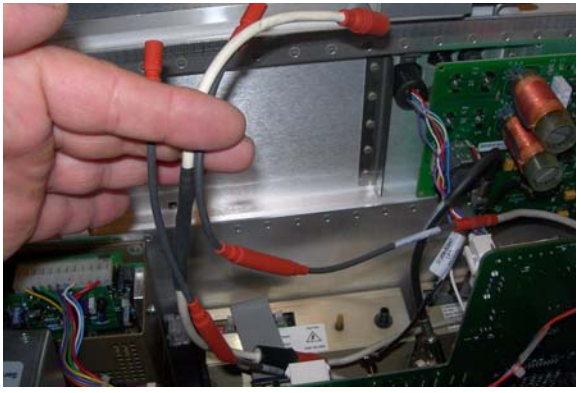


Figure 5 Three cables connected in series with power supply outputs

3 Connect the other M-F 10MΩ ballast MIDGI cable (p/n G1978-60806) in series with the VChamber power supply cable and plug it back into to VChamber power supply output.

4 Connect the M-F 10MΩ ballast SCID cable (p/n G1978-60805) in series with the Vcap cable then plug it back into to VCap output of the power supply.

Figure 6 Cables tucked to the side of the power supplies

5 Install the analyzer board if it was not already installed.

6 Arrange the cables down to the side of the power supplies so the middle foam will fit when replaced.

7 Replace all electronic tub components and reconnect all cables that were disconnected.

Step 5. Install the HV control PCA and cables

1 Attach the attach the RS-232 cable to the HV and control PCA power supply RS 232 connector.

Figure 7 Attaching RS-232 Cable

2 Remove the cover from the HV module (p/n G1978-60050)

Figure 8 Removing HV Module Cover

3 Attach the HV and control PCA to the tube. The instrument front cover, top cover, safety cover with magnet, and side panel access door should be off.

4 Remove the plastic cable clamp from the desolvation heater cable. Pull the cable down so the HV Module can fit in the location.

Figure 9 Plastic cable clamp

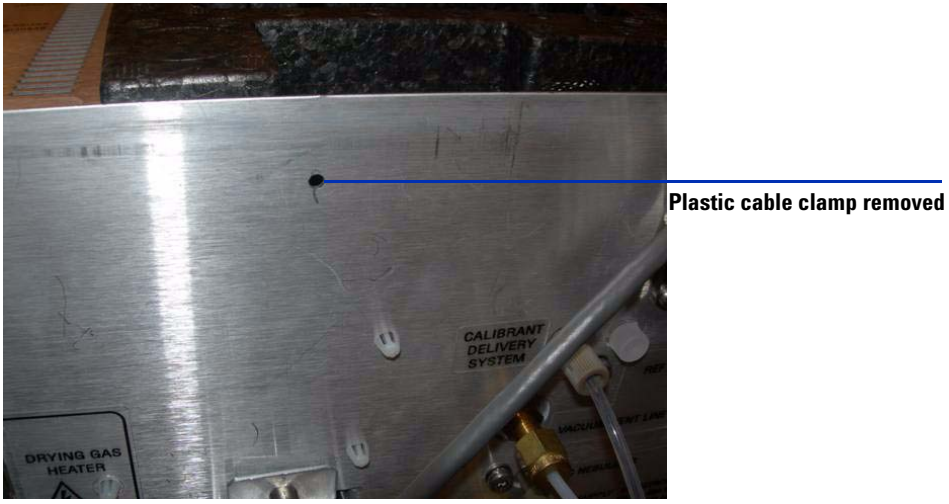


Figure 10 Cable clamp removed and cable moved down

5 Attach the HV and control PCA power supply to the tube with the self-trapping screw supplied.

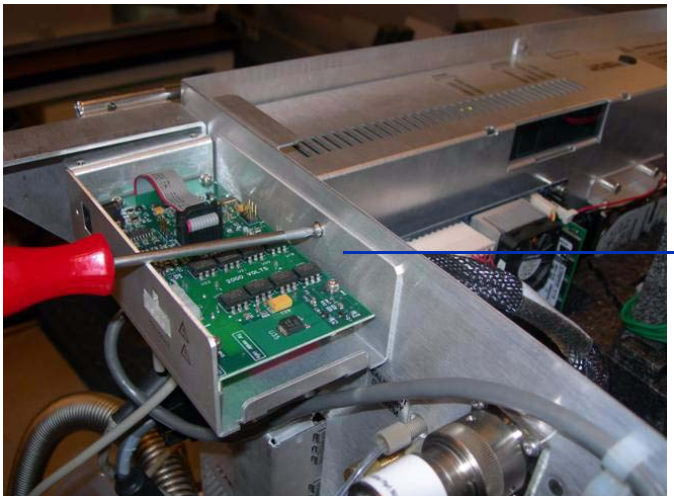


Figure 11 Self tapping screw

6 Clamp the top cover of the HV and control PCA power supply with screws provided to the support bracket.

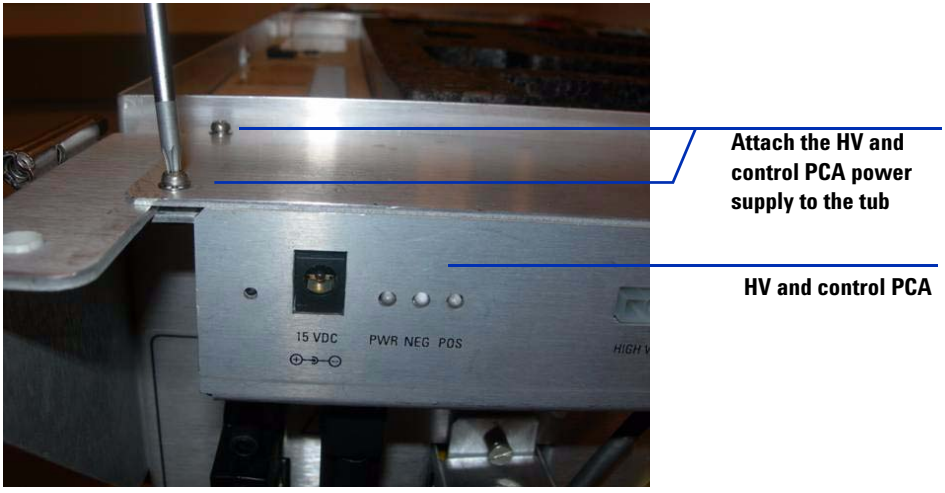


Figure 12 Clamping to support bracket

Figure 13 RS-232 cable connections

7 Connect the (RS-232) from HV module to the Serial connector on Smart card 4 interface. See Figure 13.

8 Connect the 15V dc power supply to the HV and control PCA. See Figure 14 and Figure 15.

9 Connect the other end of the 15V dc power supply into an 110V ac outlet using the power cord supplied with the 15V dc power supply. See See Figure 14 and Figure 15.

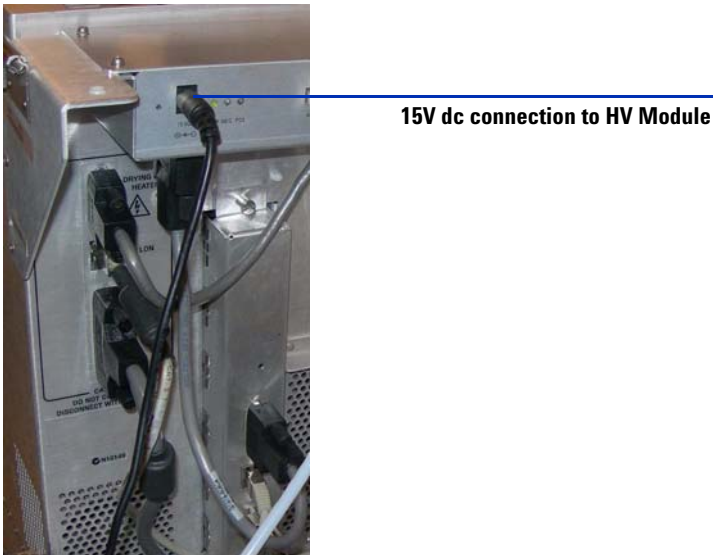


Figure 14 RS 232 cable connections

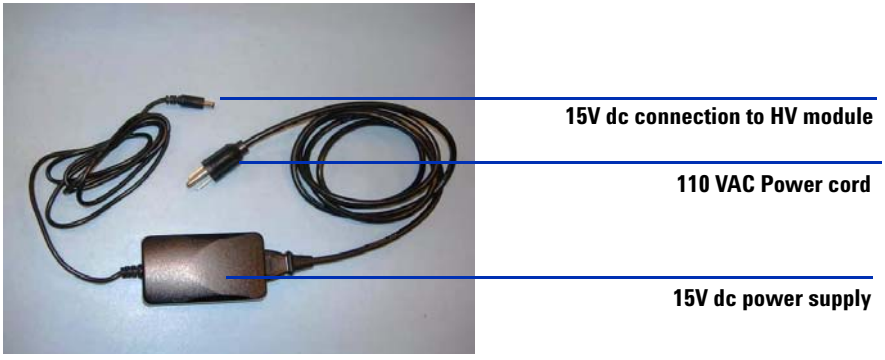


Figure 15 Power cord and 15V dc supply

Step 6. Attach the multimode source to the instrument

1 Remove the currently installed spray chamber (if applicable) from the spray chamber mount. Remove the shipping cover from the multimode source spray chamber.

