



Analyst® TF 1.7.1 Software
SelexION™ Technology for TripleTOF® Systems

User Guide



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Introduction to DMS Technology

1

Note: For safety information, refer to the *System User Guide* for the mass spectrometer.



WARNING! Electrical Shock Hazard. Do not remove the cover or attempt to service the SelexION™ controller module. It contains no serviceable parts.

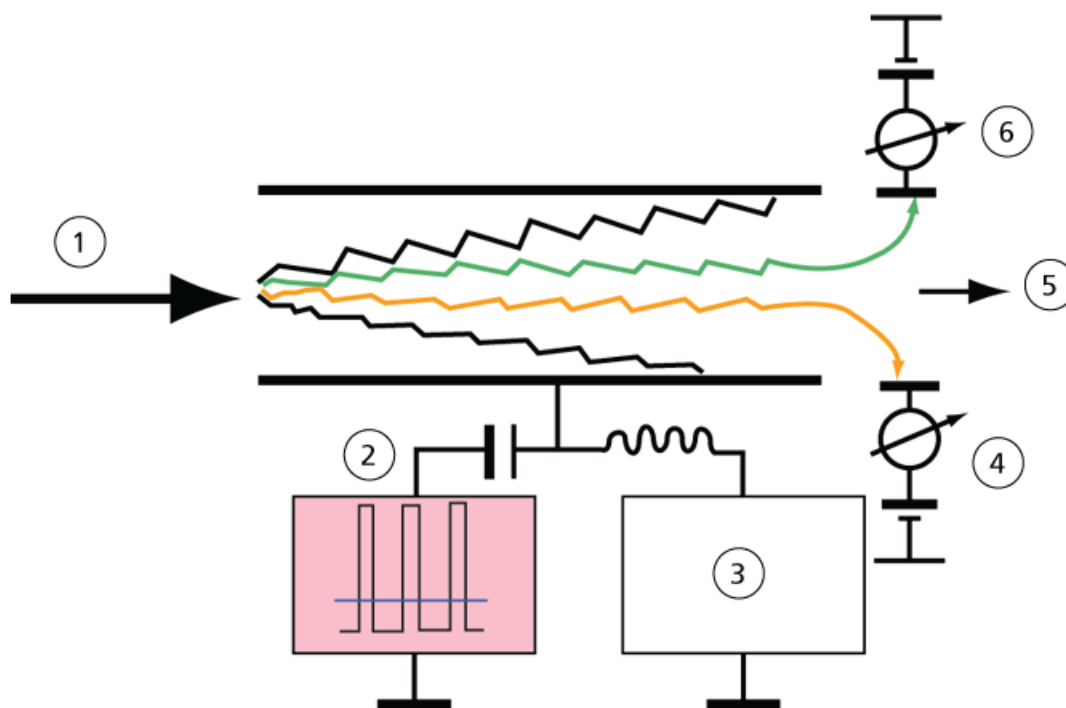
This section describes Differential Mobility Spectrometry (DMS) technology and its benefits, and the role of modifiers. The DMS Off operation mode is also discussed here.

About DMS Technology

DMS is a method of separating ions based on the difference between ion mobility in high and low electric fields in gases at or near atmospheric pressure. DMS is a variant of ion mobility spectrometry (IMS).

In DMS technology, Separation Voltages (SV) are applied across the ion transport channel, perpendicular to the direction of the transport gas flow, as shown in [Figure 1-1](#). Due to the difference between high- and low-electric-field ion mobility coefficients, ions migrate toward the walls and leave the flight path. Their trajectory is corrected by a counterbalancing DC voltage called Compensation Voltage (COV).

Figure 1-1 DMS Technology



Item	Description
1	Ion species in gas stream
2	Separation Voltage (SV)
3	Compensation Voltage (COV)
4	Positive ions
5	To mass spectrometer
6	Negative ions

Instead of recording the flight time of an ion through the ion transport channel, the DMS technology records the COV required to correct the trajectory of a particular ion for a range of SV amplitudes. The COV can be scanned to serially pass ions according to their differential mobility, or set to a fixed value to pass only the ion species with a particular differential mobility.

Certain combinations of SV and COV fields allow the target ion to pass through the SelexION™ device analytical region without colliding with the electrodes. Therefore, by scanning or fixing SV and COV, the SelexION device can operate in the following modes:

- A particular SV and COV combination can be selected, resulting in continuous filtration of particular ion species.
- When SV is fixed and COV scanned, a linear DMS spectra can be recorded.

Benefits of DMS Technology

The SelexION™ differential mobility separation technology device adds an additional dimension of separation to the TripleTOF® system.

- It enhances the quality of mass analysis and quantitative accuracy by reducing chemical noise, and by pre-separating ions of similar mass.
- It provides fast ion transit times and offers a transparent mode of operation (similar to when the SelexION technology is not installed on the system) that allows all ions to be transmitted without discrimination when SV and COV are set to zero.
- It supports simultaneous transmission of ions of both polarities and subjects each to separation based on their differential mobility constants.
- It reduces interferences in the product ion spectra.

Role of Modifiers in DMS Technology

Modifiers can be added to the gas transporting the ions through the SelexION™ device to increase the peak capacity and separation power of this device. The presence of these modifiers, which are typically common chromatography solvents (for example, isopropanol [2-propanol], acetonitrile, or methanol), affects the mobilities of ions in the device. Ions entering the mobility cell form clusters with the modifier molecules which alters their mobility characteristics. The clusters can form under low electric field conditions but fall apart again under high electric fields, which is referred to as the dynamic cluster-decluster model. The net effect of the cluster formation is that the differences between high- and low-field mobilities are amplified, yielding better separation power and increased peak capacity. Moreover, since cluster formation itself depends on the specific interaction between an analyte ion and a user-selected modifier, the use of modifiers offers an additional separation dimension to traditional chromatographic and mass spectrometric approaches. Further information on the effects of modifiers can be found in the following journal article: B.B. Schneider, T.R. Covey, S.L. Coy, E.V. Krylov, and E.G. Nazarov, *Anal. Chem.* **2010**, *82*, 1867-1880.

Because modifier use involves gas-phase ion chemistry, certain general behaviors can be expected. In positive ion mode, if the modifier has a greater proton affinity than the analyte ion, the charge may be stripped from the analyte resulting in lower signal but not necessarily lower signal-to-noise. Alternatively, if the modifier has greater gas-phase acidity than the analyte, the negative ion current will be reduced. Knowing the characteristics of the analyte and modifier can inform the appropriate choice of modifier. Using 2-propanol as a modifier is a good starting point for investigating the effect of modifiers on a given DMS separation because it has been observed to improve the separation power for a wide range of compounds.

Instrument Tuning

Before installing the SelexION™ device on the mass spectrometer, make sure that it is tuned and calibrated.

DMS Off Operation Mode

When the SelexION™ device is installed on the mass spectrometer, users might need to acquire spectral data without using the SelexION device. Instead of removing the SelexION device from the system, users can use the DMS Off operation mode to acquire data. The Analyst® TF software provides a DMS Off operation mode, which allows the user to work in an environment similar to when the SelexION device is not installed on the mass spectrometer. However, in the DMS Off mode, signal intensities will be significantly decreased as compared to the signal intensities of data acquired with the SelexION device physically removed from the mass spectrometer.

To work in the DMS Off operation mode, select the **DMS Off** check box available on the **MS** tab in the **Acquisition method** window or on the **MS** tab in the **Tune Method Editor** window.

Figure 1-2 DMS Off Check Box in the Tune Method Editor

The screenshot shows the 'MS' tab in the 'Tune Method Editor' window. The 'Advanced MS' sub-tab is active. The interface includes several control panels: 'Scan type' set to 'TOF MS', 'Accumulation time' at 0.250006 (secs), 'TOF Masses (Da)' with 'Min' at 100 and 'Max' at 2000, 'Polarity' set to 'Positive', and 'Display Mass' with a checked 'Center/Width' checkbox and a table with one row. The 'Period' section shows 'Duration' at 4.998 (mins), 'Cycles' at 1086, and 'Delay Time' at 0 (secs). At the bottom left, the 'DMS Off' checkbox is circled in red.

	Center (Da)	Width (Da)
1		

In the DMS Off operation mode, the following changes occur:

- Most of the DMS parameters are no longer available. Refer to [State of DMS Parameters in the DMS Off Mode on page 67](#). Only the **DMS Temperature (DT)** parameter is visible in the **DMS Off** mode, and it can be optimized in this mode to obtain the best sensitivity.
- The DMS parameters (SV, COV, and DMO) are removed from the parameter list in the **Ramp Parameter Settings** dialog.

- The default settling time becomes 19.974 ms.

Using the SelexION Technology

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An AB SCIEX TripleTOF® 5600+ or 6600 system with SelexION™ technology includes an Field Service Employee (FSE) installed controller module and associated electronics, along with a customer installed interface device.

Figure 2-1 6600 System with SelexION Technology



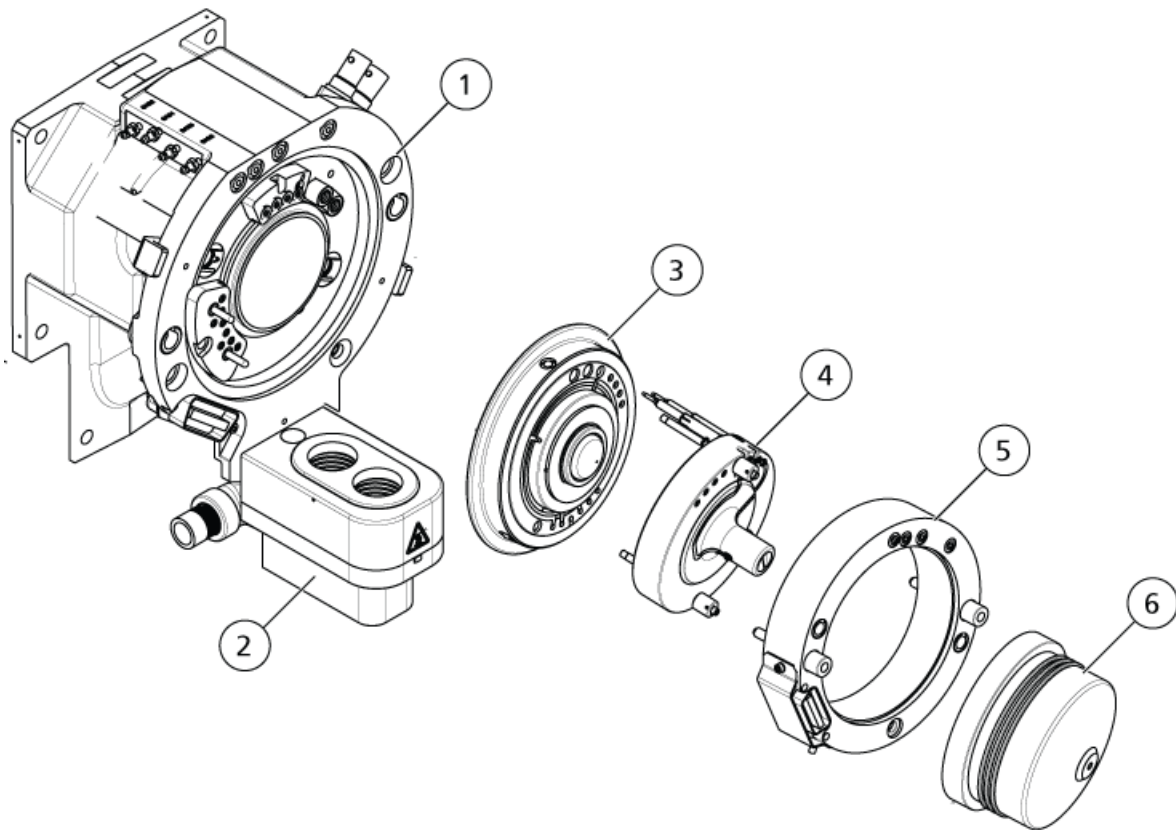
Item	Description	Comments
1	Controller module with side tray	FSE upgrade
2	Ion Source	The photo shows the IonDrive™ Turbo V ion source on a TripleTOF 6600 system.

Note: The NanoSpray[®] ion source can be installed on a TripleTOF system equipped with SelexION technology. However, modifier use is not available. Users can create acquisition methods that include modifier information and flows, but when executed the modifier pump will be disabled.

The SelexION device includes the following customer replaceable components:

- Ion mobility cell
- Adapter ring
Two adapter rings are available, the NanoSpray ring, used with the NanoSpray ion source, and the standard ring, used with all other supported ion sources.
- SelexION curtain plate

Figure 2-2 SelexION Technology



Using the SelexION Technology

Item	Description	Comments
1	Vacuum interface housing	FSE upgrade
2	Dual drain assembly	5600+: FSE upgrade 6600: Factory-installed
3	Ceramic orifice plate	FSE upgrade
4	Ion mobility cell	Customer installable
5	Adapter ring	Customer installable
6	SelexION curtain plate	Customer installable

Install the SelexION™ Technology



WARNING! Hot Surface Hazard. Let the ion source and vacuum interface components cool for at least 30 minutes before starting any maintenance procedures. With the IonDrive™ Turbo V ion source, let the ion source cool for at least 90 minutes.

CAUTION: Potential System Damage. Handle vacuum interface components with care. They are fragile and expensive.

CAUTION: Potential System Damage. Make sure that the vacuum interface components are kept clean and free of chemical or dust contamination. To prevent contamination, always wear powder-free gloves when handling the vacuum interface components.

Follow these steps to install the ion mobility cell, adapter ring, and SelexION curtain plate.

Prerequisite Procedures

- Make sure that both the ion mobility cell and the vacuum interface are clean. Use methanol to clean the surfaces.
- If the NanoSpray[®] interface components are installed, remove them and install the standard interface components. For detailed instructions, refer to the *NanoSpray[®] Ion Source Operator Guide*.

Note: The mass spectrometer must be shut down and vented before the interface components are changed.