Figure 16 Multimode source

2 Install the multimode source on the spray chamber mount. See Figure 17.

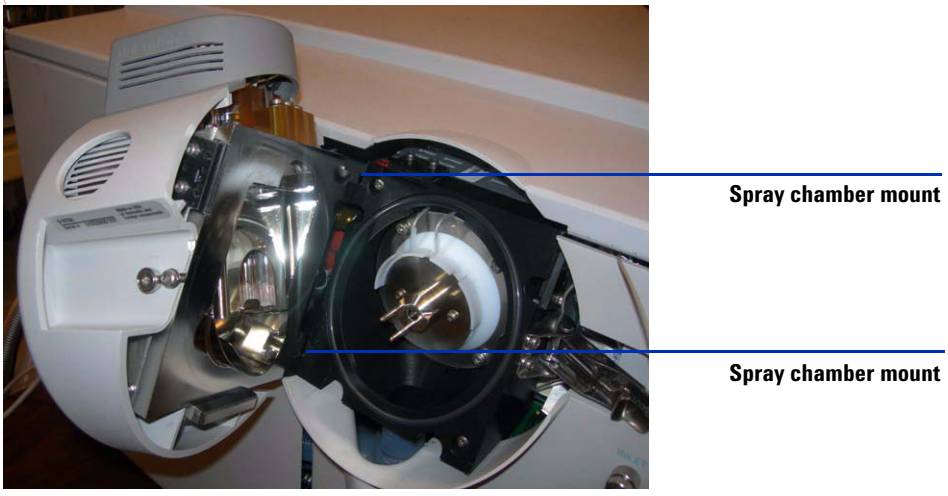


Figure 17 Multimode source attached to the TOF instrument

3 Screw the End Cap Assembly into the holder for the end cap. See Figure 18.

Note that the field shaping electrodes are in the 9 o'clock and 6 o'clock positions.

4 Loosen the end plate screws on each side to adjust the field shaping electrodes position.

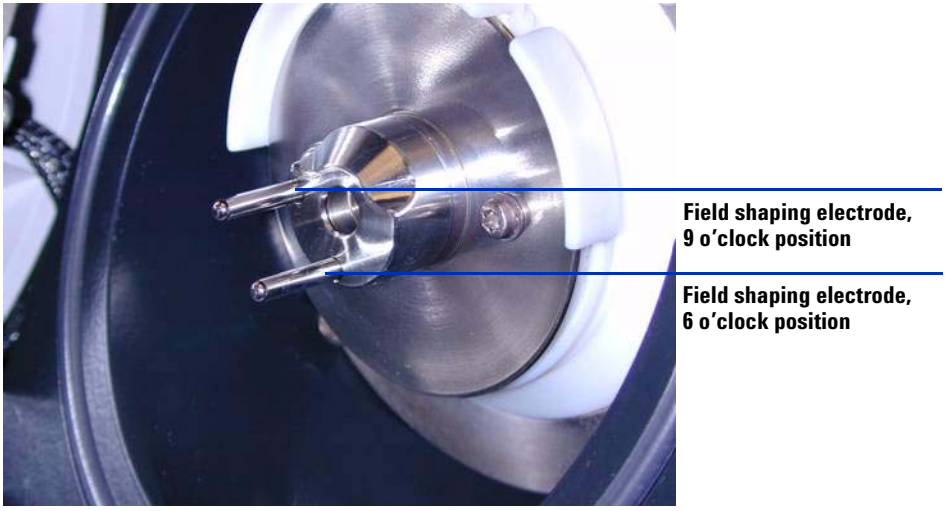


Figure 18 Multimode End Cap Assembly (p/n G1978-60060)

5 Connect the vaporizer heater, APCI high voltage, and HV and control PCA cables. The APCI heater connector, APCI high voltage connector, and HV and control PCA connector located on the left side of the instrument chassis. See Figure 19.

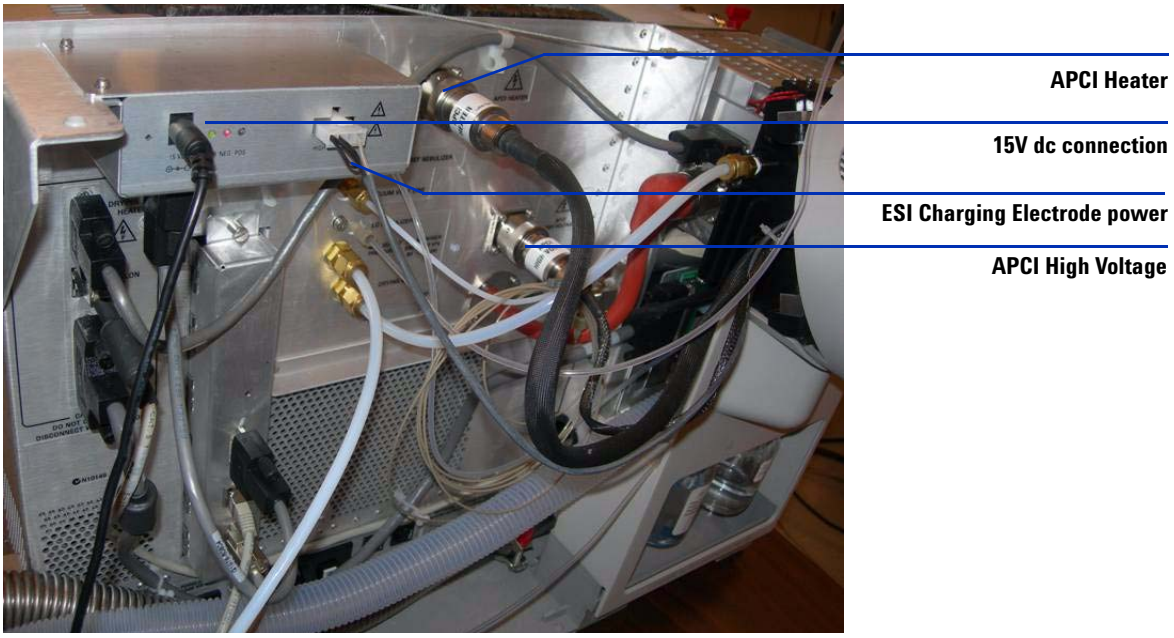


Figure 19 Cable connections

Step 7. Install the nebulizer, corona needle, and gas connections

1. Install the nebulizer on the multimode source spray chamber. Never use a nebulizer spacer on a multimode source.
2. Connect the 1/8-inch nebulizing gas tubing from the LC/MS instrument mainframe to the nebulizer gas fitting
3. Connect the LC/MS sample tubing to the nebulizer zero dead volume fitting. See Figure 20.
4. Connect the LC to the Inlet connection on the TOF instrument. Never connect LC tubing directly to the Nebulizer. See Figure 20.
5. Install the corona needle. Make sure the corona needle is pushed all the way in.

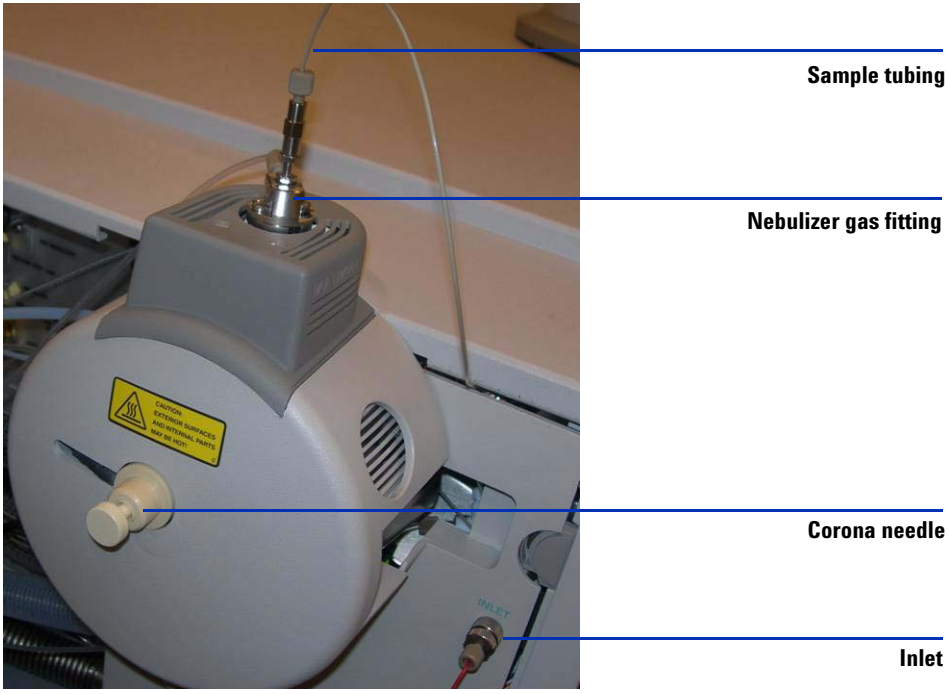


Figure 20 Nebulizer, nitrogen gas and corona needle installed

6 Switch Calibrant Bottle B to the Multimode Calibrant (p/n G1969-85020) for TOF.

Figure 21 Calibrant For TOF (p/n G1969-85020)

7 Re-install all covers.

Figure 22 All covers re-installed

Changing Sources

To convert between the ESI, APCI or APPI and the multimode ion source

Do this step if you want to change the source between ESI, APCI or APPI and the multimode source. To change to the multimode source for the first time, go to "Installation" on page 7 instead.

1. Change the **Source** setting to minimum **for drying gas, nebulizer gas, vaporizer temp, and drying gas temp**.
2. Disconnect the nebulizer gas tube from the current ion source.
3. Disconnect cables for source type that is installed.
4. Remove the current ion source.
5. Unscrew and remove the spray shield.

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

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

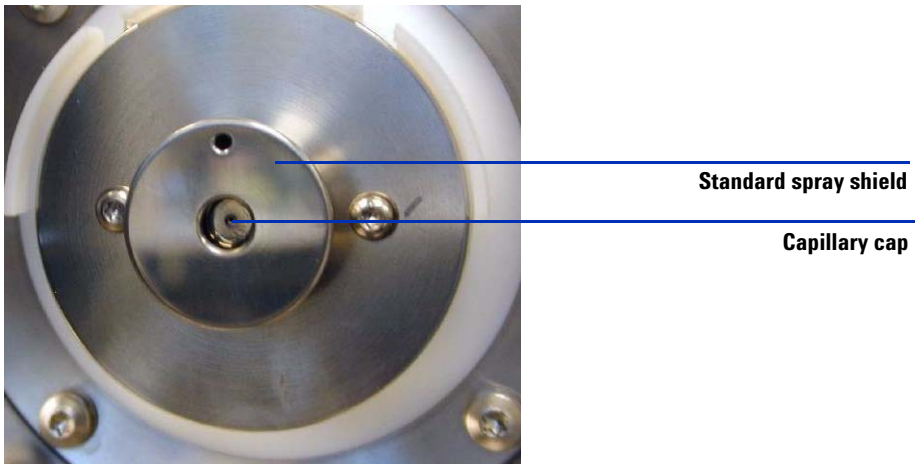


Figure 23 Standard spray shield

6 Remove the capillary cap. If needed, moisten a clean cloth with isopropyl alcohol and wipe the capillary cap See Figure 24.