Required Materials

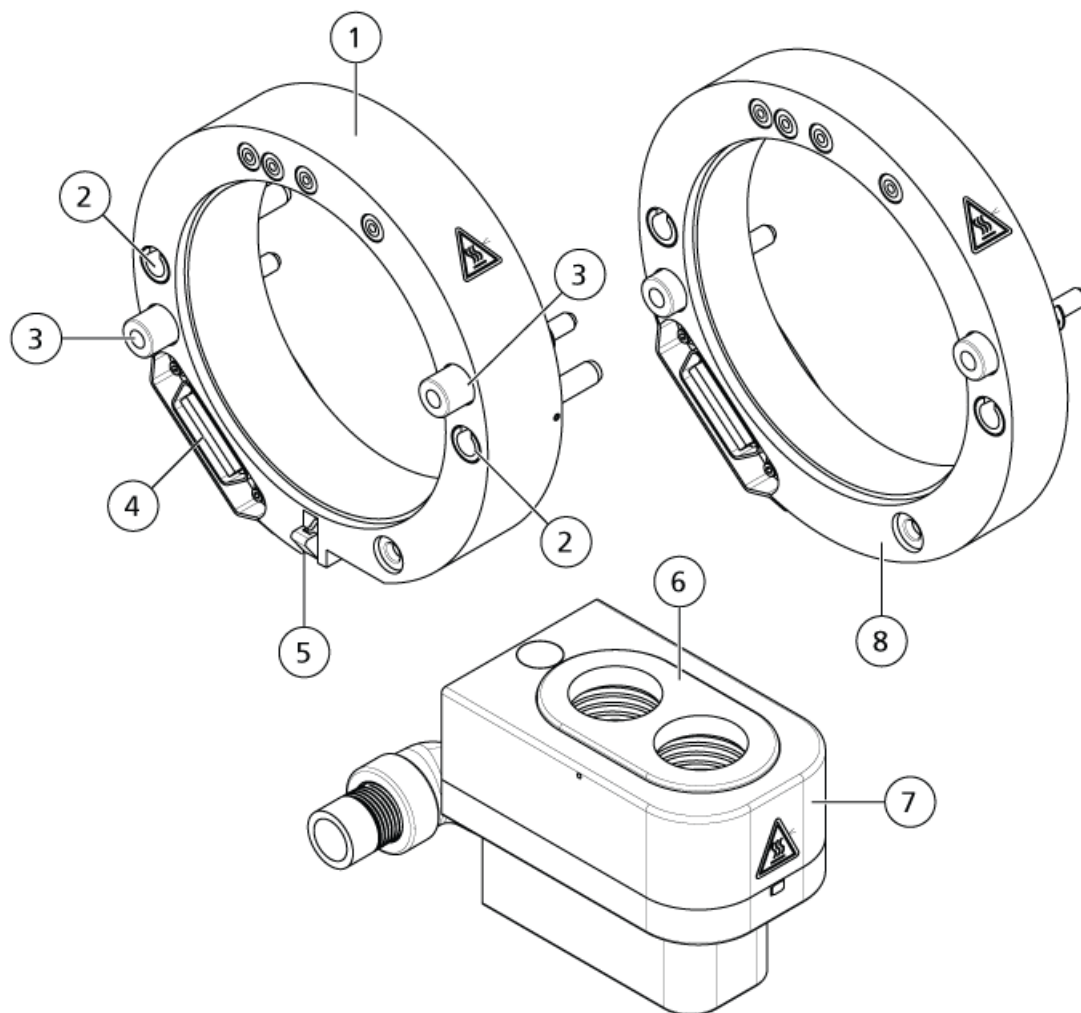
- Powder-free gloves (nitrile or neoprene recommended)

1. Complete any ongoing scans or click **Acquire > Abort Sample**.
2. Shut off the sample flow to the mass spectrometer.
3. Deactivate the active hardware profile.

Note: Failure to deactivate the active hardware profile before turning the SelexION[™] controller module on or off (to temporarily add or remove the SelexION technology to or from the system), may cause the mass spectrometer to enter an unstable state resulting in loss of control from within the Analyst[®] TF software. If the hardware profile is not deactivated and the mass spectrometer enters this unstable state, control can be recovered by removing and re-seating the ion source, or by turning both the mass spectrometer and controller module off and then on, and then reactivating the hardware profile.

4. Turn the two source latches upward to the 12 o'clock position to release the ion source.
5. Pull the ion source gently away from the vacuum interface.
6. Remove the curtain plate by pulling it straight off the vacuum interface. It is held in place by three retaining ball catches mounted on the orifice plate.
7. Position the SelexION adapter ring on the vacuum interface housing, aligning the connector on the ring with the source connector on the vacuum interface, and fitting the two thumbscrews on the adapter ring into the receptacles in the vacuum interface. Make sure that the source connector is fully seated, and that there are no gaps between the adapter ring and the vacuum interface.

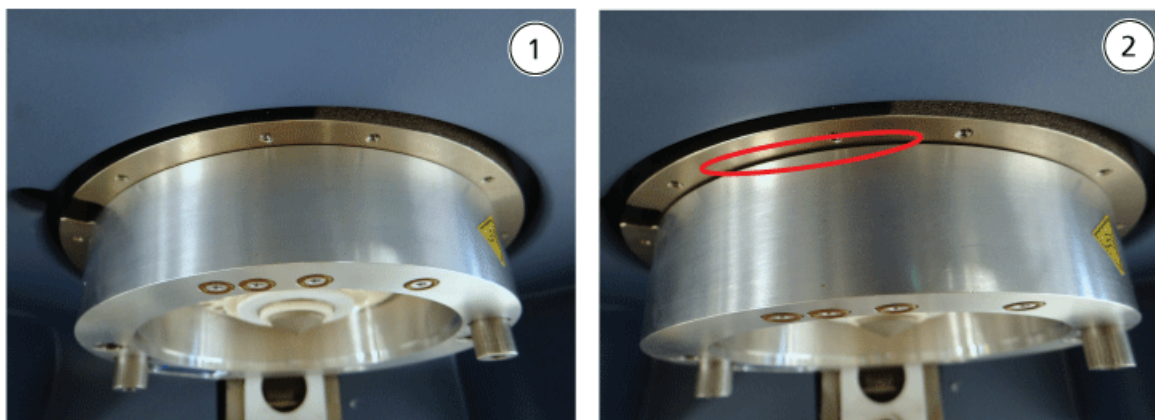
Figure 2-3 SelexION Adapter Ring and Dual Drain



Item	Description
1	Standard adapter ring
2	Receptacles (for ion source guide pins)
3	Thumbscrew
4	Interface connector
5	Latch
6	Spring-loaded plate

Item	Description
5	Dual drain
7	Latch
8	NanoSpray adapter ring

Figure 2-4 Ring Correctly (left) and Incorrectly (right) Installed



Item	Description
1	Correctly installed (no gap)
2	Incorrectly installed (gap highlighted)

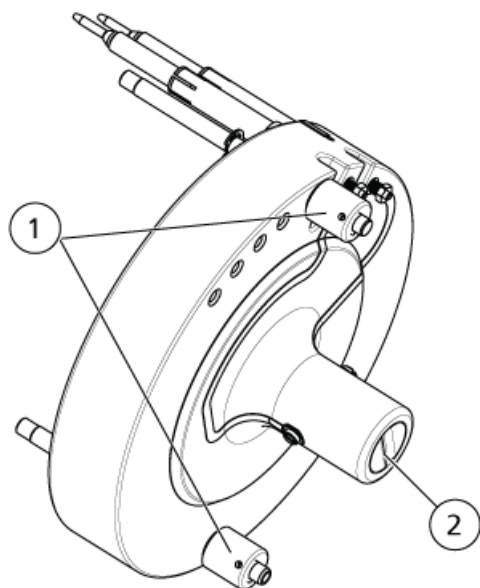
8. Tighten the thumbscrews evenly (alternating between the two thumbscrews), applying constant pressure.

Tip! After tightening the thumbscrews fully, pull on the extension ring to make sure that it is secured properly. If a gap appears, tighten the ring further.

Tip! To verify that the ring is installed correctly, install the ion source and then open the Analyst® TF software. In Manual Tune mode, set GS1 and GS2 to 80. If a loud hissing is audible at the front of the instrument, there is a gap. (The ring is not installed correctly.)

Tip! To tighten the thumbscrews on the NanoSpray ring, use a screwdriver.

Figure 2-5 SelexION Ion Mobility Cell

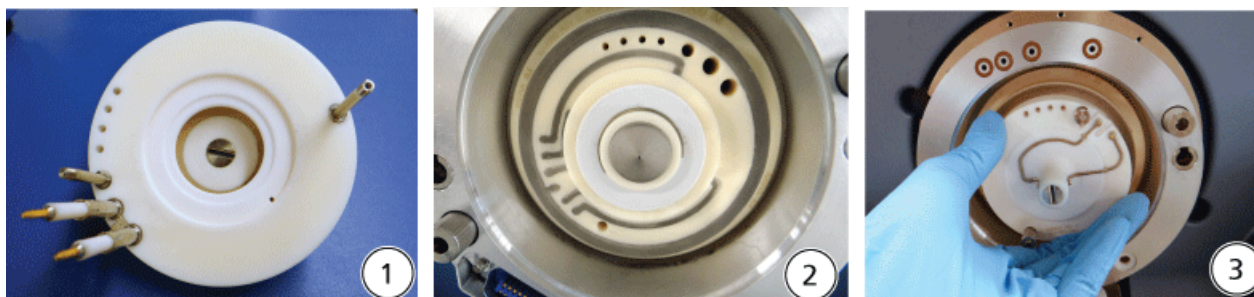


Item	Description
1	Thumbscrew
2	Electrodes

9. Position the SelexION ion mobility cell on the SelexION orifice plate, keeping the ion mobility cell vertical (perpendicular to the plane of the orifice plate), and making sure that the connectors are aligned with the sockets on the orifice plate.

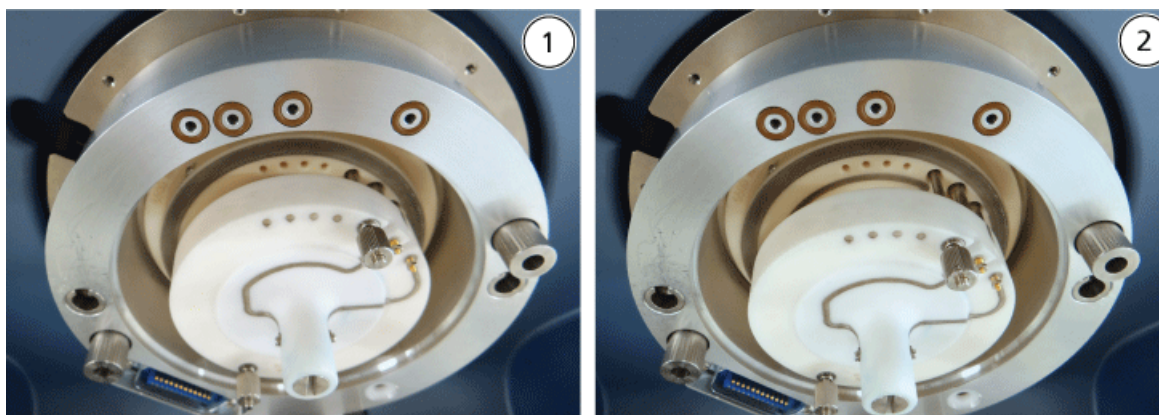
Note: Keep the surfaces of the orifice plate and the ion mobility cell clean, and do not scratch the ceramic seal on the ion mobility cell.

Figure 2-6 Ion Mobility Cell Installation



Item	Description
1	Ion mobility cell
2	Vacuum interface with the ring installed
3	Installation of the ion mobility cell

Figure 2-7 Ion Mobility Cell Correctly (left) and Incorrectly (right) Positioned



Item	Description
1	Correct position (vertical)
2	Incorrect position (angled)

10. Tighten the thumbscrews evenly, applying constant pressure.

Note: Do not loosen the nuts on the pins close to the thumbscrews.

11. Align the pins of the SelexION curtain plate with the holes in the ion mobility cell, and then press the SelexION curtain plate onto the ion mobility cell.

Using the SelexION Technology

12. Make sure that the two source latches on the ion source are pointing upwards in the 12 o'clock (open) position.
13. Position the ion source on the SelexION adapter ring. Make sure that the guide pins on the ion source fit into the receptacles in the adapter ring, push the ion source toward the interface until it is fully seated, and then rotate the source latches downward to the 6:30 (locked) position to lock the ion source in place. Refer to [Figure 2-3 on page 14](#).
14. Turn on the power to the SelexION technology.

The power switch is located on the back of the SelexION controller module.



WARNING! Toxic Chemical Hazard. Take care when filling or re-filling modifier bottles. Refer to chemical Safety Data Sheets and take appropriate safety precautions. Do not refill the modifier bottle while it is in the side tray. Disconnect the fluid line from the bottle, refill the bottle in a safe location, then reinstall the bottle and fluid line in the side tray.

15. If SelexION experiments using modifiers will be run, then purge the modifier pump. Refer to [Purge the Modifier on page 31](#).

Remove the SelexION™ Technology

Follow these steps to remove the SelexION™ curtain plate, adapter ring, and ion mobility cell, and to install the standard curtain plate. This procedure restores the TripleTOF® system to standard performance.

Required Materials

- Powder-free gloves (nitrile or neoprene recommended)



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

CAUTION: Potential System Damage. Handle vacuum interface components with care. They are very fragile and expensive.

CAUTION: Potential System Damage. Make sure that the vacuum interface components are kept clean and free of chemical or dust contamination. To prevent contamination, always wear powder-free gloves when handling the vacuum interface components.

1. Complete any ongoing scans or click **Acquire > Abort Sample**.
2. Shut off the sample flow to the mass spectrometer.

3. Deactivate the active hardware profile.

Note: Failure to deactivate the active hardware profile before turning the SelexION™ controller module on or off (to temporarily add or remove the SelexION technology to or from the system), may cause the mass spectrometer to enter an unstable state resulting in loss of control from within the Analyst® TF software. If the hardware profile is not deactivated and the mass spectrometer enters this unstable state, control can be recovered by removing and re-seating the ion source, or by turning both the mass spectrometer and controller module off and then on, and then reactivating the hardware profile.

4. Turn off the power to the SelexION technology.

The power switch is located on the back of the SelexION controller module.

5. Remove the adapter ring by loosening the thumbscrews and then pulling the adapter ring off the vacuum interface.
6. Remove the SelexION ion mobility cell by loosening the thumbscrews and then pulling the ion mobility cell off the orifice plate. Refer to [Figure 2-5 on page 16](#).
7. Install the standard curtain plate.

Note: Removal of the SelexION orifice plate and the dual drain assembly is not required. The IonDrive Turbo V ion source functions with the SelexION orifice plate, and uses the drain hole of the dual drain assembly closest to the interface housing.

8. Make sure that the two source latches on the ion source are pointing upwards in the 12 o'clock (open) position.
9. Position the ion source on the SelexION adapter ring. Make sure that the guide pins on the ion source fit into the receptacles in the adapter ring, push the ion source toward the interface until it is fully seated, and then rotate the source latches downward to the 6:30 (locked) position to lock the ion source in place. Refer to [Figure 2-3 on page 14](#).

Clean and Align the Ion Mobility Cell Electrodes

Clean and align the ion mobility cell electrodes when contamination is observed on the surfaces, or when repeated high-voltage discharge errors occur.

Required Materials

- Powder-free glove
- Small slotted screwdriver
- #600 sandpaper
- 1:1 methanol:water solution
- Spacer tool

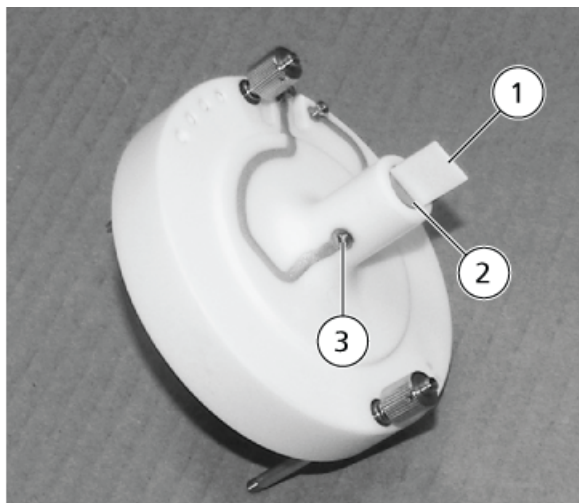


WARNING! Hot Surface Hazard. Let the ion source and vacuum interface cool for at least 30 minutes before starting any maintenance procedures. Some surfaces of the vacuum interface and the ion source become hot during operation.

CAUTION: Potential System Damage. Make sure that the vacuum interface components are kept clean and free of chemical or dust contamination. To prevent contamination, always wear powder-free gloves when handling the vacuum interface components.

1. Remove the ion mobility cell. Perform step 1 to step 8 in [Remove the SelexION™ Technology on page 18](#).
2. Using the small slotted screwdriver, loosen the adjusting screws until the electrodes move freely in the ion mobility cell and then remove the electrodes from the ion mobility cell.