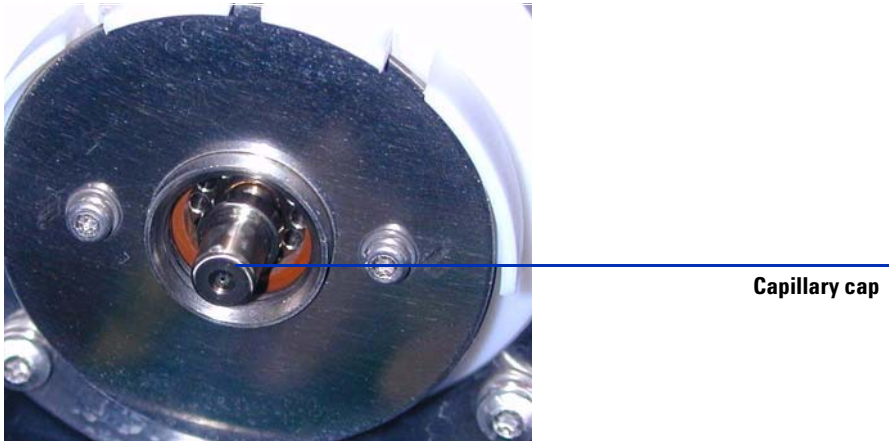


Figure 24 Capillary Cap

7 If needed, moisten a clean cloth with isopropyl alcohol and gently wipe the front of the capillary then reinstall capillary cap.

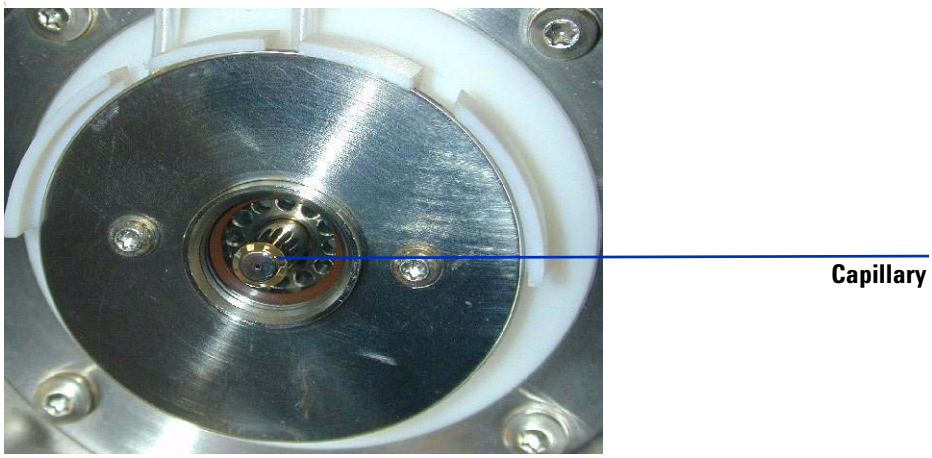


Figure 25 Capillary

8 After cleaning the capillary and cap, place the capillary cap back on capillary. Install the new spray shield with field shaping electrodes.

Figure 26 End Cap Assembly, Multimode (p/n G1978-60060)

9 Screw the multimode spray shield into the holder for the spray shield. See Figure 27.

Note that the field shaping electrodes are in the 9 o'clock and 6 o'clock positions.

10 Loosen the end plate screws on each side to adjust the field shaping electrodes position.

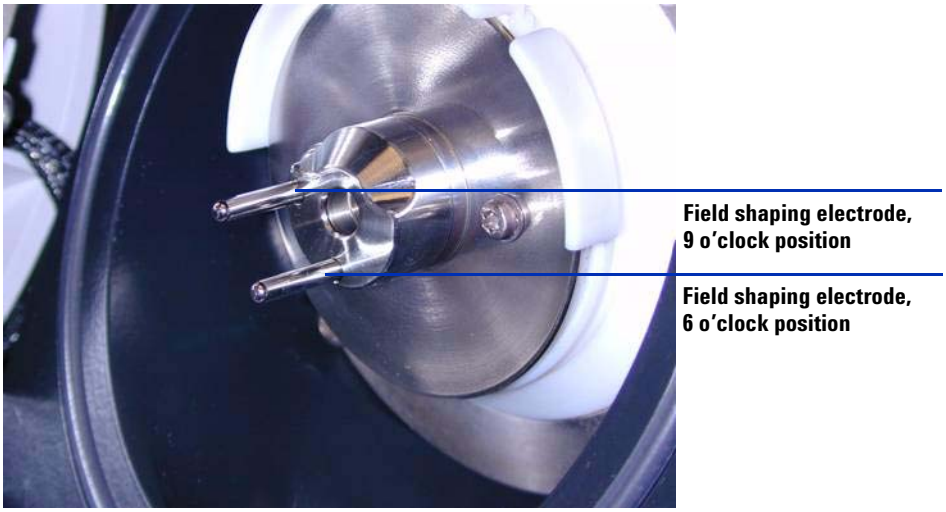


Figure 27 Multimode End Cap Assembly (p/n G1978-60060)

11 Remove any cables such as APCI vaporizer heater cable and APCI high voltage cable and any other cables such as RS 232 cable on APPI source.

CAUTION When converting back to any of the sources other than the G1978A the HV module, disconnect the +15V DC power from the module.

1 Installation

2
TOF Software and TOF Firmware Upgrade for Multimode

This section describes upgrading the G3300AA TOF Software to Revision A.02.02 and upgrading the TOF firmware to 5.30 or higher for the multimode source.

Step 1. Upgrade the TOF Software

1. Back up the following folders in the **C:\Program Files\Agilent\TOF Software** folder to a safe location.
   - DA methods
   - methods
   - worklists

   Methods and mass lists will be overwritten when the new software is installed. Also, if you have modified any Agilent supplied files, these files may be overwritten when the software is upgraded. Back up any modified Agilent files to a safe location. It is recommended that VBA projects provided by Agilent should not be modified.
2. Disconnect the House LAN from the computer.
3. Use Windows Add-Remove Programs to remove the previous installation of TOF Software.
4. When you are asked whether to remove all files and folders, click **No**. Your methods, worklists, and data analysis scripts will be preserved.
5. Use Windows Add-Remove Programs to remove the previous installation of Analyst QS.
6. Use File Explorer and open the CD-ROM drive for the Installation CD. Open the directory **Analyst**. Double-click **setup.exe**.
7. Click **Next** on the Welcome screen.
8. Click **Yes** to accept the software license agreement.
9. Click **Next** after specifying the destination location for the installed software. It is recommended to use the default location.
10. When the dialog box appears for selecting the data file storage location, select the location **D:\PE Sciex Data**.
11. Click **Next** to proceed with the rest of the installation.
12. When the dialog box appears to install the o-MALDI server, click **Cancel**. This software is not required for the LC/MSD TOF.
13. Click **Yes** when prompted to reboot the computer.
14. Use File Explorer and open the CD-ROM drive for the Installation CD. Open the directory **G3300**. Double-click **setup.exe**.
15. Click **Next** on the Welcome screen.
16. 16.Click Yes to accept the software license agreement.

17 Click **Next** after specifying the destination location for the installed software. It is recommended to use the default location.

18 Mark the **Install BootP** check box. SmartCard 4 uses a fixed IP address (192.168.254.12). Therefore the BootP service is not needed for the TOF instrument. However, the LAN card for the LC may be configured to use BootP.

You can also configure the LC with a fixed IP addresses. Please refer to the CD labeled “Agilent Technologies LAN Card G1369A” (p/n G1369-90000) for more information.

19 Click **Next** after specifying the location for data like methods and reports to be stored. You may wish to put the data on a different drive to make backups easier. For bundled systems, the default location for TOF data is **D:\TOF_Data**. You need to change the value in the location text box to this folder name.

20 Click **Next** on the Start Copying Files dialog box that allows you to review your setup choices.

21 When you are asked to update the list of masses, click **Yes**. The upgrade from A.00.00, A.01.00, or A.01.01 to A.02.00 requires the list of masses to be updated.

22 Click **Yes** when you are prompted to restart the computer.

23 Connect the House LAN to the computer.

24 Add the MAC address for the LC LAN card to the BootP Manager and assign the IP address 192.168.254.11 to the LC.

You can also configure the LC with a fixed IP addresses. Please refer to the CD labeled “Agilent Technologies LAN Card G1369A” (p/n G1369-90000) for more information.

25 After reloading software, configure the logical instrument. The TOF and optionally the LC and ADC are configured into one logical instrument. This must be done before using the TOF Software system.

a Click **Start > Programs > Agilent > TOF Software > Tools > Instrument Configuration**.

b Click **Add**.

c In the Add Devices window, click **OK** to accept the default connection value for the LC/MSD TOF.

d Continue to add instruments until all desired instruments have been added.

e Change the Instrument Name if desired. This is only used for reporting purposes.

f Click **OK** to create the instrument configuration.

g When the instrument is successfully configured, click **OK** to close the information box that appears.

26 Check that the HOSTS file were correctly changed. The TOF Software adds an entry for the TOF and the HPLC modules.

a Use Notepad to open the file **HOSTS** in the **C:\WINNT\System32\drivers\etc** folder.

b Under the entry for the local host, check that the entries appear for the TOF system and LC (if configured).

c Click **File > Save** to close the file.

Step 2. Upgrade the TOF firmware

1. Install the TOF Firmware Update tool. Use File Explorer and open the CD-ROM drive for the Installation CD.
2. Open the folder **Support\TOF Firmware**.
3. Double-click **MSFirmwareUpdate_1.16.exe**.

   The WinZip self-extractor dialog appears. Use the default installation path.
4. Click **Unzip**.
5. Click **OK** when you are informed that the files have been unzipped.
6. Click **Close** to complete the installation.
7. Double-click **tofupdate.exe** in the copied directory.
8. Enter the IP address of the TOF. By default, this is 192.168.254.12
9. Enter **Y** when prompted to continue the update.
10. When the TOF firmware has been updated, press the reset button on the communication card (SmartCard 4) to reboot it. The reset button can be accessed via the small opening above the SmartCard 4 serial port.
11. After the SmartCard 4 has finished initializing, start the TOF Software.
12. Click **Print > Instrument Configuration**.
13. Verify that the SmartCard 4 firmware revision is 5.30 or higher.

Step 3. Pump down the LC/MSD TOF and condition the high voltage electronics

Before you try tuning the LC/MSD TOF, the high voltage electronics need to be conditioned.

1. Click **Start > Programs > Agilent > TOF Software > Tools > TOF Diagnostics**.
2. Click **Connection > Connect**.

   By default, the IP address 192.168.254.12 for the LC/MSD TOF appears.
3. Click **OK**.

   Once you are connected, the MS Status line will say Instrument Responding. Also, the connection box at the bottom right of the screen will be green.
4. In the **HV Conditioning** group box, select the **0.6 Hour Cycle (Quick Vent)** option, since the TOF instrument was vented under nitrogen. Select the **Condition HV** button to initiate the high voltage conditioning process. Tuning and Calibration cannot proceed until this process has completed.

3
Installation Verification

In this chapter, you create and run methods to check out the system. See “ESI + APCI LC Demo Sample” on page 105 for structural information on the demo sample that is used in this chapter.

Step 1. Auto tune

MassHunter TOF Acquisition for TOF A.02.02

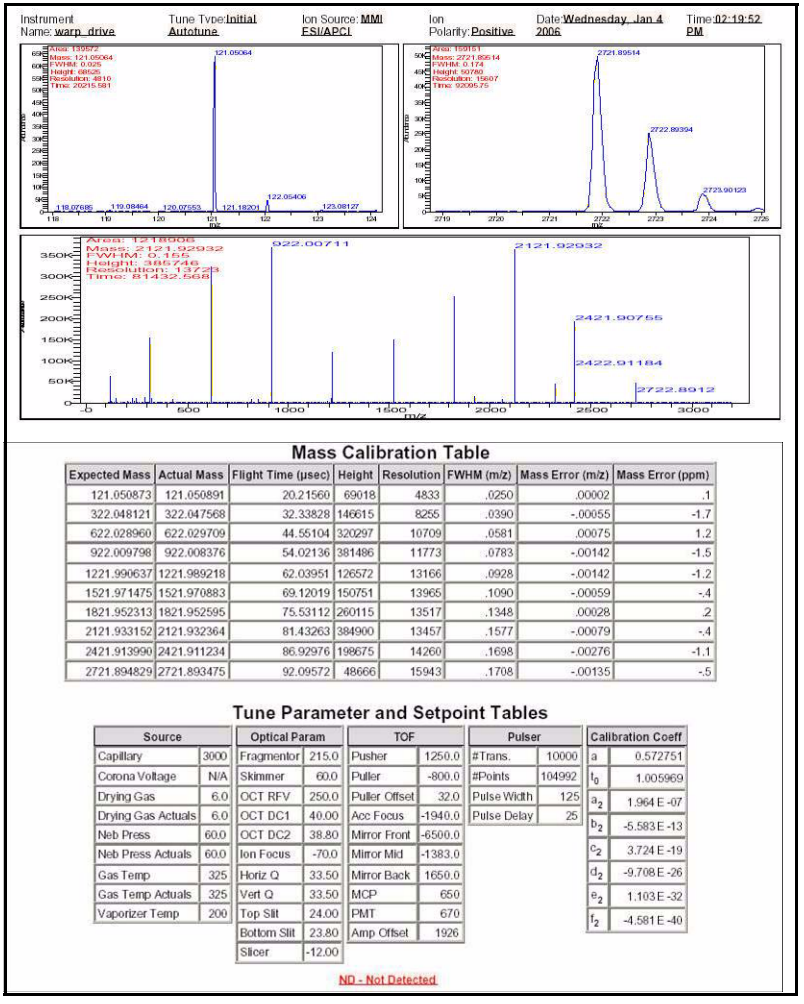
Before the TOF system with multimode source can be used, the installation and verification tasks must be completed. Auto tune is done in mixed mode, with the TOF G1969-85000 ESI-L Low Concnetration Tuning Mix.

1 Click **File > Open > Method**.

2 Load the **MMIautotune.m** file.

3 Click the **Tune** tab and select **Autotune**.

The instrument will generate a positive Autotune report for the multimode source. See Figure 28 on page 39.



Mass Calibration Table

Expected Mass	Actual Mass	Flight Time (µsec)	Height	Resolution	FWHM (m/z)	Mass Error (m/z)	Mass Error (ppm)
121.050873	121.050891	20.21560	69018	4833	.0250	.00002	.1
322.048121	322.047568	32.33828	146615	8255	.0390	-.00055	-1.7
622.028960	622.029709	44.55104	320297	10709	.0581	.00075	1.2
922.009798	922.008376	54.02136	381486	11773	.0783	-.00142	-1.5
1221.990637	1221.989218	62.03951	126572	13166	.0928	-.00142	-1.2
1521.971475	1521.970883	69.12019	150751	13965	.1090	-.00059	-.4
1821.952313	1821.952595	75.53112	260115	13517	.1348	.00028	.2
2121.933152	2121.932364	81.43263	384900	13457	.1577	-.00079	-.4
2421.913990	2421.911234	86.92976	198675	14260	.1698	-.00276	-1.1
2721.894829	2721.893475	92.09572	48666	15943	.1708	-.00135	-.5

Tune Parameter and Setpoint Tables

Source	
Capillary	3000
Corona Voltage	N/A
Drying Gas	6.0
Drying Gas Actuals	6.0
Neb Press	60.0
Neb Press Actuals	60.0
Gas Temp	325
Gas Temp Actuals	325
Vaporizer Temp	200

Optical Param	
Fragmentor	215.0
Skimmer	60.0
OCT RFV	250.0
OCT DC1	40.00
OCT DC2	38.80
Ion Focus	-70.0
Horiz Q	33.50
Vert Q	33.50
Top Slit	24.00
Bottom Slit	23.80
Slicer	-12.00

TOF	
Pusher	1250.0
Puller	-800.0
Puller Offset	32.0
Acc Focus	-1940.0
Mirror Front	-6500.0
Mirror Mid	-1383.0
Mirror Back	1650.0
MCP	650
PMT	670
Amp Offset	1926

Pulser	
#Trans.	10000
#Points	104992
Pulse Width	125
Pulse Delay	25

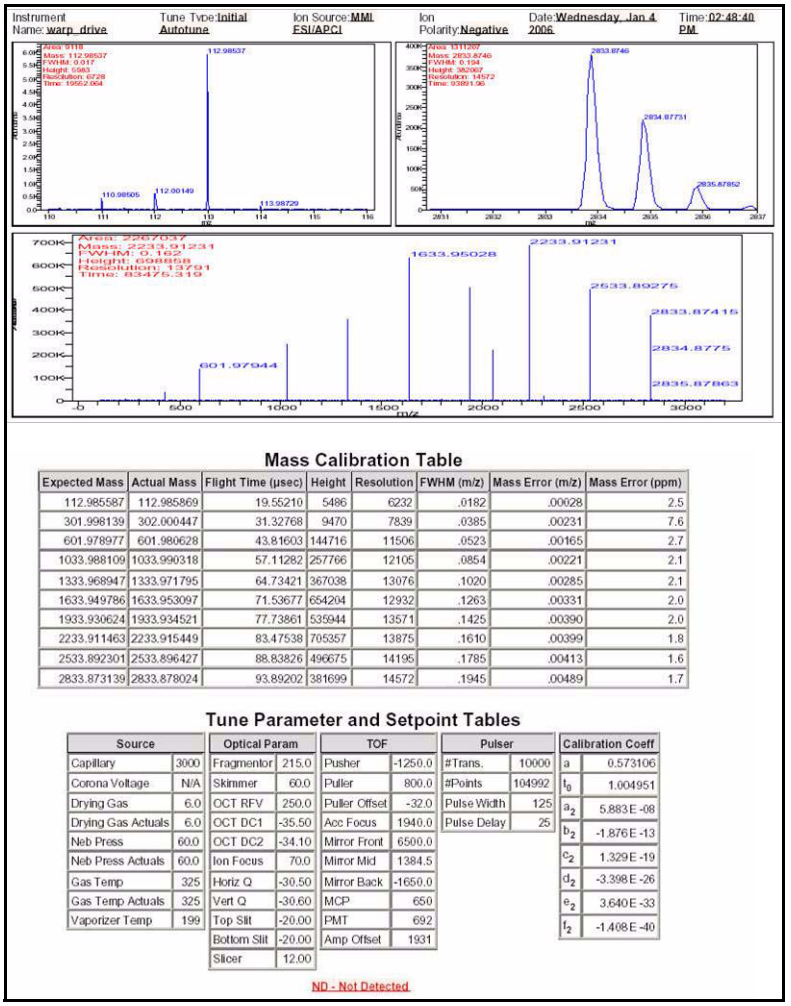
Calibration Coeff	
a	0.572751
l_0	1.005969
a_2	1.964 E -07
b_2	-5.583 E -13
c_2	3.724 E -19
d_2	-9.708 E -26
e_2	1.103 E -32
f_2	-4.581 E -40

ND - Not Detected

Figure 28 Positive Autotune report for multimode source

4 Switch the polarity to negative and run autotune.

The instrument will generate a negative Autotune report for the multimode source.