Figure 2-8 SelexION Ion Mobility Cell



Item	Description	Comment
1	Spacer tool	Used to align the electrodes
2	Electrode	—
3	Adjusting screw	—

Note: If the adjusting screws are completely removed from the ion mobility cell, make sure that the bowed washers are replaced in the original orientation.

3. Using the #600 sandpaper, lightly scrub the flat surface of each electrode and then wash the electrodes with a 1:1 methanol:water solution.
4. Allow the electrodes to dry and then insert them into the ion mobility cell.
5. Move the spacer tool through the gap in the front of the electrodes and then, using the small slotted screwdriver, align the electrodes in the ion mobility cell so that the spacer tool is centered in the ion mobility cell.
Make sure that the spacer tools fits between the electrodes and then adjust the screws on each side of the ion mobility cell to center the electrodes.
6. Position the SelexION™ ion mobility cell on the SelexION orifice plate and then tighten the thumbscrews. Refer to [Install the SelexION™ Technology on page 12](#).

Refill the Modifier Bottle



WARNING! Toxic Chemical Hazard. Take care when filling or re-filling modifier bottles. Refer to chemical Safety Data Sheets and take appropriate safety precautions. Do not refill the modifier bottle while it is in the side tray. Disconnect the fluid line from the bottle, refill the bottle in a safe location, then reinstall the bottle and fluid line in the side tray.

1. Disconnect the fluid line from the modifier bottle in the side tray.
2. Refill the modifier bottle in a safe location, taking the appropriate safety precautions if needed.
3. Reinstall the modifier bottle in the side tray and then reconnect the fluid line.

Clean the SelexION™ Technology Surfaces

Clean the external surfaces of the SelexION™ technology after a fluid spill, or when they become dirty.

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

Use the SelexION™ Technology with the CDS

The SelexION™ technology can be used with the optional calibrant delivery system (CDS). To use the SelexION technology with the CDS:

1. Make sure that the CDS is installed on top of the modifier tray.
2. Plumb the ion source and CDS as described in the Appendix, "Single-Probe Configuration," in the *Calibrant Delivery System Operator Guide*.
3. Use the ESI calibration solution kits.

The DMS parameters must be optimized to obtain the best signal and separation of compounds of interest. For more information about DMS parameters, refer to [DMS Parameter Descriptions on page 64](#).

Optimize the DMS parameters with or without a modifier in the **Manual Tuning** mode. The DMS parameters can be optimized in the **Tune and Calibrate** mode in one of the following ways:

- As a starting point, use an existing acquisition method that was created for the compound to be analyzed, and that contains optimized compound parameters, source parameters, and LC flow rate, and then optimize the DMS parameters.
- Create an acquisition method, optimizing the compound parameters, source parameters, and the LC flow rate first, and then optimizing the DMS parameters.

This section describes the second method of optimizing the DMS parameters. The first method is a subset of the second method described in this section.

Optimize DMS Parameters in Manual Tuning

This section describes how to:

- Create an acquisition method in the **Manual Tuning** mode and optimize DMS parameters without a modifier.
- Purge the modifier.
- Create an acquisition method and optimize DMS parameters in the **Manual Tuning** mode, with a modifier selected.

Optimize DMS Parameters

Note: To acquire data using a modifier, create the acquisition method and then optimize the DMS parameters with the modifier selected in the method. The DMS parameters—Separation Voltage (SV), Compensation Voltage (COV), and DMS Offset (DMO)—are affected by the choice of a modifier. Therefore, adding or changing the modifier or the modifier concentration after optimizing the SV, COV, and DMO parameters will require a re-optimization of these parameters.

Prerequisites

- The SelexION™ technology is installed on the mass spectrometer and the controller module is turned on.
-

Note: Before turning the SelexION controller module on or off (to temporarily add the SelexION technology to or remove it from the system), first deactivate the active hardware profile within the Analyst® TF software. Failure to do so might cause the mass spectrometer to enter an unstable state resulting in loss of control from within the Analyst TF software. If the hardware profile is not deactivated and the mass spectrometer enters this unstable state, control can be recovered by removing and re-seating the ion source, or by turning both the mass spectrometer and controller module off and on and then reactivating the hardware profile.

Create an Acquisition Method and Optimize DMS Parameters without a Modifier

Use this procedure to create an acquisition method and optimize the DMS parameters for the compound in the **Manual Tuning** mode. A modifier is not required for this procedure.

1. Activate a hardware profile containing a syringe pump. Refer to *Creating Hardware Profiles and Projects* in the *Getting Started Guide* or the *System User Guide*.
2. T-infuse (or split-infuse) the sample into the LC stream. Refer to [T-Infuse Sample into LC Stream on page 69](#).
3. On the Navigation bar, click **Tune and Calibrate**, double-click **Manual Tuning**.
4. Select a scan type and then type the mass ranges and other required information. Optimize the compound and ion source parameters. Then, optimize the LC flow rate for the chromatographic method setup. Refer to the *Manual Optimization Tutorial*.
5. Click the **DMS** tab.

Figure 3-1 Default DMS Parameter Settings

Source/Gas	Compound	DMS	Resolution	Detector
DMS Temperature Reached				
DMS Temperature (DT)		Low		
Modifier (MD)		None		
Separation Voltage (SV)		0.0		
Compensation Voltage (COV)		0.0		
DMS Offset (DMO)		-3.0		
DMS Resolution Enhancement (DR)		Off		

All of the DMS parameters have default values. The **Separation Voltage (SV)** and the **Compensation Voltage (COV)** are set to zero.

6. Optimize the DMS parameters to get the best separation and sensitivity. The following parameters must be optimized in the specified order:
 - a. **DMS Temperature (DT):** Click **Start** to test this parameter with the default value **Low**. For the test, use the default values for other DMS parameters (SV = 0; COV = 0; Modifier = None) or switch to the DMS Off mode by selecting the **DMS Off** check box on the **MS** tab.

Figure 3-2 Tune Method Editor with Default DMS Parameter Settings

Source/Gas	Compound	DMS	Resolution	Detector	MS	Advanced MS						
DMS Temperature Reached					Scan type: Product Ion							
DMS Temperature (DT)		Low			Product Of: 30 (Da)	TOF Masses (Da) Min: 100 Max: 2000						
Modifier (MD)		None			Accumulation time: 0.100021 (secs)	<input checked="" type="radio"/> High Resolution <input type="radio"/> High Sensitivity						
Separation Voltage (SV)		0.0			Polarity: <input checked="" type="radio"/> Positive <input type="radio"/> Negative	Display Mass <input checked="" type="checkbox"/> Center/Width						
Compensation Voltage (COV)		0.0			<table border="1"> <thead> <tr> <th></th> <th>Center (Da)</th> <th>Width (Da)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td></td> <td></td> </tr> </tbody> </table>			Center (Da)	Width (Da)	1		
	Center (Da)	Width (Da)										
1												
DMS Offset (DMO)		-3.0			Period Duration: 5.000 (mins) Cycles: 2968 Delay Time: 0 (secs)							
DMS Resolution Enhancement (DR)		Off			<input type="checkbox"/> DMS Off							

Data is shown in the panes below the **Tune Method Editor**. If the signal obtained for the peak of interest is not satisfactory, then change the DT value to either **Medium** or **High** and then evaluate the signal again until the best signal is obtained.

Note: For each DT value change, let the system equilibrate for at least 30 minutes before optimizing the DMS parameters.

Optimize DMS Parameters

- b. **Modifier (MD):** Make sure that the value of this parameter is **None**.
- c. **Separation Voltage (SV) and Compensation Voltage (COV)** The SV and COV are tested together iteratively to find the SV and COV combination that gives the best signal and separation. Step SV through 0 to the maximum allowed SV range while ramping COV through the full COV range. Refer to [Ramp the Separation Voltage and Compensation Voltage on page 27](#).

Note: The full COV range is –100 volts to 100 volts. However, most compounds optimize between –20 volts to 30 volts in the absence of a modifier. Some compounds might optimize even higher than 30 volts. In the presence of a modifier, we recommend using at least –60 volts to 20 volts COV range because the negative COV shifts can be very large for some compounds. The maximum SV value is linked to DT and TEM parameters.

- d. **DMS Offset (DMO):** Ramp DMO for the optimized SV and COV combination. Refer to [Ramp DMO for the Optimized SV and COV Combination on page 27](#)
- e. **DMS Resolution Enhancement (DR):** For a single compound, use the **Off** (no throttle gas is being added) DR value. Other DR values, **Low**, **Medium**, or **High**, are used when the separation of compounds needs to be improved. For example, when two compounds have close COV and need to be baseline separated, test the Low, Medium, or High DR values to get the best separation. Select the required value (**Low**, **Medium**, or **High**) for the DR parameter and then click **Start** to ramp COV at a particular SV value to evaluate the signal and separation of the compounds. Test the different DR values until you are satisfied with the separation of the compounds.
[Table 3-1](#) shows the different DR values and the corresponding settling times.

Table 3-1 DR Values and the Corresponding Settling Times

DR Values	Settling Time Values	
	5600+	6600
Off	20 ms	30 ms
Low	30 ms	40 ms
Medium	40 ms	50 ms
High	50 ms	60 ms

Note: The DR readbacks show the actual pressure in the **Mass Spec Detailed Status** dialog. Double-click the **Mass Spec** icon on the status bar to open this dialog.

Note: When the value of DR is set to **Low**, **Medium**, or **High**, gas flow is enabled between the SelexION™ device exit and the orifice inlet into the mass spectrometer, which improves the resolution of the SelexION device.

7. Save the acquisition method after all of the DMS parameters have been successfully optimized.

Ramp the Separation Voltage and Compensation Voltage

1. Start with an **SV** value of **0**.

2. Click **Edit Ramp**.

The **Ramp Parameter Settings** dialog opens.

3. Select **Compensation Voltage** in the **Parameter** field.

4. Type **-20** in the **Start** field.

5. Type **30** in the **Stop** field.

6. Use the default value in the **Step** field or type a required step size and then click **OK**.

The **Ramp Parameter** check box is selected.

7. Click **Start**.

Data is shown in the panes below the **Tune Method Editor**. Note the maximum signal intensity. The COV value at which this maximum sensitivity is achieved should be zero.

8. Change the SV value to a number between 0 and the maximum allowed SV range, for example 2000.

Use SV in increments of 500 or more because the acceptable SV range is large.

9. Use the same COV range for ramping and then click **Start** to evaluate the signal again.

Data is shown in the panes below the **Tune Method Editor**. Note the maximum signal intensity and COV value at which the maximum signal was achieved.

10. Repeat the process of stepping SV and ramping COV and then note the SV value that gives the best signal intensity. After the signal intensity starts to decrease, stop the process. Further fine tune the SV value by repeating the above process with smaller SV steps in the 100 volt to 200 volt range as used above, and by ramping COV.

After the optimal SV and COV pair is determined, set the SV and COV parameters to these values in the method.

Ramp DMO for the Optimized SV and COV Combination

1. Click **Edit Ramp**.

The **Ramp Parameter Settings** dialog opens.

2. Select **DMS Offset** in the **Parameter** field.

3. Type **-30** in the **Start** field.

4. Type **30** in the **Stop** field.

5. Use the default value in the **Step** field or type a number and click **OK**.

Optimize DMS Parameters

6. Click **Start**.

Data is shown in the panes below the **Tune Method Editor**. The allowed range for DMO is –100 volts to 100 volts.

Create an Acquisition Method with a Modifier Selected and Optimize DMS Parameters

Note: Modifiers cannot be used with the NanoSpray[®] ion source. Users are able to create acquisition methods that include modifier information and flows, but when executed the modifier pump will be disabled.

If the compounds of interest did not get adequately separated in the DMS mode, a modifier can be introduced to help separate these compounds. A modifier is a chemical that is added into the Curtain Gas[™] flow to help improve the separation of compounds.

Select a modifier and optimize the DMS parameters in **Manual Tuning** mode and then create an acquisition method to save the optimized parameter settings.

Before selecting a modifier for the first time or when changing the modifier, purge the modifier line. Refer to [Purge the Modifier on page 31](#).

Prerequisites

- There is sufficient modifier in the modifier bottle for acquisition. For more information about calculating modifier consumption, refer to [Example Modifier Consumption Calculation](#).
- To refill the modifier bottle, refer to [Refill the Modifier Bottle on page 22](#).

1. T-infuse the sample into the LC stream. [T-Infuse Sample into LC Stream on page 69](#).
2. On the Navigation bar, under **Tune and Calibrate**, double-click **Manual Tuning**.
3. Select a scan type and then type the mass range and other required information. Optimize the compound and source parameters. Then, optimize the LC flow rate according to your chromatographic method setup. Refer to the [Manual Optimization Tutorial](#).

Tip! As a starting point, an existing acquisition method that has been optimized for the compound to be analyzed can be used. The existing method can use no modifier, or it can use a different modifier than the one currently in use. The method used as a starting point provides optimized source and compound parameters and an LC flow rate. The DMS parameters must be modified for the required modifier.

4. Click the **DMS** tab.
5. Optimize the DT parameter as described in [Create an Acquisition Method and Optimize DMS Parameters without a Modifier on page 24](#).

- In the **Modifier (MD)** parameter, select a modifier from the list. Select one of the pre-defined modifiers. To use a modifier other than the pre-defined ones, select **Custom**.

Figure 3-3 DMS Parameter Settings

Source/Gas	Compound	DMS	Resolution	Detector
DMS Temperature Reached				
DMS Temperature (DT)	Low			
Modifier (MD)	None			
Separation Voltage (SV)	None			
Compensation Voltage (COV)	2-Propanol			
	Acetonitrile			
	Methanol			
	Acetone			
	Custom			
DMS Offset (DMO)				
DMS Resolution Enhancement (DR)	Off			

The **Modifier Composition (MDC)** parameter is shown with its default value, which is set to **Low**.

- In the **MDC** parameter, if required, select **High** to test the modifier concentration that would provide the optimal separation.

Low is 1.5% or higher, and **High** is 3.0% concentration of modifier.

The software uses the **Curtain Gas** flow rate value and the density and molecular weight of the selected modifier to calculate the flow rate of the modifier and then applies that flow rate automatically.

- If **Custom** was selected for the **Modifier (MD)** parameter in step 6, then provide the density and molecular weight of the custom modifier as shown in [Figure 3-4](#) so that the software can calculate the flow rate for the modifier for the specified setting (**Low** or **High**) and then apply it.

Optimize DMS Parameters

Figure 3-4 DMS Parameter Settings

Source/Gas	Compound	DMS	Resolution	Detector
DMS Temperature Reached <input type="checkbox"/>				
DMS Temperature (DT)		Low		
Modifier (MD)		Custom		
Modifier Composition (MDC)		Low		
Modifier Density (g/mL) (MDD)		0.0000		
Modifier MW (MDW)		0.00		
Separation Voltage (SV)		0.0		
Compensation Voltage (COV)		0.0		
DMS Offset (DMO)		-3.0		
DMS Resolution Enhancement (DR)		Off		

Parameter	Description
Modifier Density (g/mL) (MDD)	Specify the density of the custom modifier. The software uses this density along with the Modifier Molecular Weight (MDW) and the Curtain Gas flow rate value to determine the flow rate of the custom modifier.
Modifier MW (MDW)	Specify the molecular weight of the custom modifier in g/mol. The software uses the value of this parameter along with the Modifier Density (MDD) and the Curtain Gas flow rate value to determine the flow rate of the custom modifier.

Tip! To view the modifier pump flow rate in the **Mass Spec Detailed Status** dialog, double-click the **Mass Spec** icon on the status bar.