Mass Calibration Table

Expected Mass	Actual Mass	Flight Time (µsec)	Height	Resolution	FWHM (m/z)	Mass Error (m/z)	Mass Error (ppm)
112.985587	112.985869	19.55210	5486	6232	.0182	.00028	2.5
301.998139	302.000447	31.32768	9470	7839	.0385	.00231	7.6
601.978977	601.980628	43.81603	144716	11506	.0523	.00165	2.7
1033.988109	1033.990318	57.11282	257766	12105	.0854	.00221	2.1
1333.968947	1333.971795	64.73421	367038	13076	.1020	.00285	2.1
1633.949786	1633.953097	71.53677	654204	12932	.1263	.00331	2.0
1933.930624	1933.934521	77.73861	535944	13571	.1425	.00390	2.0
2233.911463	2233.915449	83.47538	705357	13875	.1610	.00399	1.8
2533.892301	2533.896427	88.83826	496675	14195	.1785	.00413	1.6
2833.873139	2833.878024	93.89202	381699	14572	.1945	.00489	1.7

Tune Parameter and Setpoint Tables

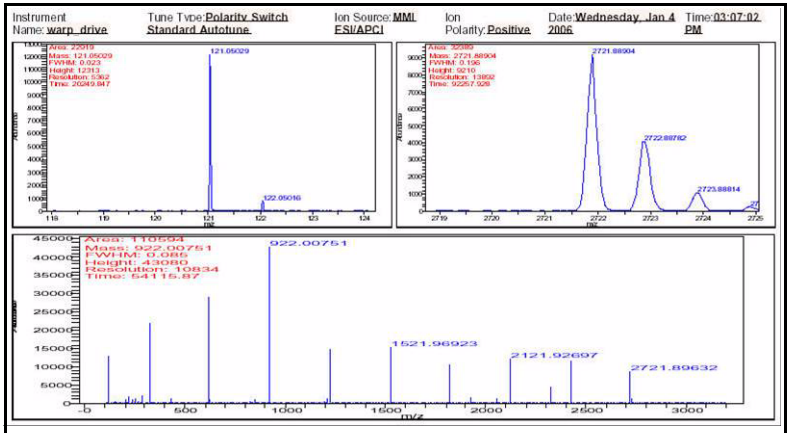
Source		Optical Param		TOF		Pulser		Calibration Coeff	
Capillary	3000	Fragmentor	215.0	Pusher	-1250.0	#Trans.	10000	a	0.573106
Corona Voltage	N/A	Skimmer	60.0	Puller	800.0	#Points	104992	t_0	1.004951
Drying Gas	6.0	OCT RFV	250.0	Puller Offset	-32.0	Pulse Width	125	a_2	5.883E-08
Drying Gas Actuals	6.0	OCT DC1	-35.50	Acc Focus	1940.0	Pulse Delay	25	b_2	-1.876E-13
Neb Press	60.0	OCT DC2	-34.10	Mirror Front	6500.0			c_2	1.329E-19
Neb Press Actuals	60.0	Ion Focus	70.0	Mirror Mid	1384.5			d_2	-3.398E-26
Gas Temp	325	Horiz Q	-30.50	Mirror Back	-1650.0			e_2	3.640E-33
Gas Temp Actuals	325	Vert Q	-30.60	MCP	650			f_2	-1.408E-40
Vaporizer Temp	199	Top Slit	-20.00	PMT	692				
		Bottom Slit	-20.00	Amp Offset	1931				
		Slicer	12.00						

Figure 29 Negative Autotune report for multimode source

5 Load the associated polarity switching method positive. Example: MMIautotunePSPos.m

6 Click the **Tune** tab and select **Autotune**.

The instrument will generate a polarity switching positive report only for MMIautotunePSPos.m.



Mass Calibration Table

Expected Mass	Actual Mass	Flight Time (µsec)	Height	Resolution	FWHM (m/z)	Mass Error (m/z)	Mass Error (ppm)
121.050873	121.050388	20.24985	12109	5421	.0223	-.00048	-4.0
322.048121	322.046844	32.39415	21261	8600	.0375	-.00128	-4.0
622.028960	622.027895	44.62864	30662	9614	.0647	-.00107	-1.7
922.009798	922.007759	54.11588	43835	11066	.0833	-.00204	-2.2
1221.990637	1221.986149	62.14826	15042	12136	.1007	-.00449	-3.7
1521.971475	1521.968707	69.24161	15559	12501	.1218	-.00277	-1.8
1821.952313	1821.946941	75.66390	10177	12733	.1431	-.00537	-2.9
2121.933152	2121.928178	81.57594	12417	12965	.1638	-.00497	-2.3
2421.913990	2421.907380	87.08284	12385	12840	.1887	-.00661	-2.7
2721.894829	2721.894859	92.25803	8810	13327	.2045	.00003	.0

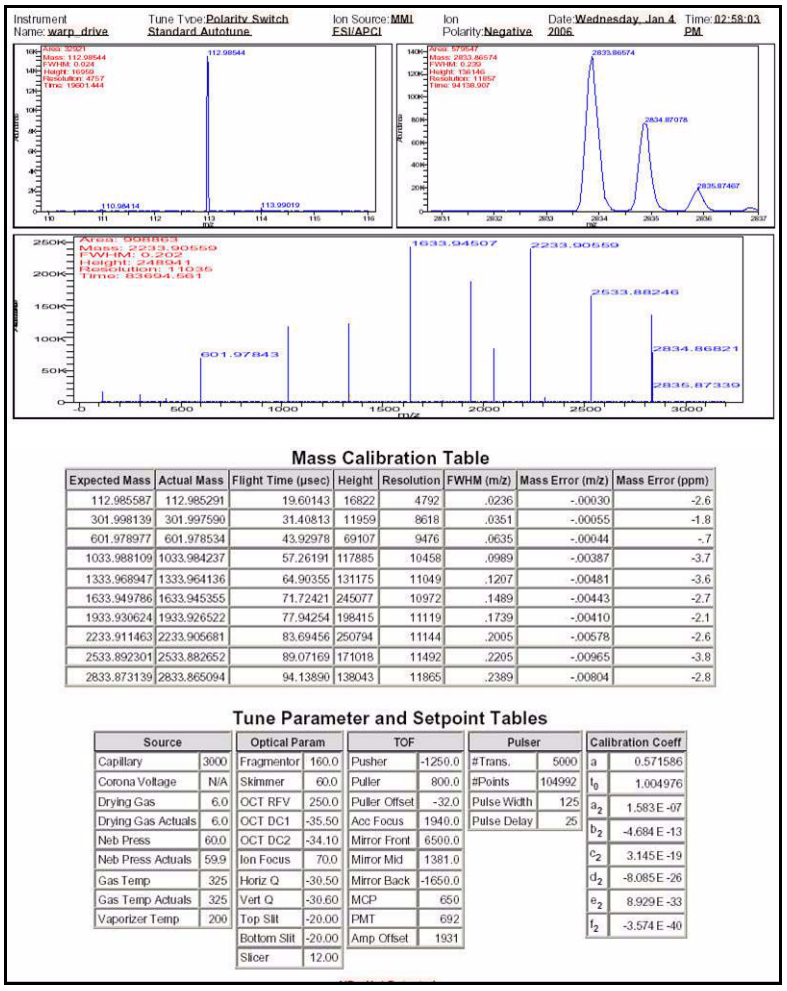
Tune Parameter and Setpoint Tables

Source		Optical Param		TOF		Pulser		Calibration Coeff	
Capillary	3000	Fragmentor	215.0	Pusher	1250.0	#Trans.	5000	a	0.571732
Corona Voltage	N/A	Skimmer	60.0	Puller	-800.0	#Points	104992	l_0	1.006036
Drying Gas	6.0	OCT RFV	250.0	Puller Offset	32.0	Pulse Width	125	a_2	1.830E-07
Drying Gas Actuals	5.9	OCT DC1	40.00	Acc Focus	-1940.0	Pulse Delay	25	b_2	-5.168E-13
Neb Press	60.0	OCT DC2	38.80	Mirror Front	-6500.0			c_2	3.373E-19
Neb Press Actuals	60.0	Ion Focus	-70.0	Mirror Mid	-1381.0			d_2	-8.570E-26
Gas Temp	325	Horiz Q	33.50	Mirror Back	1650.0			e_2	9.563E-33
Gas Temp Actuals	325	Vert Q	33.50	MCP	650			f_2	-3.953E-40
Vaporizer Temp	199	Top Slit	24.00	PMT	670				
		Bottom Slit	23.80	Amp Offset	1926				
		Slicer	-12.00						

ND - Not Detected

7 Load the associated polarity switching method negative. Example: MMIautotunePSNeg.m.

The instrument will generate a polarity switching negative report only for MMIautotunePSNeg.m.



Instrument Name: warp_drive | Tune Type: Polarity Switch Standard Autotune | Ion Source: MMI ESI/APCI | Ion Polarity: Negative | Date: Wednesday, Jan 4 2006 | Time: 02:58:03 PM

Mass Calibration Table

Expected Mass	Actual Mass	Flight Time (µsec)	Height	Resolution	FWHM (m/z)	Mass Error (m/z)	Mass Error (ppm)
112.985587	112.985291	19.60143	16822	4792	.0236	-.00030	-2.6
301.998139	301.997590	31.40813	11959	8618	.0351	-.00055	-1.8
601.978977	601.978534	43.92978	69107	9476	.0635	-.00044	-.7
1033.988109	1033.984237	57.26191	117885	10458	.0989	-.00387	-3.7
1333.968947	1333.964136	64.90355	131175	11049	.1207	-.00481	-3.6
1633.949786	1633.945355	71.72421	245077	10972	.1489	-.00443	-2.7
1933.930624	1933.926522	77.94254	198415	11119	.1739	-.00410	-2.1
2233.911463	2233.905681	83.69456	250794	11144	.2005	-.00578	-2.6
2533.892301	2533.882652	89.07169	171018	11492	.2205	-.00965	-3.8
2833.873139	2833.865094	94.13890	138043	11865	.2389	-.00804	-2.8

Tune Parameter and Setpoint Tables

Source		Optical Param		TOF		Pulser		Calibration Coeff	
Capillary	3000	Fragmentor	160.0	Pusher	-1250.0	#Trans.	5000	a	0.571586
Corona Voltage	N/A	Skimmer	60.0	Puller	800.0	#Points	104992	l_0	1.004976
Drying Gas	6.0	OCT RFV	250.0	Puller Offset	-32.0	Pulse Width	125	a_2	1.583 E -07
Drying Gas Actuals	6.0	OCT DC1	-35.50	Acc Focus	1940.0	Pulse Delay	25	b_2	-4.684 E -13
Neb Press	60.0	OCT DC2	-34.10	Mirror Front	6500.0			c_2	3.145 E -19
Neb Press Actuals	59.9	Ion Focus	70.0	Mirror Mid	1381.0			d_2	-8.085 E -26
Gas Temp	325	Horiz Q	-30.50	Mirror Back	-1650.0			e_2	8.929 E -33
Gas Temp Actuals	325	Vert Q	-30.60	MCP	650			f_2	-3.574 E -40
Vaporizer Temp	200	Top Slit	-20.00	PMT	692				
		Bottom Slit	-20.00	Amp Offset	1931				
		Slicer	12.00						

The instrument is ready for use with fast polarity switching tunes.