- For the selected modifier and the MDC value, tune the SV, COV, and DMO parameters as described in [Create an Acquisition Method and Optimize DMS Parameters without a Modifier on page 24](#), until the signal and separation are satisfactory.

Note: For each change in modifier type or concentration, allow the system to equilibrate for at least 30 min before optimizing the DMS parameters.

To test a different modifier concentration (High or Low) of the same modifier (selected in step 6), select a different MDC value (Low or High) and then re-optimize the SV, COV, and DMO parameters as described in [Create an Acquisition Method and Optimize DMS Parameters without a Modifier on page 24](#).

To use a different modifier do the following:

- a. Purge the modifier line. Refer to [Purge the Modifier on page 31](#).
 - b. Select a different modifier in the acquisition method and then specify the MDC value for the new modifier.
 - c. Re-optimize the SV, COV, and DMO parameters as described in [Create an Acquisition Method and Optimize DMS Parameters without a Modifier on page 24](#).
10. If needed, optimize the DR parameter as described in [Create an Acquisition Method and Optimize DMS Parameters without a Modifier on page 24](#).
11. Save the acquisition method.

Real-Time Modifier Parameters Control

If data is acquired in **Manual Tuning** using the acquisition method created in the previous topic, and the user changes the MDC value from **Low** to **High** or **High** to **Low** during acquisition, then the software immediately calculates the required modifier pump flow rate and adjusts the modifier pump accordingly.

Similarly, if during acquisition the user changes the molecular weight or molecular density of the custom modifier specified in the acquisition method, then the software immediately calculates the required modifier pump flow rate and then adjusts the modifier pump accordingly.

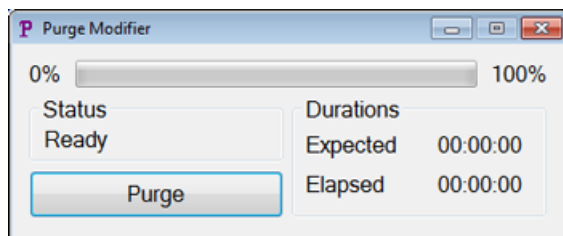
Purge the Modifier

Before using a new modifier, purge the modifier currently being used from the modifier pump. Purging the modifier will take about four minutes during which the mass spectrometer will be unavailable for use.

A modifier can be purged or cleared from the modifier pump from the **Manual Tuning** or **Acquire** mode when the SelexION™ device is turned on.

1. Make sure that the SelexION controller module is turned on and then activate a hardware profile. Refer to [Creating Hardware Profiles and Projects in the System User Guide](#).
2. Connect the bottle containing the other modifier to the modifier pump.
3. Do one of the following:
 - If the software is in **Acquire** mode with samples in the acquisition queue, then refer to [Purge Modifiers from Acquire Mode with Samples in the Acquisition Queue on page 34](#).
 - If the software is already in **Manual Tuning** or **Acquire** mode, then go to step 4.
 - If the software is not in either **Manual Tuning** or **Acquire** mode, then on the Navigation bar, click **Acquire** or **Tune and Calibrate**.
4. Click the **Purge Modifier** icon on the toolbar.

Figure 3-5 Purge Modifier Dialog



The **Purge Modifier dialog** opens. The status shows as **Ready**, which indicates the system is ready to start the purge process.

5. Click the **Purge** button.

The purge process starts. If the modifier purge was initiated from the **Manual Tuning** mode, the system is automatically entered into a non-Tuning mode, and the **Reserve Instrument for Tuning** icon becomes deselected on the toolbar. Refer to [About the Purge Process on page 32](#).

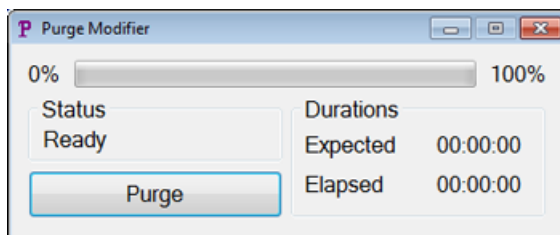
6. Click **X** to close the **Purge Modifier** dialog.

When the purge finishes, equilibrate the system for approximately 30 minutes. To equilibrate the system, open the acquisition method to be run, and start it. Then stop the acquisition. Wait 30 minutes.

About the Purge Process

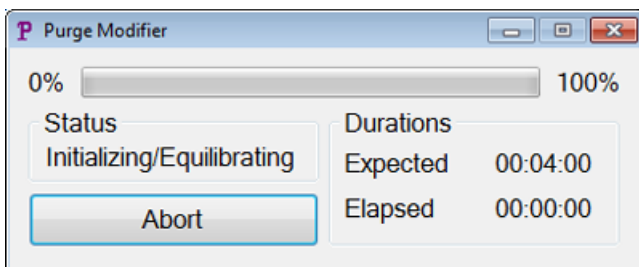
If the modifier purge was initiated in Manual Tuning mode, the system is automatically entered into a non-tuning mode, and the **Reserve Instrument for Tuning** icon becomes deselected on the toolbar.

Figure 3-6 Purge Modifier Dialog



The purge process enters the **Initializing/Equilibrating** mode. While in the initializing mode, an acquisition method and a batch file are created in the background. During the **Equilibrating** mode, the system is equilibrating.

Figure 3-7 Purge Modifier Dialog

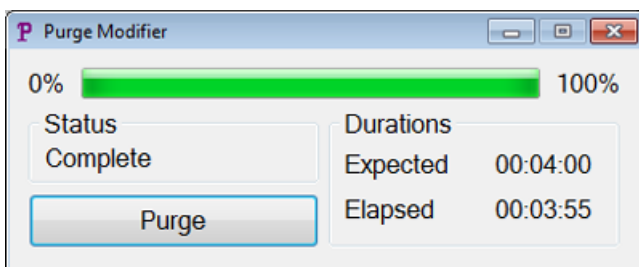


The status in the **Purge Modifier** dialog then changes from **Initializing/Equilibrating** to **Purging**, which indicates that the modifier is being cleared from the modifier pump. During the modifier purge, the mass spectrometer performs a scan and collects data in the API Instrument\Data folder. After the purge is complete, the purge acquisition method, batch file, and data are automatically deleted.

During purging, the **Purge** button changes to **Abort**. The expected purge time (four minutes) and the time elapsed in the purge cycle are shown. The Analyst® TF software automatically sets the DMS and source parameters to new values for four minutes (expected purge time). To view these values, refer to [Values of DMS and Source Parameters Used During Modifier Purge on page 67](#).

Tip! Users can view the status of the modifier purge process in the **Mass Spec Detailed Status** dialog. Double-click the **Mass Spec** icon on the status bar to view this dialog.

Figure 3-8 Purge Modifier Dialog



Purging the modifier from the modifier pump takes about four minutes. After the Purge process is complete, the status in the **Purge Modifier** dialog changes to **Complete**. The **Abort** button changes back to **Purge**. The system automatically re-enters Manual Tuning mode if the modifier purge was initiated from Manual Tuning mode. The values of some DMS and source parameters are reset. To view the reset values, refer to [Values of DMS and Source Parameters After Modifier Purge is Completed or Aborted on page 68](#).

Abort the Purge Process

- In the **Purge Modifier** dialog, click **Abort**.

Optimize DMS Parameters

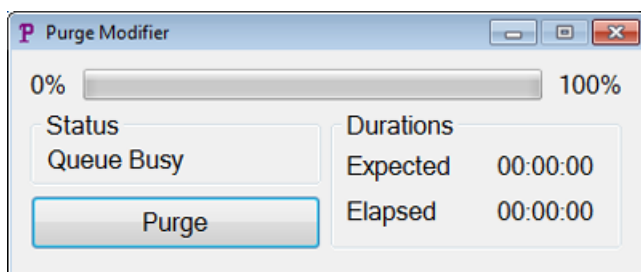
The purge cycle is terminated, and the values of some DMS and source parameters are reset. To view the reset values, refer to [Values of DMS and Source Parameters After Modifier Purge is Completed or Aborted on page 68](#).

The **Status** changes to **Aborted**, and the **Abort** button changes to **Purge**. If the modifier purge was initiated from Manual Tuning mode, after abort, the system is set back into Manual Tuning mode. After the modifier purge is aborted, allow the system to equilibrate for approximately 10 minutes with the required source conditions and the new modifier running before acquiring new samples.

Purge Modifiers from Acquire Mode with Samples in the Acquisition Queue

If the system is in the **Acquire** mode with samples in the acquisition queue, and the user selects the **Purge Modifier** icon, then a Queue Busy message is shown in the **Purge Modifier** dialog.

Figure 3-9 Purge Modifier Dialog



If the **Purge** button is clicked, then a message is shown indicating that the acquisition is currently in progress. For the purge to continue, complete or cancel the acquisition process and then make sure that no samples are waiting in the queue.

Modifier Purge Status

Purge Status	Description
Ready	The system is ready to start the Purge process.
Initializing/Equilibrating	An acquisition method and batch files are created during Initializing mode. The system is equilibrated during Equilibrating mode.
Purging	Modifier purge is in progress.
Aborted	The purge cycle is terminated.
Queue Busy	Acquisition is in progress. Purge is not possible.
Complete	The purge process is complete.

Instrument Optimization

Instrument optimization with the SelexION™ device installed should only be used for troubleshooting or correcting minor resolution or calibration issues. For full instrument optimization, we recommend that the SelexION ion mobility cell be removed from the ion source before instrument optimization is performed.

This section describes how to do the following:

- Create an acquisition method in the Acquire mode to optimize COV by ramping in two different ways during batch acquisition.
- Learn about the capability of the SelexION™ technology to separate isobaric compounds.
- Create an MRM^{HR} acquisition method with DMS parameters.
- Learn about modifier consumption calculations.

Prerequisites

- The SelexION™ technology is installed on the mass spectrometer and the controller module is turned on.

For separation of compounds using the liquid chromatography method, the SelexION device can be used with the **Ramp COV in LC Mode** option to ramp COV during batch acquisition.

For analysis of samples by infusion, for example metabolism using surface sampling techniques, the SelexION device can be used for separation of compounds along with the **Ramp COV for Cycle** option to mimic the LC gradient.

Use the methods created in this section to submit batches to acquire data. Refer to the *System User Guide* for the mass spectrometer.

Optimize the COV parameter Using the Ramp COV in LC Mode

A single-period, multiple-experiment acquisition method can be created using the **Ramp COV in LC Mode** option, where each experiment has a different COV value. This acquisition method can be run alongside an LC gradient to determine the optimal COV value for analytes eluding during an LC run. The data acquired using this method will generate a COV map on an LC timescale.

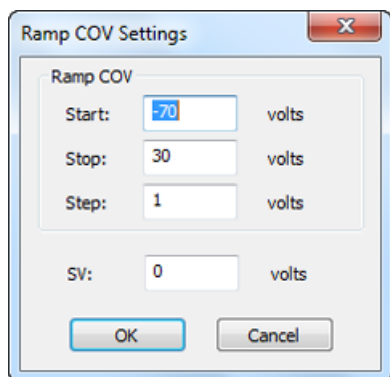
The Ramp COV in LC Mode works for TOF MS or Product Ion scan types.

Use this procedure after values or acceptable default values for all the DMS parameters except COV have been optimized.

1. Activate a hardware profile containing the necessary devices. Refer to *Create a Hardware Profile* in the *System User Guide* for the mass spectrometer.
2. On the Navigation bar, under **Acquire**, double-click **Build Acquisition method**.

3. Select the **TOF MS** or **Product Ion** scan type, type the mass range, acquisition time, and other required information.
4. Click **Edit Parameters**.
The **Parameter Settings** dialog opens.
5. Type the optimized values of the compound parameters on the **Compound** tab. Refer to the *Manual Optimization Tutorial*.
6. Type the optimized values of the ion source and gas parameters on the **Source/Gas** tab. Make sure that the source temperature (TEM) specified here is the same value as the one used for optimizing the DMS parameters. Refer to the *Manual Optimization Tutorial*.
7. Click the **DMS** tab and do the following:
 - a. Select the required values for the **DMS Temperature (DT)**, **Modifier (MD)**, and **DMS Resolution Enhancement (DR)** parameters. Make sure that the DMS temperature specified here is the same as the one used for optimizing the DMS parameters.
 - b. Type the optimized **DMO** value for all the compounds in the **DMS Offset (DMO)** field.
 - c. Click **OK**.
8. Click **Ramp COV in LC Mode** and provide the following COV values in the allowed COV range of –100 volts to 100 volts:

Figure 4-1 Ramp COV Settings Dialog



Field	Description
Start	Type the voltage at which the ramping starts.
Stop	Type the voltage at which the ramping stops.
Step	Set the step size.
SV	Type the separation voltage to use to ramp the COV value.

9. Click **OK**.
10. Type the LC gradients and flow rates according to the desired chromatographic method setup.
11. If required, provide values for the parameters of the peripheral devices included in the active hardware profile.
12. Save the acquisition method. It can be used to ramp COV in LC mode during batch acquisition of samples and acquiring data.

Optimize the COV parameter Using the Ramp COV for Cycle Option

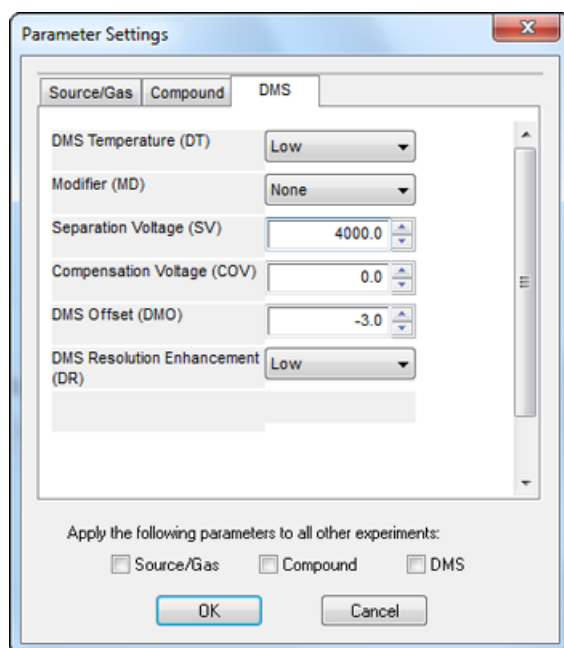
Use this procedure when the optimized values or acceptable default values for all the DMS parameters except COV have been obtained.

The **Ramp COV for Cycle** option can be used to create a single-period, single-experiment DMS acquisition method. The COV values to be ramped are inserted automatically during the batch acquisition process. The number of COV values determines the number of cycles that the mass spectrometer will run. The COV parameter is treated as a cycle-dependant parameter which means that each cycle will have a different value for the COV parameter. In case of an IDA method, one COV value per cycle is run for both the survey and dependent experiments.

The **Ramp COV for Cycle** option works with TOF MS or Product Ion scan types. The IDA, SWATHTM acquisition, and MRM^{HR} workflows are also supported.