For MassHunter Workstation Software - Acquisition for TOF B.01.03

- Run autotune with the G1969-85000 Tune 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_2O + 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

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:

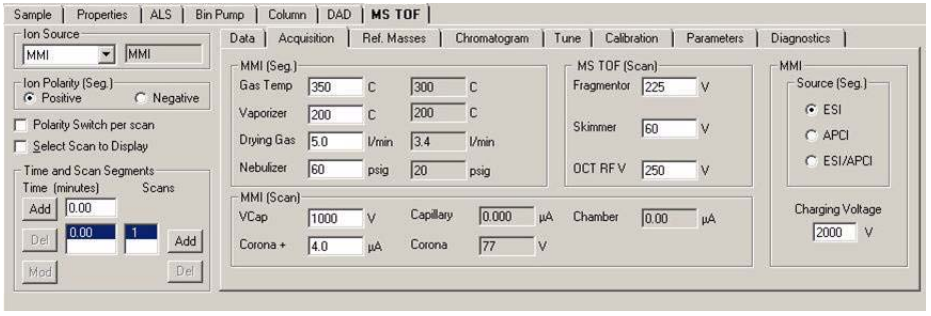


Figure 30 Acquisition parameters

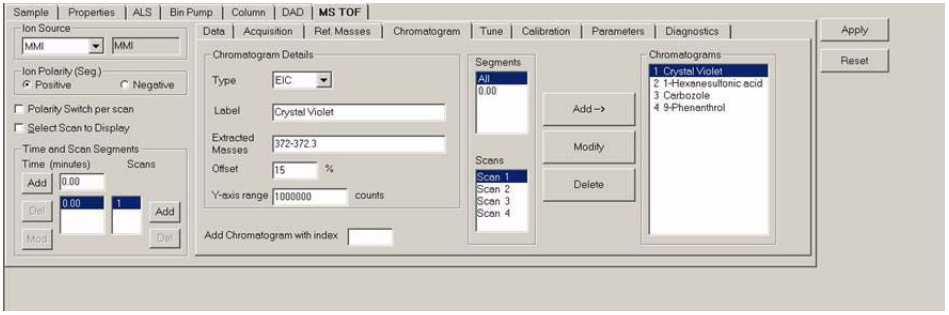


Figure 31 Chromatogram

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_2O + 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	

Step 4. Create MMCHECKTOF_EI_NEG.m

- Set the parameters for MMCHECKTOF_EI_NEG.m:

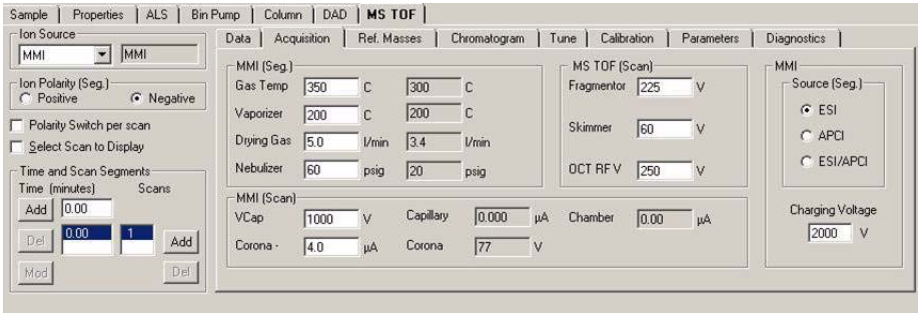


Figure 32 Acquisition

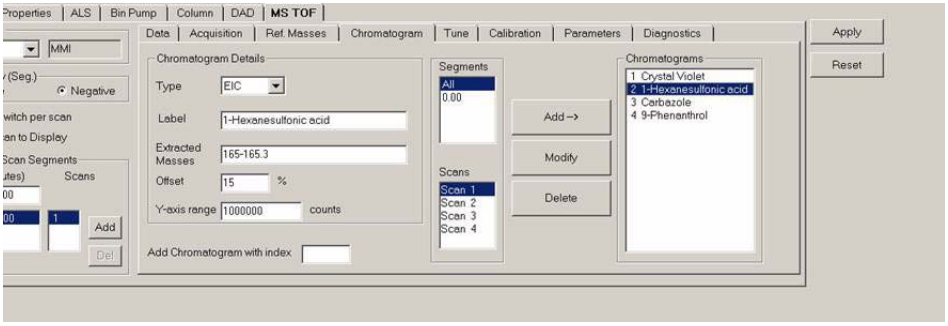


Figure 33 Chromatogram

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_2O + 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	

Step 5. Create MMCHECKTOF_CI_POS.m

- Set the parameters for MMCHECKTOF_CI_POS.m:

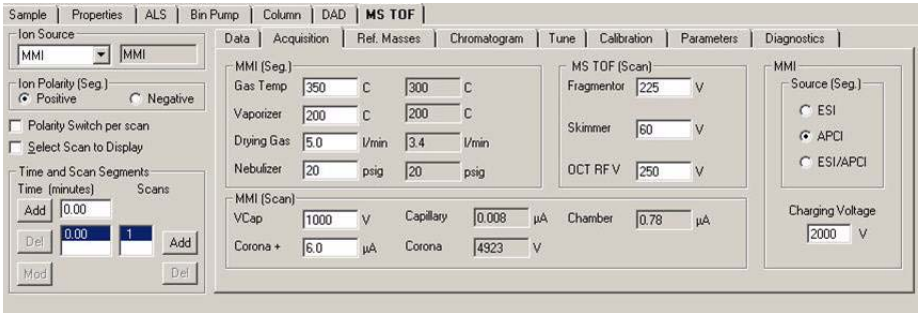


Figure 34 Acquisition

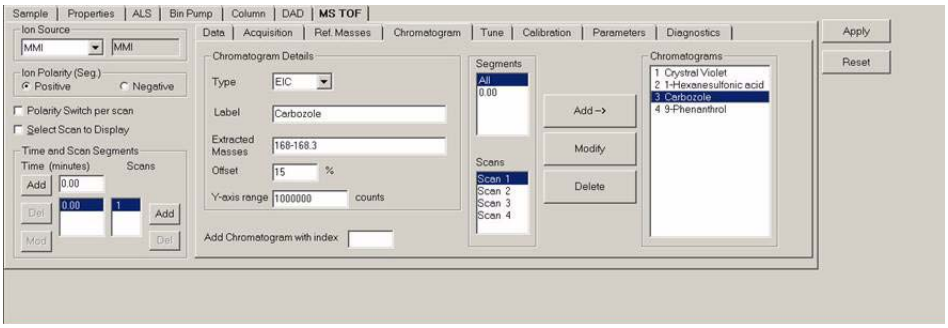


Figure 35 Chromatogram

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_2O + 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	

Step 6. Create MMCHECKTOF_CI_NEG.m

- Set the parameters for MMCHECKTOF_CI_NEG.m:

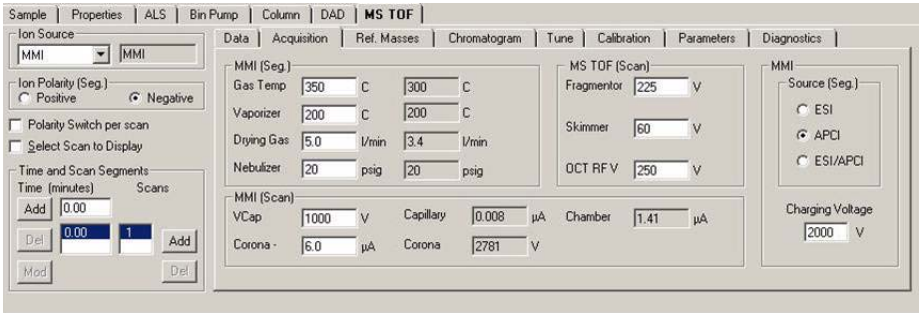


Figure 36 Acquisition

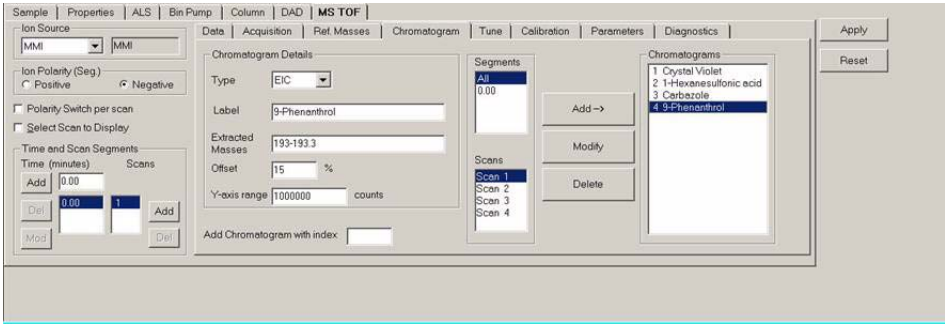


Figure 37 Chromatogram

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_2O + 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	

Step 7. Create MMCHECKTOF_MX_EI POS_CI POS.m

- Set the parameters for MMCHECKTOF_MX_EI POS_CI POS.m.