1. Activate a hardware profile containing the necessary devices. Refer to *Create a Hardware Profile* in the *System User Guide* for the mass spectrometer.
2. On the Navigation bar, under **Acquire**, double-click **Build Acquisition method**.
3. Click **Mass Spectrometer** in the **Acquisition method** pane.
4. Select a scan type and then, as applicable, enter the mass range, acquisition time, and other required information for all the compounds. Refer to the *Manual Optimization Tutorial*.
5. Click **Edit Parameters**.
The **Parameter Settings** dialog opens.
6. Type the optimized values of the compound parameters on the **Compound** tab. Refer to the *Manual Optimization Tutorial*.
7. Type the optimized values of the ion source and gas parameters on the **Source/Gas** tab. Make sure that the source temperature (TEM) specified here is the same value as the one used for optimizing the DMS parameters. Refer to the *Manual Optimization Tutorial*.
8. Click the **DMS** tab and do the following:

- a. Select the required values for the **DMS Temperature (DT)**, **Modifier (MD)**, and **DMS Resolution Enhancement (DR)** parameters. Make sure that the DMS temperature specified here is the same as the one used for optimizing the DMS parameters.
- b. Type the optimized SV value for all the compounds in the **Separation Voltage (SV)** field.
- c. Type the optimized DMO value for all the compounds in the **DMS Offset (DMO)** field.
- d. Click **OK**.

Figure 4-2 Parameter Settings Dialog

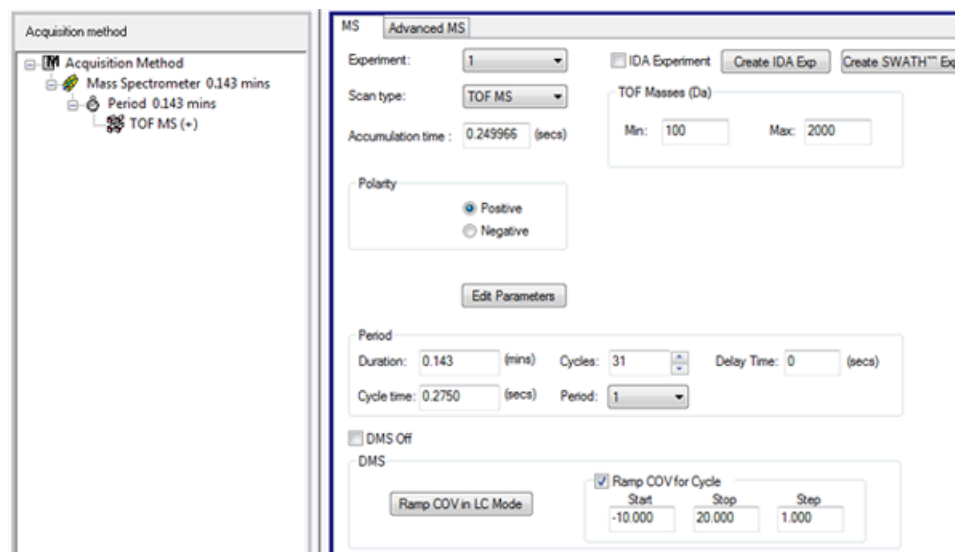
Note: Most compounds optimize between –20 volts to 30 volts in the absence of a modifier. Some compounds might optimize even higher than 30 volts. In the presence of a modifier, we recommend using a COV range of at least –60 volts to 20 volts because the negative COV shifts can be dramatic for some compounds.

9. Select the **Ramp COV for Cycle** check box on the MS tab page and provide the following COV values in the allowed COV range of –100 volts to 100 volts.

Table 4-1 COV Values

Label	Description
Start	Type the voltage at which the ramping starts.
Stop	Type the voltage at which the ramping stops.
Step	Set the step size.

Figure 4-3 Ramp COV for Cycle on MS tab



10. If required, provide values for the parameters of the peripheral devices included in the active hardware profile.

Note: When an acquisition method with **Ramp COV for Cycle** option is used for acquisition, only one cycle of the COV ramp is executed. If more cycles of the COV ramp are needed, use the **Ramp COV in LC Mode** option.

11. Save the acquisition method. It can be used for ramping COV during batch acquisition of samples and acquiring data.

Create an MRM^{HR} Acquisition Method Using the DMS Parameters

The Analyst[®] TF software supports the use of DMS parameters in an MRM^{HR} workflow for the best separation and quantitative analysis of the compounds of interest in a sample.

1. Activate a hardware profile. Refer to *Create a Hardware Profile* in the *System User Guide* for the mass spectrometer.
2. On the Navigation bar, under **Acquire**, double-click **Build Acquisition Method**.
The **Acquisition Method** window opens.
3. Click **Mass Spectrometer** in the **Acquisition method** pane.
4. Create an experiment with the **TOF MS** scan type.
5. Create the desired number of experiments with the **Product Ion** scan type.
6. Select the **Period** and then click **Edit Parameters**.
7. Type the optimized values of the compound parameters on the **Compound** tab. Refer to the *Manual Optimization Tutorial*.
8. Enter the optimized values of the ion source and gas parameters on the **Source/Gas** tab. Make sure that the source temperature (**TEM**) specified here is the same value as the one used for optimizing the DMS parameters. Refer to the *Manual Optimization Tutorial*.
9. Click the **DMS** tab and then type the following values:
 - a. Select the required values for the **DMS Temperature (DT)**, **Modifier (MD)**, **Separation Voltage (SV)**, **Compensation Voltage (COV)**, and **DMS Resolution Enhancement (DR)** parameters. Make sure that the DMS temperature specified here is the same value as the one used for optimizing the DMS parameters.
 - b. Select the **Source/Gas**, **Compound**, and **DMS** check boxes to copy the same values of these parameters in all experiments.
10. Click **OK**.
11. Select the **TOF MS** experiment.
12. Click **Edit Parameters**.
13. Click the **DMS** tab and then set the following values:
 - For the **Separation Voltage (SV)** and **Compensation Voltage (COV)** parameters type **0**.
 - For the **DMS Resolution Enhancement (DR)** parameter, select **Off**.

Create and Submit Batches

14. To change the COV parameter for individual Product Ion experiments, click the experiment and type the desired **Compensation Voltage (COV)**.
15. Click **OK**.
16. If required, provide values for the parameters of the peripheral devices included in the active hardware profile.
17. Save the acquisition method.

Separate Isobaric Compounds Using the SelexION Technology

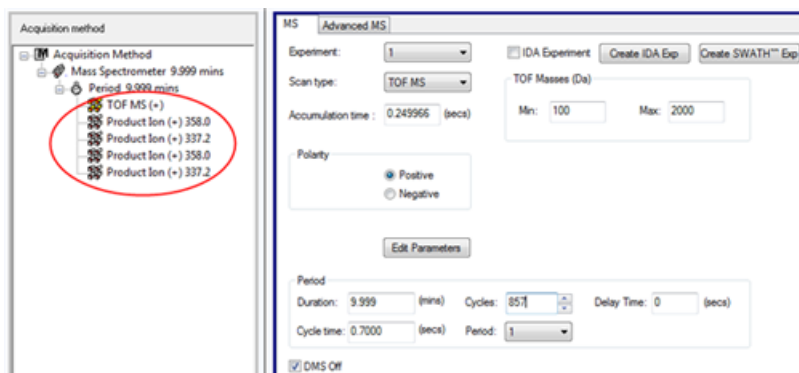
Isobaric compounds have the same nominal mass and, thus, cannot be distinguished by the mass spectrometer. The SelexION™ technology automatically eliminates crosstalk and separates isobaric compounds.

When creating an MRM^{HR} acquisition method (TOF MS experiment with Product Ion experiments) for multiple isobaric compounds, we recommend alternating isobaric masses with product ion masses of other compounds if possible, and avoiding having (product ion) isobaric masses in consecutive Product Ion scans.

Figure 4-4 shows an example of how to create an experiment containing two isobaric compounds and two non-isobaric compounds in an MRM^{HR} workflow.

1. Type the product ion mass of one isobaric compound.
2. Type the product ion mass of one non-isobaric compound.
3. Type the mass of the second isobaric compound.
4. Type the mass of the second non-isobaric compound.

Figure 4-4 Non-consecutive Arrangement of Isobaric Compounds in an MRM-HR Method



In an MRM^{HR} acquisition method, the software takes precautions to avoid crosstalk at the expense of a slightly longer cycle time. The settling time field is populated to avoid crosstalk, resulting in the slightly longer cycle time.

Modifier Consumption Calculation

The modifier pump flow rate for the pre-defined modifiers in the Analyst[®] TF software is calculated by the software using the modifier density and the modifier molecular weight. The density and molecular weight of the pre-defined modifiers in the Analyst TF software are listed in [Table 4-2](#).

Table 4-2 Density and Molecular Weight of Pre-defined Modifiers

Modifier	Molecular Weight (g/mol)	Density (g/cm ³)
2-propanol	60.10	0.7860
Acetonitrile	41.05	0.7822
Methanol	32.04	0.7918
Acetone	58.08	0.7925

The Analyst TF software uses the following formula to calculate the modifier pump flow rate in $\mu\text{L}/\text{min}$:

$$\text{Modifier Pump Flow Rate} = \frac{(0.1636 \times \text{CUR} + 1.7726) \times \text{MDC} \times 0.04089 \times \text{MDW} \times 1000}{(100 - \text{MDC}) \times \text{MDD}}$$

where:

- **MDW** is the Modifier Weight in g/mol
- **MDC** is the Modifier Composition
- **MDD** is the Modifier Density in g/mL
- **CUR** is the Curtain Gas[™] flow value

Example Modifier Consumption Calculation

As an example, approximate modifier consumption calculations for all the pre-defined modifiers in the Analyst[®] TF software at a Curtain Gas[™] flow of 20 psi and at different modifier concentrations for a 24 hour batch is shown in [Table 4-3](#).

Table 4-3 Approximate Modifier Consumption (in mL) at a Curtain Gas Flow Rate of 20 psi for a 24 Hour Batch

Modifier\Concentration	Low (1.5%) (mL/24hrs)	High (3.0%) (mL/24hrs)
2-Propanol	240.2	487.8
Acetonitrile	164.9	334.8

Table 4-3 Approximate Modifier Consumption (in mL) at a Curtain Gas Flow Rate of 20 psi for a 24 Hour Batch (continued)

Modifier\Concentration	Low (1.5%) (mL/24hrs)	High (3.0%) (mL/24hrs)
Methanol	127.1	258.1
Acetone	230.2	467.5

Calculate the Appropriate Modifier Consumption for a Batch

1. Determine the duration of the batch.
2. Determine the modifier pump flow rate from the **Mass Spec Detailed Status** dialog by clicking the **Mass Spec** icon on the **Status** bar in the bottom right corner of the Analyst[®] TF software window, while running the method from the Analyst[®] TF software.

Note: We recommend using a 2 L bottle for the modifier when running long batches at high CUR value and high modifier concentration.

3. Multiply the modifier pump flow rate ($\mu\text{L}/\text{min}$) with the batch duration (minutes) to obtain the approximate volume of modifier required for a batch.

This section describes how to do the following:

- View DMS parameters in **File Information** while viewing data files.
- Report data.
- Review a data file acquired with the ramped COV parameter.
- Display a contour plot for data acquired with the ramped COV parameter

Analyze Quantitative Data

View DMS Parameters Used for Acquisition in File Information While Viewing Data Files

The experimental conditions used to collect data are stored in the data file along with the results. The DMS parameters that were used to acquire samples are shown in the **File Information** pane of the data file.

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

The **Select Sample** dialog opens.

2. In the **Data Files** pane, select a .wiff file to view.
3. In the **Samples** pane, select the sample to view and then click **OK**.

The data acquired from the sample opens.

4. To view the file information, click the **Show File Info** icon.

The **File information** pane opens below the graph.

5. Expand the required period in the left pane of the **File Information** pane and then click the required period experiment link.

All of the DMS parameters (except COV, SV, and DMO) and modifier parameters used during the sample acquisition are recorded in the section for the selected period and experiment.

The COV, SV, and DMO start and stop values for each compound are recorded under the period experiment section.

The start, stop, and step values of the ramped COV parameter used during sample acquisition are recorded under the period section.

Analyze and Process Data

Refer to the *Analyze and Process Data* section in the Analyst® TF *Getting Started Guide* or the *System User Guide* for the mass spectrometer.

Report Data

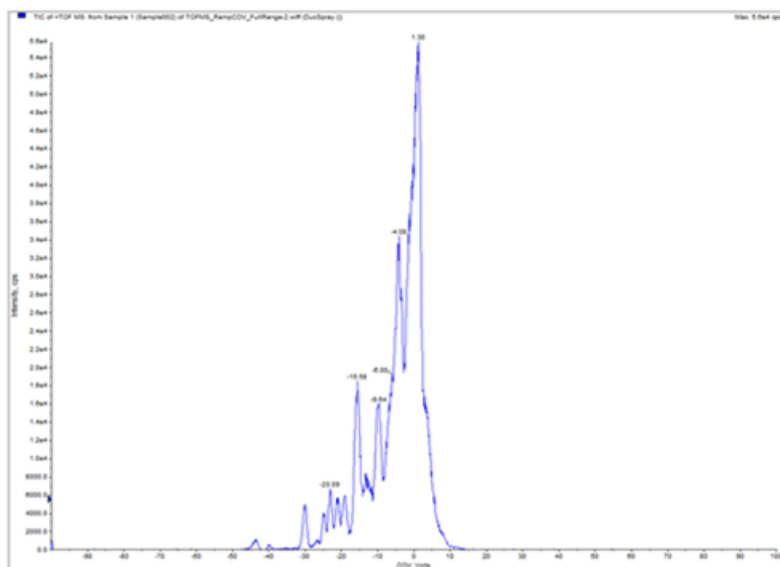
The MultiQuant™ software is used to quantitate data, and its reporting functionality, using the Reporter Software, can be used to create reports.

Analyze Qualitative Data

Review a Data File Acquired with the Ramp COV for Cycle Option

1. Open the project folder containing the acquired data.
2. On the Navigation bar, under **Explore**, double-click **Open Data File**.
The **Select Sample** dialog opens.
3. From the **Data Files** list, select the .wiff file containing the acquired data.
4. If required, in the **Samples** list, click a sample, and then click **OK**.

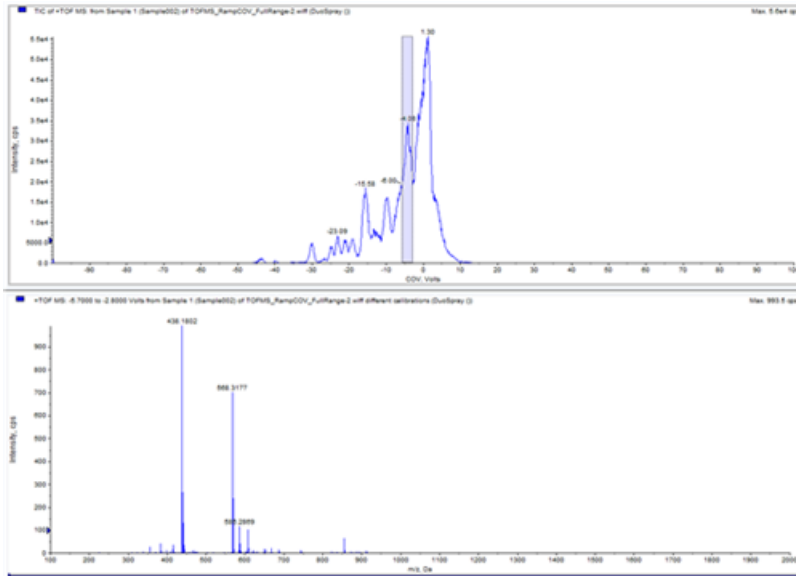
Figure 5-1 TIC



The TIC for the selected data file opens. The x-axis displays the COV in volts and the y-axis displays the intensity in cps.