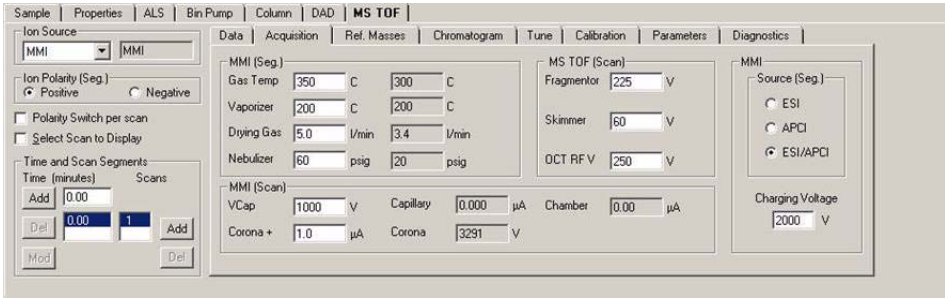


Figure 38 Acqusition

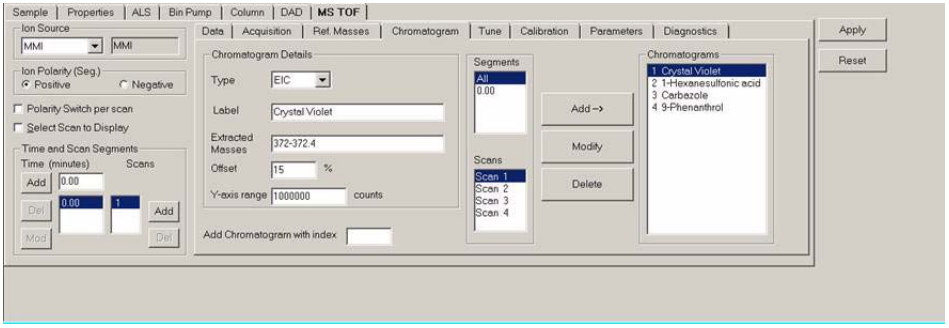


Figure 39 Chromatogram

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_2O + 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	

Step 8. Create MMCHECKTOF_MX_EI NEG_CI NEG.m

- Set the parameters for MMCHECKTOF_MX_EI NEG_CI NEG.m:

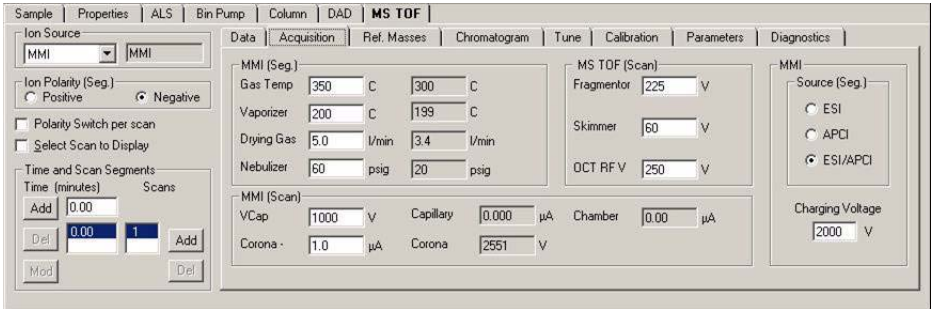


Figure 40 Acqusition

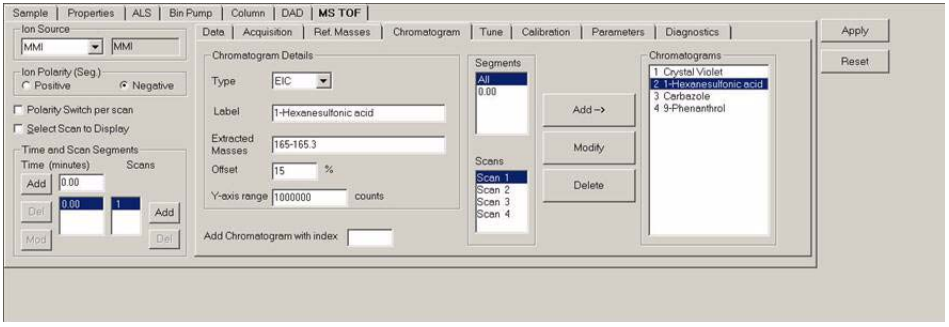


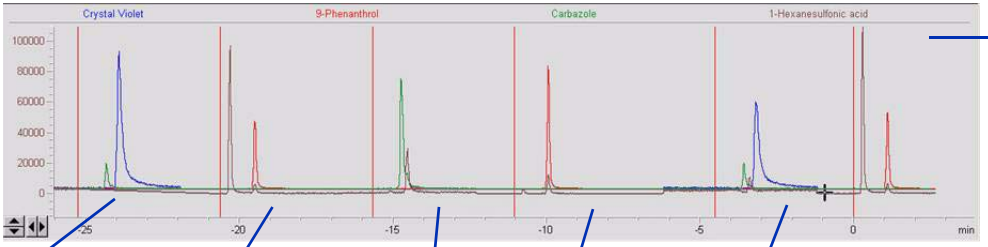
Figure 41 Chromatogram

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_2O + 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	

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.



ESI +APCI NEG
1-Hexanesulfonic acid &
9-Phenanthrol

ESI POS
Crystal Violet

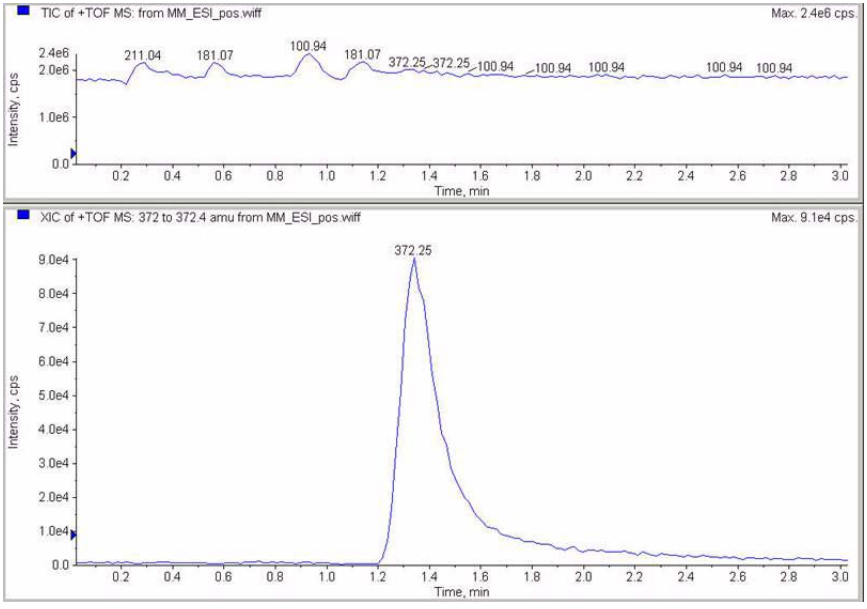
ESI NEG
1-Hexanesulfonic acid

APCI POS
Carbazole

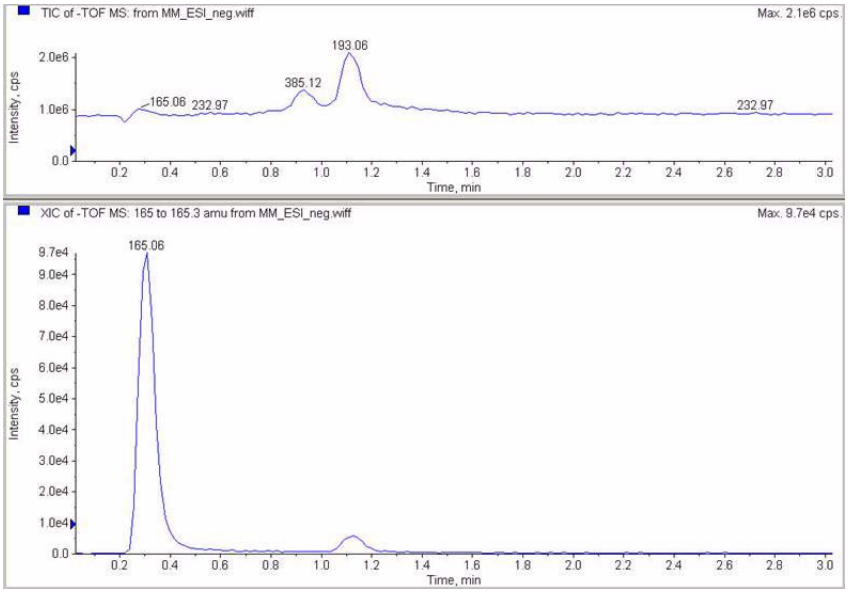
APCI NEG
9-Phenanthrol

ESI +APCI POS Crystal Violet & Carbazole

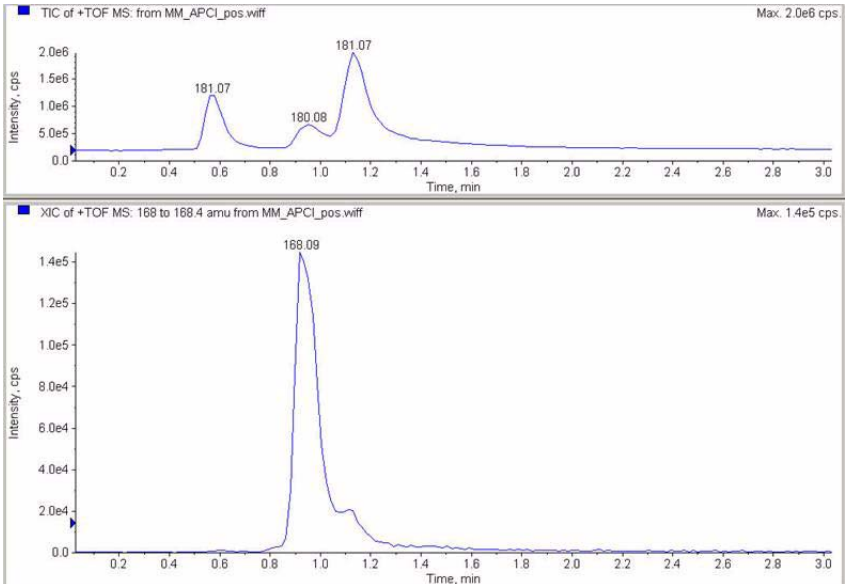
2 View the data from Analyst for MM_ESI_pos.wif. Exstract Ion 372- 372.4. Record peak height Example: 91,000.