5. Select a COV range in the TIC, right-click and then select **Show Spectrum**.

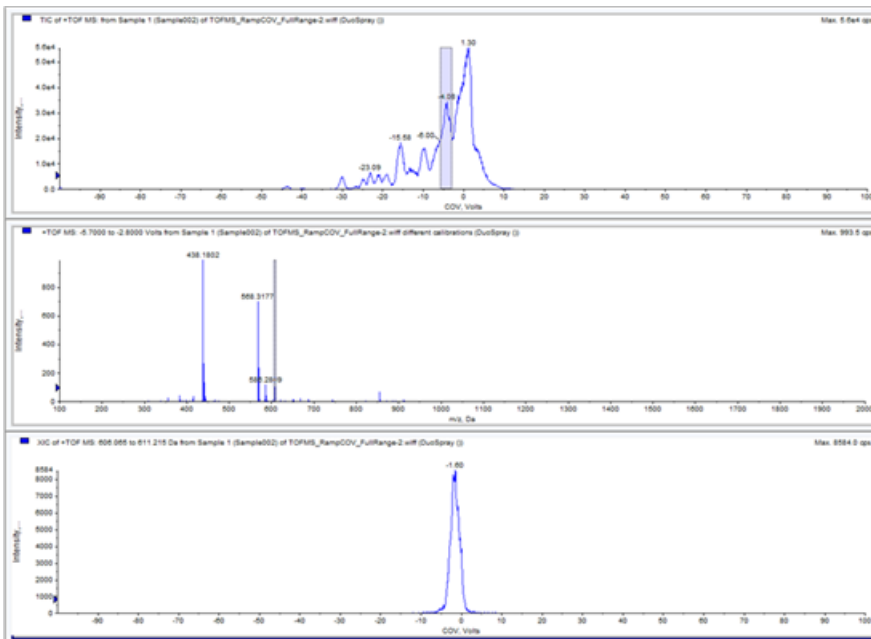
Figure 5-2 Spectrum



The spectrum for the selected COV range is shown under the TIC, with intensity on the y-axis and masses in Da (daltons) on the x-axis. It displays the intensity of all the compounds that appear in the SelexION™ ion mobility cell in the selected COV range. The selected COV range appears in the title of the open spectrum.

6. Select a mass in the spectrum, right-click, and then click **Extract Ions (Use Range)**.

Figure 5-3 XIC



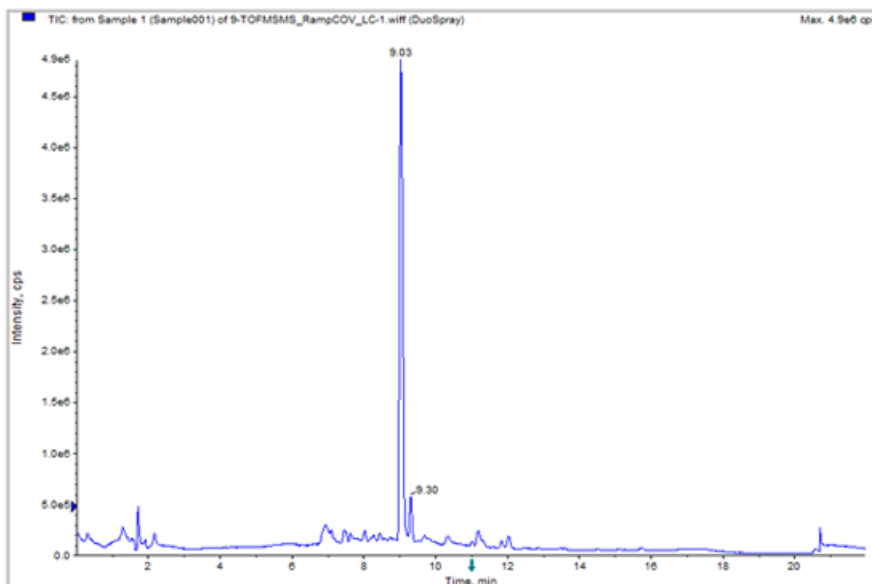
Analyze and Process Data

The TIC for the selected mass opens. The COV ramp is shown on the x-axis and the intensity on the y-axis.

Review a Data File Acquired using the Ramp COV in LC Mode Option

1. Open the project folder containing the acquired data.
2. On the Navigation bar, under **Explore**, double-click **Open Data File**.
The **Select Sample** dialog opens.
3. From the **Data Files** list, select the .wiff file containing the acquired data.
4. If required, in the **Samples** list, click the required sample and then click **OK**.

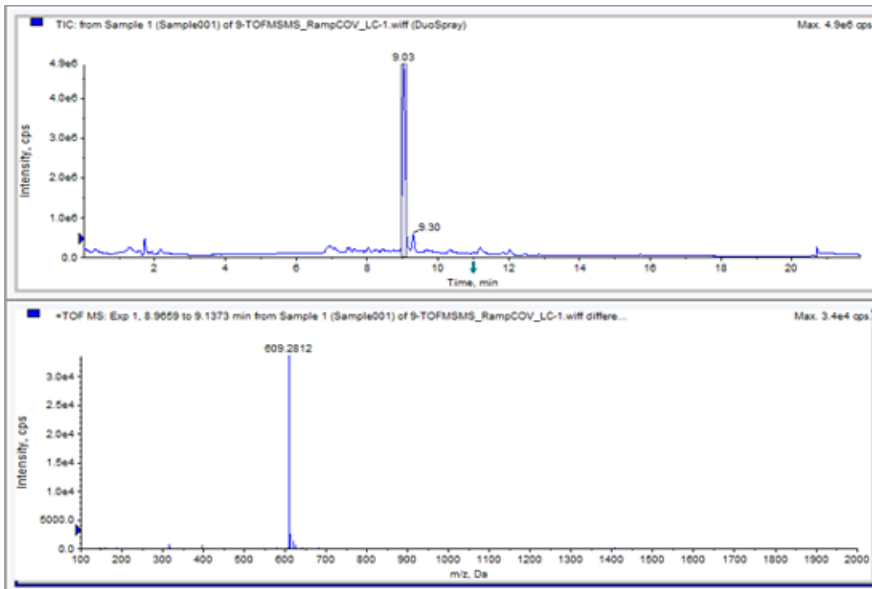
Figure 5-4 TIC



The TIC for the selected data file opens. The x-axis displays the time in min and the y-axis displays the intensity in cps.

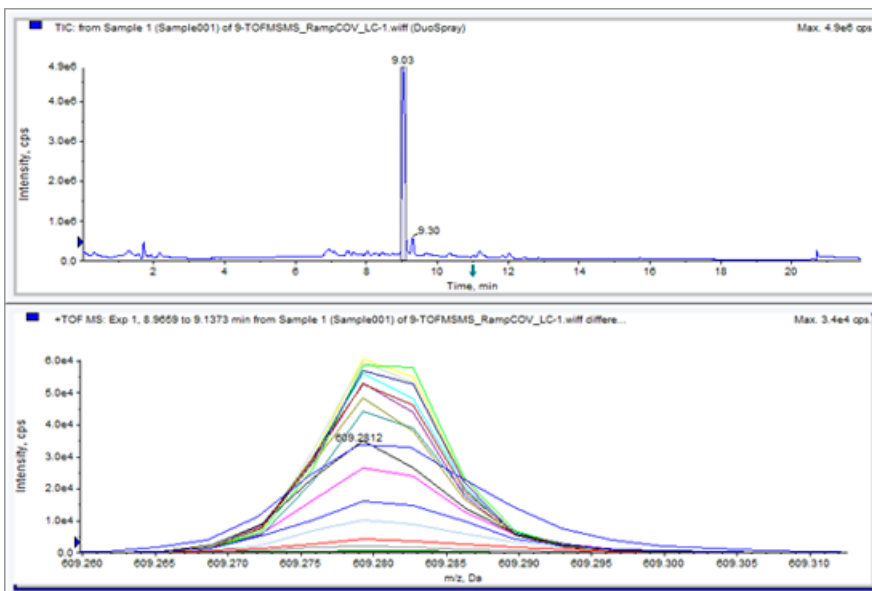
5. Select an area in the TIC, right-click and then click **Show Spectrum**.

Figure 5-5 Spectrum



The spectrum for the selected time range is shown under the TIC with intensity on the y-axis and masses in Da on the x-axis. The spectrum shows the intensity of all of the compounds that are found in the SelexION™ ion mobility cell in the selected time range. The selected time range is shown in the title of the open spectrum. Zoom into the required mass range in the spectrum. The peaks for all the analytes that elute during the selected time range are shown in the spectrum.

Figure 5-6 Peaks Displayed in the Spectrum



Analyze and Process Data

- Note the color of the highest peak, right-click on the legend (small rectangle) in the top left corner of the spectrum, and then note the experiment number for the color of the highest peak.

Tip! Raise the threshold (little blue arrow on the y-axis) to show more or fewer traces in the legend. Only the XIC traces above the blue arrow are shown in the legend.

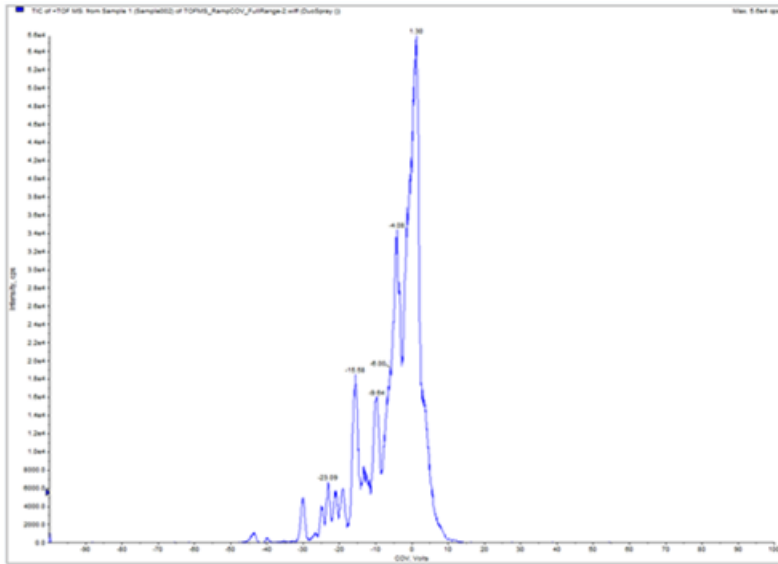
- Click the **Show File Info** icon.
- Expand the **Period** section and then click the experiment number from step 6.
The information about the selected period and experiment combination is shown in the right pane. The COV value along with other DMS parameters is also shown.

Show a Contour Plot for Data Acquired with the Ramped COV Parameter (Ramp COV for Cycle Option Only)

The Analyst® TF software can show a contour plot for the data that is acquired using an acquisition method with a ramped COV parameter and a full scan type. Contour plots provide visualization of the separation of the compounds. For more information about contour plots, refer to *Contour Plots* in the *Analyze and Process Data* section in the Analyst® TF *Getting Started Guide*, and *Qualitative Data Analysis* in the Analyst® TF *Advanced User Guide*.

- On the Navigation bar, under **Explore**, double-click **Open Data File**.
- In the **Select Sample** dialog, in the **Data Files** list, select a data file (.wiff file).
- In the **Samples** pane, select a sample.
- Click **OK**.

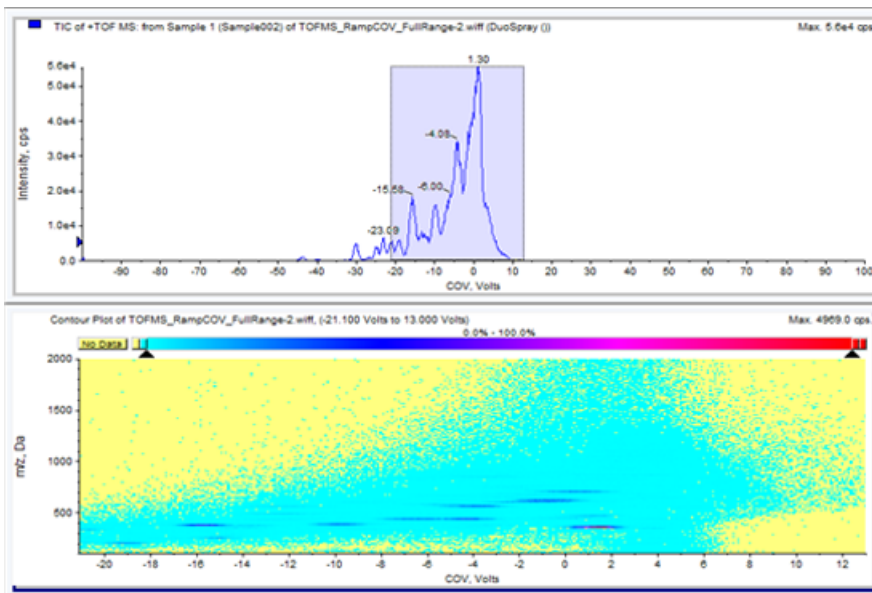
Figure 5-7 TIC



The TIC for the selected sample opens. The x-axis shows the COV in volts and the y-axis shows the intensity in cps.

5. Highlight the range to view in the contour plot. If a selection is not made, then the whole range is shown.
6. Right-click in the TIC and then click **Show Contour Plot**.

Figure 5-8 Contour Plot

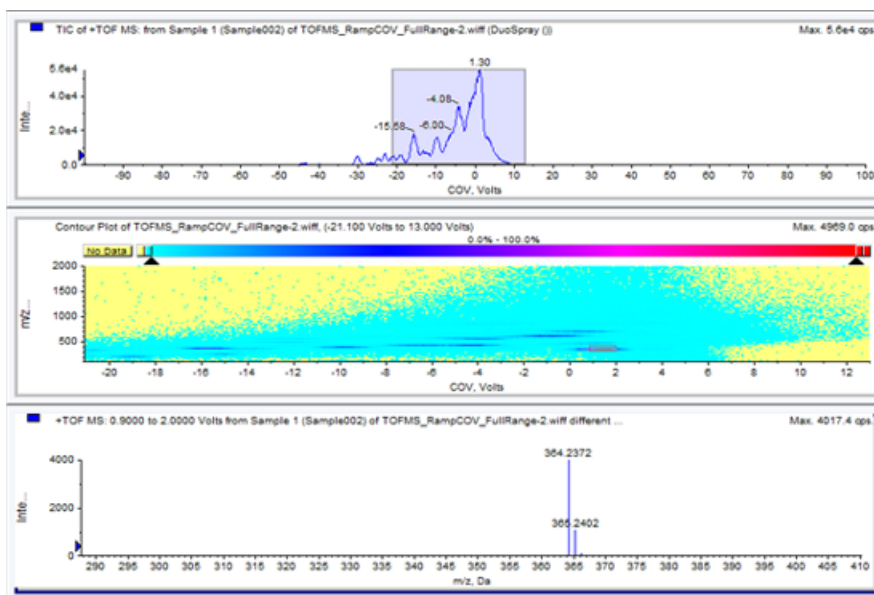


Analyze and Process Data

The contour plot for the selected sample is shown under the TIC window. The x-axis shows the COV in volts and the y-axis shows the m/z in Da.

7. To view the spectrum, select a region in the contour plot, right-click and then click **Show Spectrum**.

Figure 5-9 Spectrum



The spectrum for the selected COV range is shown below the contour plot window. It shows the intensity (y-axis) of all m/z values (x-axis) in the selected COV range. The selected COV range is shown in the title of the open spectrum.

This section describes how to:

- Create an Information Dependent Acquisition (IDA) method to ramp Compensation Voltage (COV) during batch acquisition mode.
- View the IDA data acquired with ramped COV in the **Explorer** window.
- View the IDA data acquired with ramped COV in the IDA Explorer.