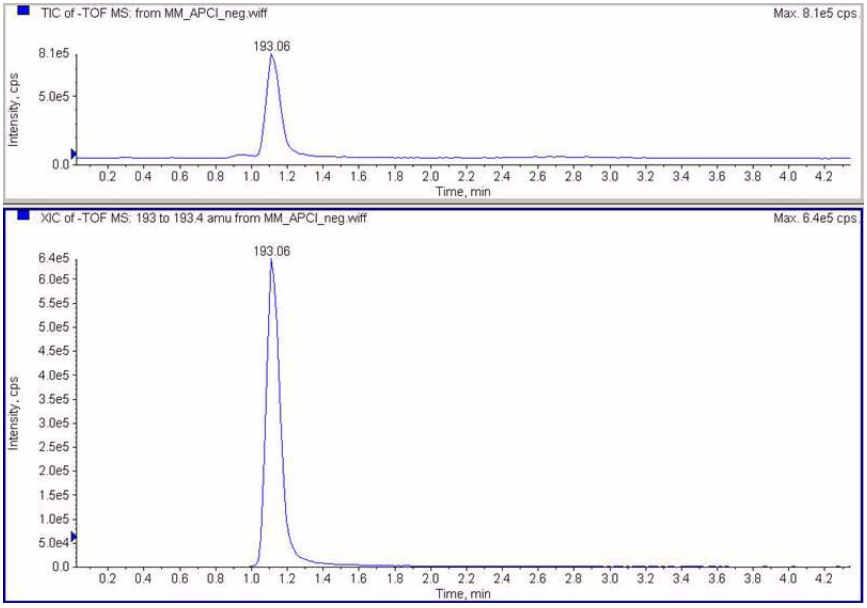
3 View the data in the data analysis program for MM_ESI_Neg. Extract Ion 165-165.4. Record the peak height Example 97,000.



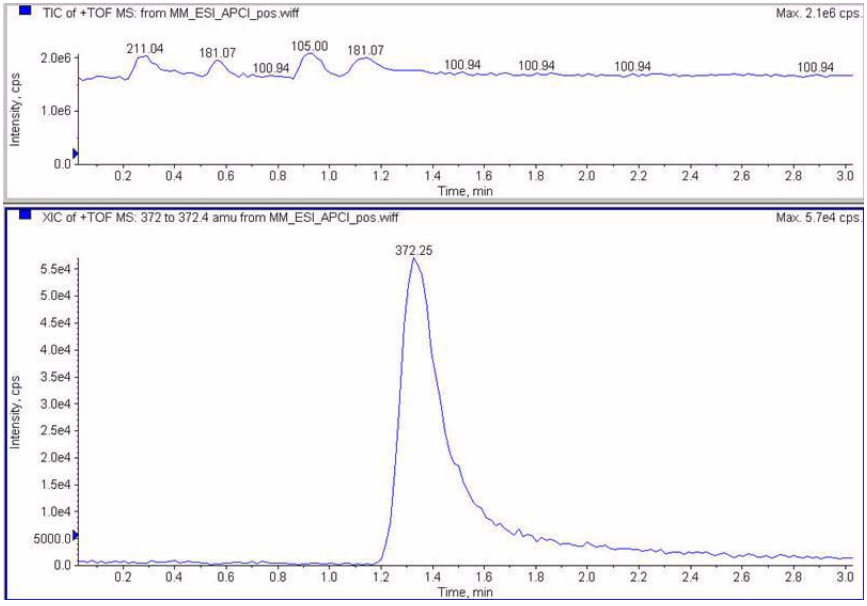
4 View the data in the data analys program for MM_APCI_POS. Extract Ion 168-168.4. Record the peak height. Example 140,000.



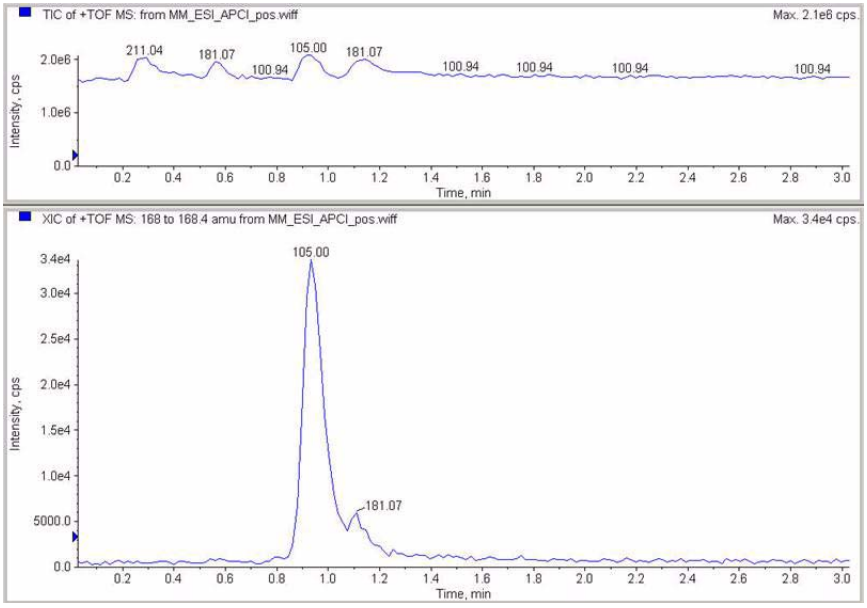
5 View the data in the data analysis program for MM_APCI_NEG. Extract Ion 193-193.4. Record the peak height. Example 640,000.



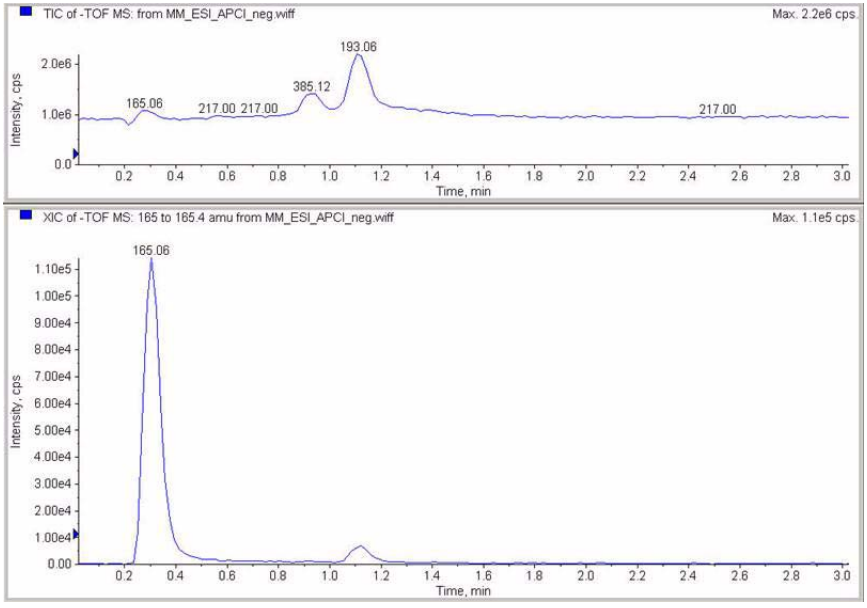
6 View the data in the data analysis program for MM_ ESI_APCI_POS. Extract Ion 372-372.4. Record the peak height. Example: 57,000.



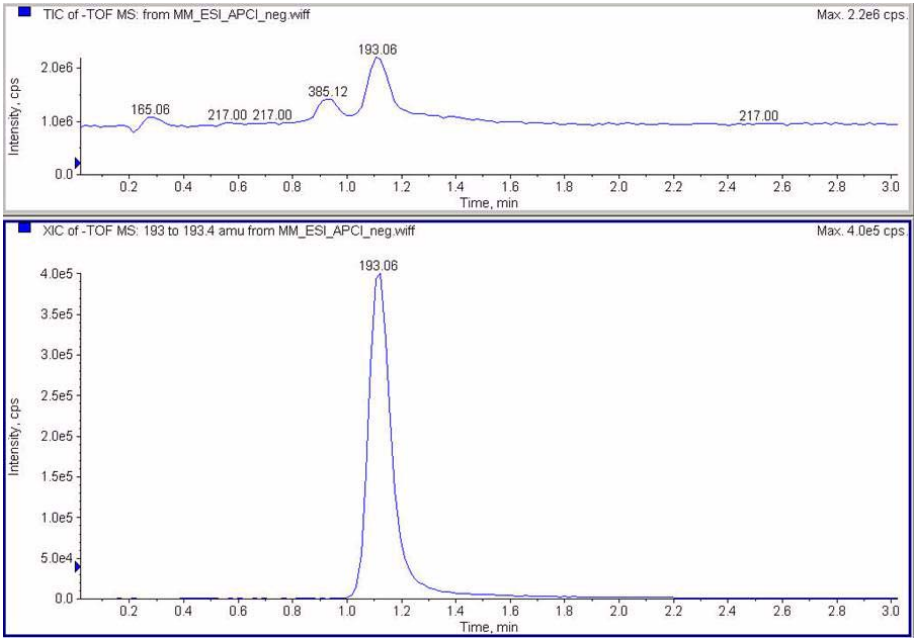
7 View the data in the data analysis program for MM_ ESI_APCI_POS. Extract Ion 168-168.4. Record the peak height. Example: 34,000.



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.



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.



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

- 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.

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In This Book

This book contains information to install, replace, and verify your Agilent G1978A Multimode for 6210/6220 TOF.

Printed in USA
First Edition, December 2008

G1978-90060

Agilent Technologies