Prerequisites

The SelexION™ technology is installed on the instrument and the controller module is turned on.

Use the IDA acquisition method to create and submit batches to acquire data. Refer to the *IDA Tutorial, System User Guide* for the mass spectrometer or the *Analyst® TF Advanced User Guide*.

Create an IDA Acquisition Method to Ramp COV During Batch Acquisition

Instead of using liquid chromatography (LC) for analysis of samples, use the SelexION™ device with infusion to separate the compounds of interest and filter out the chemical noise or interference. With the SelexION device, the ramping COV feature for Cycle option of the Analyst® TF software can be used to mimic the LC gradient.

In addition to the Manual Tuning mode, the COV parameter can also be ramped during batch acquisition by selecting the check box to activate the **Ramp COV for Cycle** option in an acquisition method in the **Acquisition Method editor**. The COV parameter is treated as a cycle-dependant parameter. The ramping COV functionality works for a single period DMS acquisition method.

The IDA methods without ramped parameter will run for the required method duration, but the IDA methods with ramped COV will run for the required number of cycles based on the ramping COV start, stop, and step values. The method run will terminate when the last step of COV is acquired, and not when the method duration is reached. The COV value is dynamically calculated and set for each cycle.

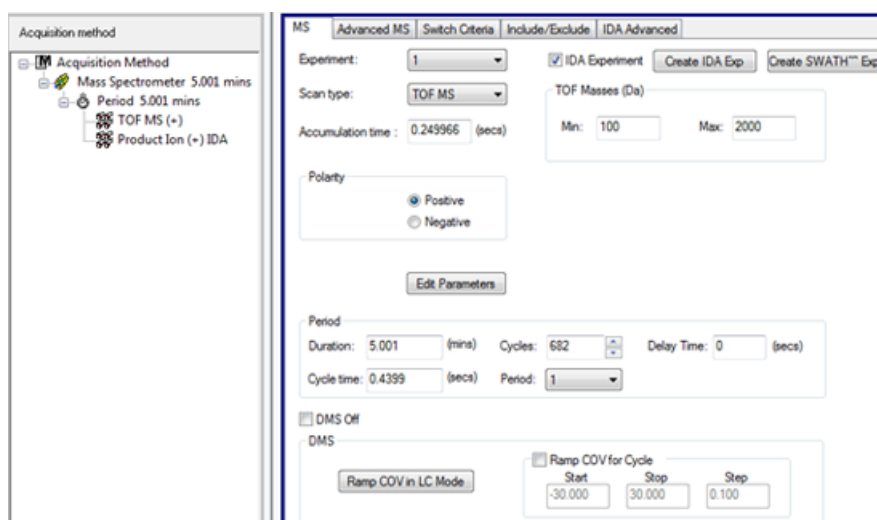
The COV, SV, DT, and DMO values in the survey scan (or any other supported IDA survey scans) are automatically propagated to the dependant scans in an IDA method.

The modifier used in the survey scan of an IDA method also gets automatically propagated to the dependant scans. Use this procedure after all of the DMS parameters have been optimized except COV.

Create an IDA Acquisition Method to Ramp COV During the Batch Acquisition Mode

1. Activate a hardware profile. Refer to the *System User Guide* for the mass spectrometer.
2. Create an IDA method with a TOF MS scan as survey scan. Refer to the *IDA Tutorial*.
3. In the **Acquisition method editor**, in the open IDA method, click **TOF MS** in the **Acquisition method** pane.

Figure 6-1 TOF MS Method



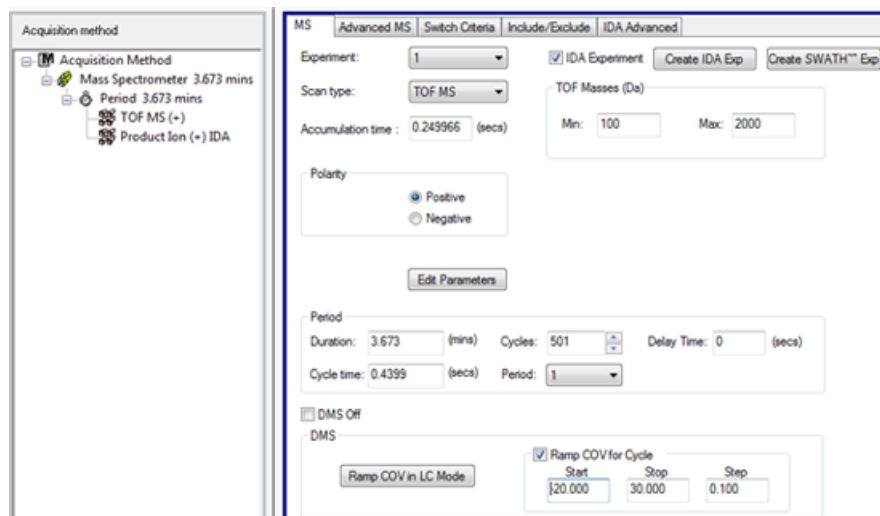
4. Select the **Ramp COV for Cycle** check box on the **MS** tab and then provide the following COV values in the allowed COV range of –100 volts to 100 volts.

Table 6-1 COV Values

Field	Description
Start	Type the voltage at which the ramping starts.
Stop	Type the voltage at which the ramping stops.
Step	Set the size of the steps on each cycle.

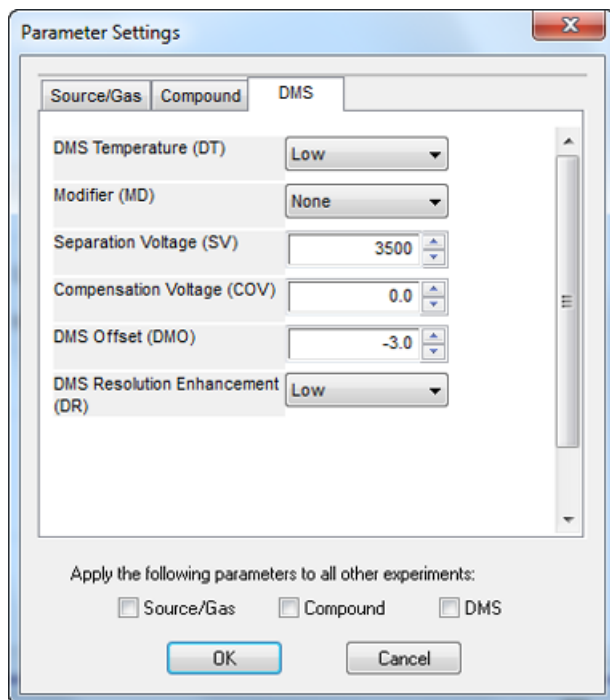
Note: Most compounds optimize between –20 volts to 30 volts in the absence of a modifier. Some compounds might optimize even higher than 30 volts. In the presence of a modifier, we recommend using a COV range of at least –60 volts to 20 volts because the negative COV shifts can be dramatic for some compounds.

Figure 6-2 MS Parameters



5. Click **Edit Parameters**.
The **Parameter Settings** dialog opens.
6. Type the optimized values of the ion source and gas parameters on the **Source/Gas** tab. Make sure that the source temperature (TEM) specified here is the same as the one used for optimizing the DMS parameters. Refer to the *Manual Optimization Tutorial*.
7. Type the optimized values of the compound parameters on the **Compound** tab. Refer to the *Manual Optimization Tutorial*.
8. Select the **DMS** tab and do the following:
 - a. Select the required values for the **DMS Temperature (DT)**, **Modifier (MD)**, and **DMS Resolution Enhancement (DR)** parameters. Make sure that the DMS temperature specified here is the same as the one used for optimizing the DMS parameters.
 - b. Type the optimized SV value for all the compounds in the **Separation Voltage (SV)** field.
 - c. Type the optimized DMO value for all the compounds in the **DMS Offset (DMO)** field.

Figure 6-3 Parameter Settings Dialog



9. Click **OK**.

A message is shown indicating that the changes to the values of DMS parameters for one IDA experiment will be automatically applied to all the other IDA experiments.

10. If required, provide values for the parameters of the peripheral devices included in the active hardware profile.
11. Save the acquisition method. It can be used to ramp COV as a cycle-dependent parameter during batch acquisition and acquire data.

View IDA Data Acquired with Ramped COV in the Explore Window

We recommend using the PeakView[®] software to view the IDA data files.

In the Analyst[®] TF software, the IDA data file with ramped COV parameter by default will open in the **Explore** window.

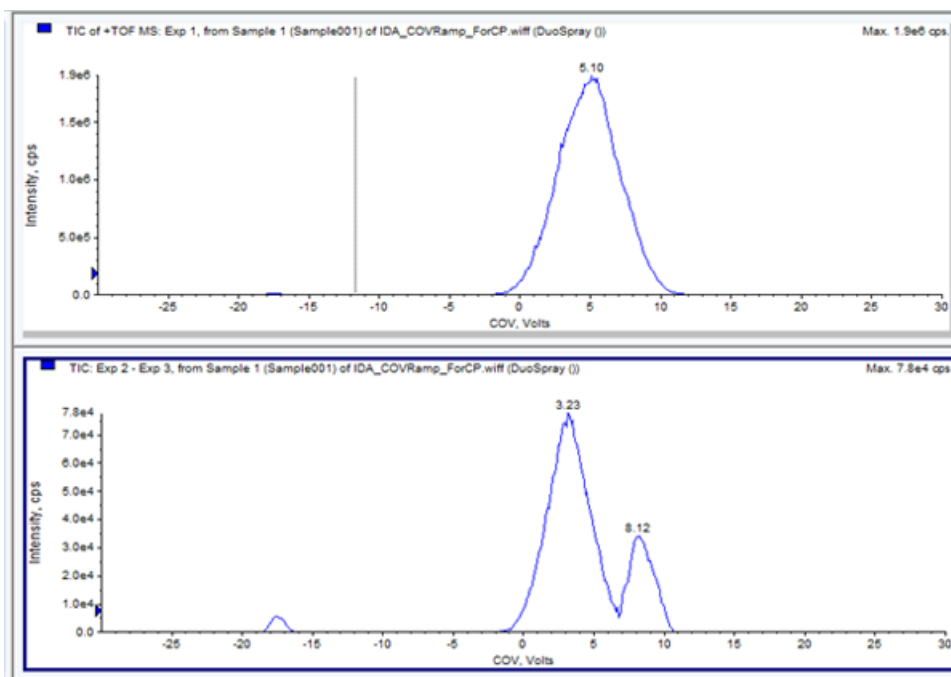
1. Open the project folder containing the acquired IDA data.
2. On the Navigation bar, under **Explore**, double-click **Open Data File**.

The **Select Sample** dialog appears.

3. From the **Data Files** list, select the .wiff file containing the acquired IDA data to view.
4. In the **Samples** list, click the required sample, and then click **OK**.

The data file opens in the **Explore** window. The TICs for the survey and dependant experiments are displayed. The x-axis displays the COV in volts and the y-axis displays the intensity in cps.

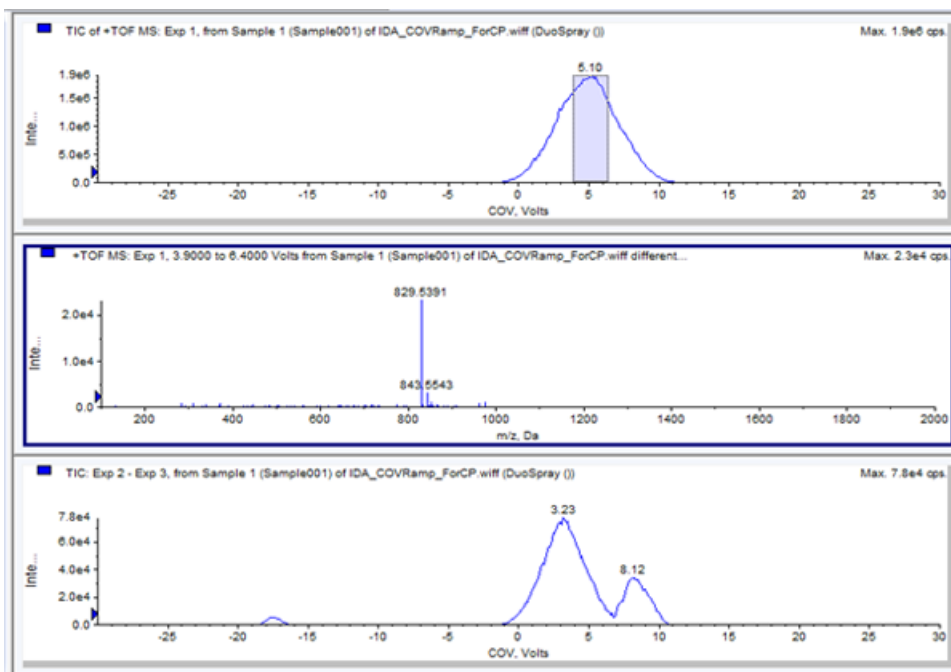
Figure 6-4 TICs



5. Select the required COV range in any of the two TICs, right-click and then click **Show Spectrum**.

The spectrum, with intensity on y-axis and masses in Da on x-axis, for the selected COV range appears under the TIC. It displays the intensity of all the compounds that appear in the SelexION™ ion mobility cell in the selected COV range. The selected COV range appears in the title of the open spectrum.

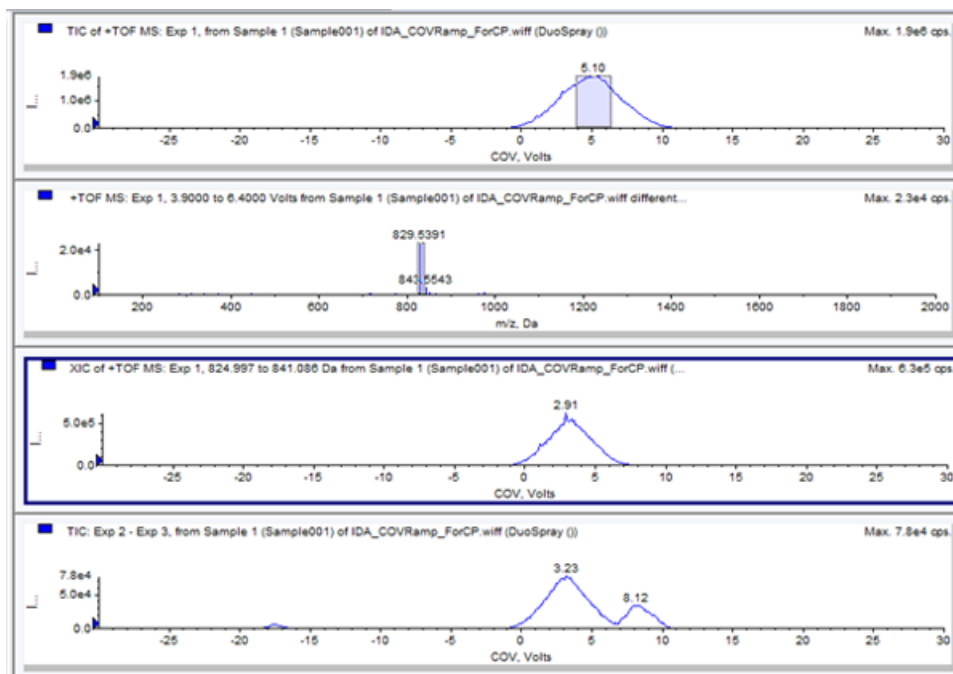
Figure 6-5 Spectrum



6. Select a mass in the spectrum, right-click and then click **Extract Ions (Use Range)**.

The XIC for the selected mass opens. The COV for the selected mass is shown on the x-axis and the intensity on the y-axis.

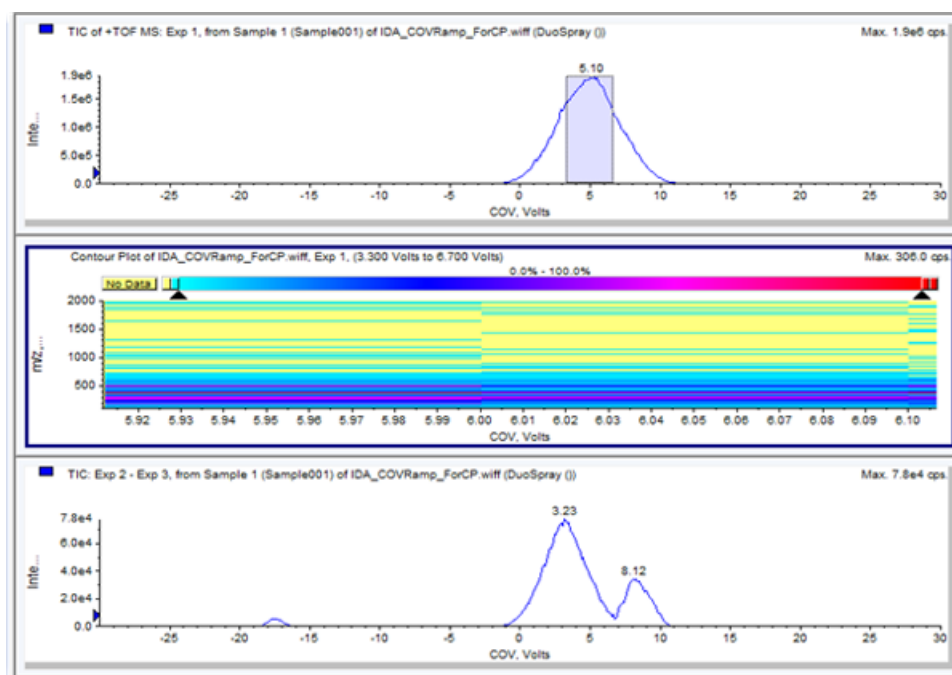
Figure 6-6 XIC



7. In the TIC of the dependant scans or the survey scan, highlight the range to view in the contour plot. Right-click and then click **Show Contour Plot**. If a selection is not made, then the whole range is shown.

The contour plot for the selected sample opens under the TIC window. COV in volts is shown on the x-axis and the m/z in Da is shown on the y-axis.

Figure 6-7 Contour Plot



View the IDA Data Acquired with Ramped COV Parameter in the IDA Explorer

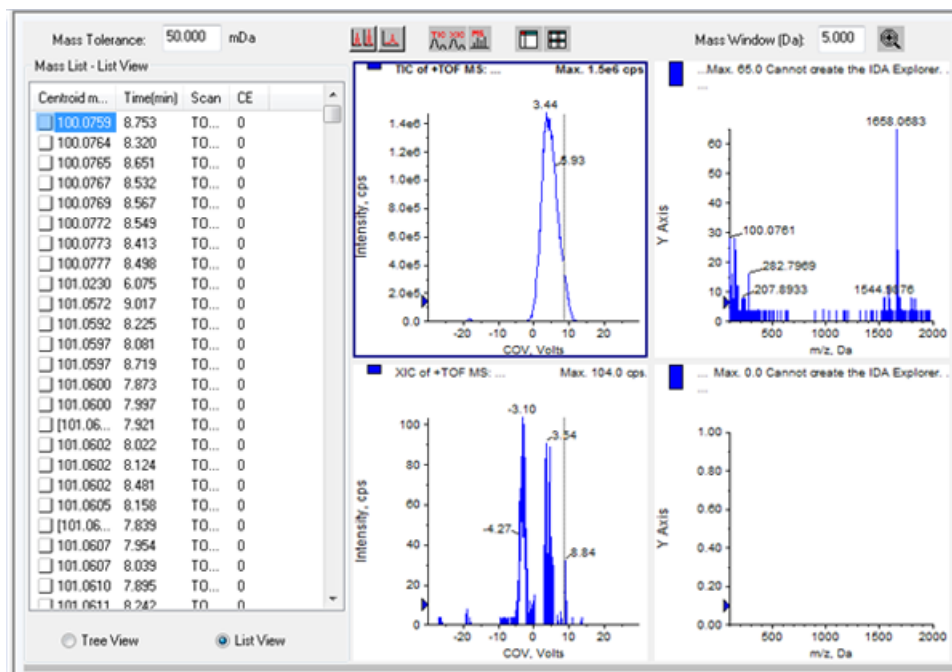
If data is acquired with an IDA method, then the data does not open in the **IDA viewer** until the acquisition has finished, but it is shown in the **Explore** window during acquisition.

To easily view IDA data, set the **IDA Explorer** as the preset viewer. Use the **IDA Explorer** tab in the **Appearance Options** dialog to use the IDA Explorer to view IDA data. Users can also select the columns for the **Mass-List List** view pane. The **IDA Explorer** is preset to show IDA samples.

For more information, refer to *View IDA Data* in the *IDA Tutorial*.

1. Open the project folder containing the acquired IDA data.
2. On the Navigation bar, under **Explore**, double-click **Open Data File**.
The **Select Sample** dialog appears.
3. From the **Data Files** list, select the .wiff file containing the acquired IDA data to view.
4. In the **Samples** list, click the required sample and then click **OK**.

Figure 6-8 IDA Explorer



The **IDA Explorer** opens. The left portion of the pane shows a list of masses sent to the dependent scan as a tree view, or as a list view. Switch between views by clicking **Tree View** or **List View** at the bottom of the **Mass List** pane.

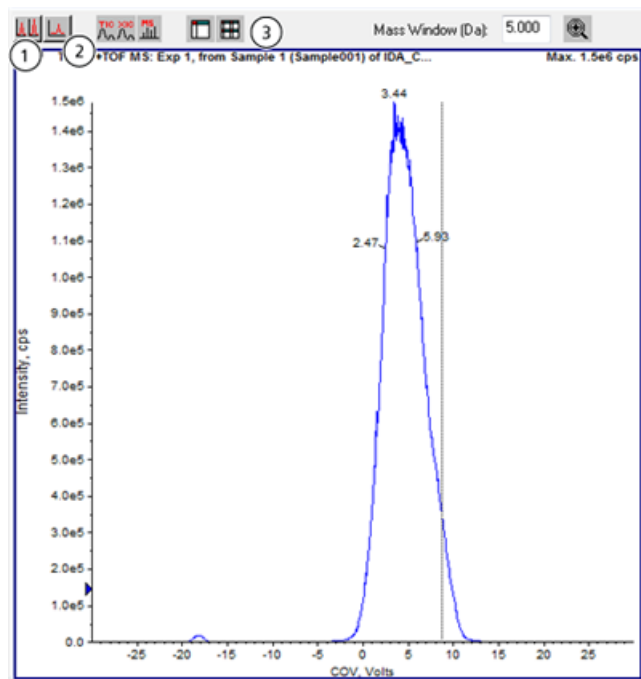
The right portion of the pane shows the acquired IDA data graphically. Instead of time, the ramped COV range is shown on the x-axis in the TIC and XIC graphs.

- Use the two buttons above the graph to switch between single graph and multiple graph displays.
 - To view the active graph only, click **Show only active graph**.
 - To return to multi-graph view, click **Show all the graphs**.

Use DMS Parameters in IDA

- To view all the graphs in **Explorer**, click **Export all the graphs to Explorer**.

Figure 6-9 Buttons in IDA Explorer



Item	Button name
1	Show all the graphs
2	Show only active graph
3	Export all the graphs to Explorer

Symptom	Corrective Action
<p>An error message reports that a discharge has been detected in the SelexION™ ion mobility cell during sample acquisition or equilibration.</p>	<p>Lower the SV by 100 volts and then re-optimize the DMS parameters.</p> <p>When a discharge is detected in the SelexION ion mobility cell during sample acquisition, the software aborts the sample acquisition and logs the error in the event log. Double-click the aborted sample in the queue to see an error message.</p> <p>If a discharge is detected in the SelexION ion mobility cell, then to avoid repeating the discharge when using the same method, use lower Separation Voltage (SV) or DMS Temperature (DT) value in the acquisition method. The DMS parameters will need to be re-optimized for the new SV or DT value.</p> <p>If there are discharges with SV and DT combinations that have worked in the past, then clean and align the SelexION ion mobility cell electrodes. Refer to Clean and Align the Ion Mobility Cell Electrodes on page 20.</p> <p>When the fault is cleared the instrument goes into the Standby mode.</p>
<p>When the SelexION controller module is turned on or off, the Mass Spectrometer icon in the Analyst® TF software turns and remains red.</p>	<p>Before turning the SelexION controller module on or off (to temporarily add or remove the SelexION technology to or from the system), first disable the active hardware profile within the software. Failure to do so may cause the mass spectrometer to enter an unstable state resulting in loss of control from within the software. If the hardware profile is not deactivated and the mass spectrometer enters this unstable state, control may be recovered by removing and re-seating the ion source, or by turning both the mass spectrometer and SelexION controller module off and then on, and then reactivating the hardware profile.</p>

DMS Parameter Descriptions

Parameter Name	Description	Possible Values
DMS Temperature (DT)	The temperature applied on the ceramic heater that is mounted in the back of the curtain plate heat exchanger. For each DT value change, allow the system to equilibrate for at least 10 minutes to 15 minutes before optimizing any DMS parameters. When the new temperature is reached, DMS Temperature reached is shown above the DT field.	<ul style="list-style-type: none"> • (Default) Low (150 °C) • Medium (225 °C) • High (300 °C)
Modifier (MD)	A chemical that is added into the Curtain Gas™ flow to help improve the separation of ions. If the MD value is set to None , the MDC, MDD, and MDW parameters are not available. If the MD value is set to a value other than None , the MDC parameter becomes available. If MD is set to Custom , the MDC, MDD, and MDW parameters become available.	<ul style="list-style-type: none"> • (Default) None • 2-propanol • Acetonitrile • Methanol • Acetone • Custom
Modifier Composition (MDC)	The parameter that controls the modifier concentration. The Analyst® TF software uses the density and molecular weight of the selected modifier and the Curtain Gas flow rate to calculate the modifier pump flow rate and then apply that flow rate automatically to the pump flow rate.	<ul style="list-style-type: none"> • Off (0) • (Default) Low (1.5% or higher) • High (3.0)
Modifier Density (g/mL) (MDD)	The density of a custom modifier. The Analyst TF software uses this density along with the Modifier MW and the Curtain Gas flow rate to determine the modifier pump flow rate.	Specify the density in g/mL for the modifier.

Parameter Name	Description	Possible Values
Modifier MW (MDW)	The molecular weight in g/mol of a custom modifier. The Analyst TF software uses the value of this parameter along with the Modifier Density and the Curtain Gas flow rate to determine the modifier pump flow rate.	Specify the molecular weight (g/mol) of the modifier.
Separation Voltage (SV)	The peak to peak amplitude of the separation voltage waveform.	Specify the Separation Voltage to be applied. <ul style="list-style-type: none">• (Default) 0.0• Range: 0 to the maximum SV value based on the DT and TEM parameters in each method
Compensation Voltage (COV)	A DC offset potential between the two electrodes of the mobility device. For example, if COV is 5 volts, then one of the two electrodes has 5 volts higher potential applied than the other one.	Specify the Compensation Voltage to be applied. <ul style="list-style-type: none">• (Default) 0.0• Range: -100 to 100

DMS Parameters

Parameter Name	Description	Possible Values
DMS Offset (DMO)	The voltage applied to the two electrodes of the SelexION™ ion mobility cell, relative to the orifice potential. For example, if the DMS offset potential is 5 volts and the orifice potential is at 100 volts, then the two electrodes in front of the orifice inlet have 105 volts potential. The DMS Offset is a way to tune the transmission out of the SelexION ion mobility cell into the mass spectrometer.	Specify the DMS Offset value. <ul style="list-style-type: none"> (Default) –3.0 volts in positive polarity, 3.0 volts in negative polarity Range: –100 to 100
DMS Resolution Enhancement (DR)	<p>Use of the DR parameter increases the residence time of ions in the SelexION™ ion mobility cell, leading to reduced sensitivity due to larger diffusional signal loss. When the DR value is changed, the settling time and the total scan time will be updated to account for ion transport through the SelexION ion mobility cell. When performing RF/DC scans (quadrupole scans), the settling time and the total scan time will be updated.</p> <p>Controls the flow of the nitrogen gas that can be enabled between the SelexION™ device exit and the orifice inlet into the mass spectrometer. When the value of DR is set to Low, Medium, or High, gas flow is enabled, which improves the resolution of the SelexION device.</p> <p>DR is also referred to as throttle gas.</p> <p>The set points for the different DR parameter values (Off, Low, Medium, and High) are configured during installation and must not be changed.</p>	<ul style="list-style-type: none"> (Default) Off (0) Low (10) Medium (25) High (40)

State of DMS Parameters in the DMS Off Mode

DMS Parameters	DMS Off Mode	
	State	Value
DMS Temperature (DT)	Visible on UI (user interface)	Low (default)
Modifier (MD)	Hidden	None
Separation Voltage (SV)	Hidden	0
Compensation Voltage (COV)	Hidden	0
DMS Offset (DMO)	Hidden	-3.0 volts in positive polarity; 3.0 volts in negative polarity
DMS Resolution Enhancement (DR)	Hidden	Off

Values of DMS and Source Parameters Used During Modifier Purge

Parameter Name	Value Set During Modifier Purge
Modifier Pump Flow Rate	1000 (µL/min)
Temperature (TEM)	300
DMS Temperature (DT)	225
DMS Resolution Enhancement (DR)	0
Separation Voltage (SV)	0
Compensation Voltage (COV)	0
DMS Offset (DMO)	3
Ion Source Gas 1 (GS1)	50
Ion Source Gas 1 (GS2)	50
Curtain Gas (CUR)	20
IonSpray Voltage Floating (ISVF)	0
Collision Gas (CAD)	System Default

Values of DMS and Source Parameters After Modifier Purge is Completed or Aborted

Parameter Name	Value After Modifier Purge is Completed or Aborted
DMS Temperature (DT)	150
Temperature (TEM)	0
Modifier Pump Flow Rate	0
GS1	20
GS2	0
CUR	30
CAD	6

T-Infuse Sample into LC Stream

B



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



WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the sample tubing nut is tightened properly before operating this equipment, to prevent leakage.

Note: T-infusion (split-infusion) can also be performed using an external tee to connect the three lines. The LC and syringe streams connect to the tee, which in turn is connected to the two-way grounding union.

1. Replace the two-way grounding union with a three-way grounding union (Fitting union 0.15 mm Bore PN 018786; Fitting Tee Ring PN 018787) on the ion source.
2. Connect the red PEEK tubing from the syringe pump to the grounding union on the ion source.
3. Connect the grounding union on the ion source to an LC pump.
4. Connect the sample tubing nut to the grounding union through a 30 cm piece of red PEEK tubing. Refer to *Connect the Tubing and Cables* topic in the ion source *Operator Guide*.

Revision History

Revision	Reason for Change	Date
A	First release of document.	September 2014
B	Updated for TripleTOF [®] 6600 system. Enhanced procedure <i>Install the SelexION[™] Technology on page 12.</i>	January 2015
C	Added warning not to remove covers.	March 2015
D	Updated settling times.	April 2015
E	Updated settling times.	May 2015