Ion Source

for Triple Quadrupole and QTRAP Systems

Tests, Specifications, and Data Log

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AB Sciex Pte. Ltd.
Blk 33, #04-06
Marsiling Ind Estate Road 3
Woodlands Central Indus. Estate.
SINGAPORE 739256

Contents

IonDrive™ Turbo V Ion Source Tests

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These tests apply to the IonDrive™ Turbo V ion source installed on a 6500 or 6500+ series system.

Run these tests in any of the following situations:

- When a new ion source is installed.
- After major maintenance to the ion source.
- Whenever the performance of the ion source must be assessed, either before starting a project or as part of a standard operating procedure.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of toxic or injurious materials used with the ion source.

WARNING! Puncture Hazard, Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Discontinue use of the ion source if the ion source window is cracked or broken and then contact a SCIEX Field Service Employee (FSE). Any toxic or injurious materials introduced into the equipment will be present in the source exhaust output. Dispose of sharps following established laboratory safety procedures.

WARNING! Toxic Chemical Hazard. Wear personal protective equipment, including a laboratory coat, gloves, and safety glasses, to avoid skin or eye exposure.

WARNING! Ionizing Radiation Hazard, Biohazard, Electrical Shock Hazard, or Toxic Chemical Hazard. In the event of a chemical spill, review product Safety Data Sheets for specific instructions. Make sure that the system is in Standby mode before cleaning a spill near the ion source. Use appropriate personal protective equipment and absorbent wipes to contain the spill and dispose of it following local regulations.

Required Materials
• Mobile phase solvent: 70:30 acetonitrile:water solution • Test Solution: 0.0167 pmol/µL (equivalent to 10 pg/µL) reserpine. Use the pre-diluted 0.0167 pmol/µL reserpine solution included in the SCIEX Standard Chemical Kit (PN 4406127). • HPLC pump (for mobile phase) • Manual injector (8125 Rheodyne or equivalent) with a 5 µL loop or an autosampler set up for 5 µL injections • PEEK tubing 1/16-inch outside diameter (o.d.), 0.005-inch inside diameter (i.d.) • Ion source with a probe installed • Syringe 250 µL to 1000 µL • Powder-free gloves (nitrile or neoprene is recommended) • Safety glasses • Lab coat

Note: All test solutions must be kept refrigerated. If they are left out of the refrigerator for longer than 48 hours, then discard them and use new solutions.

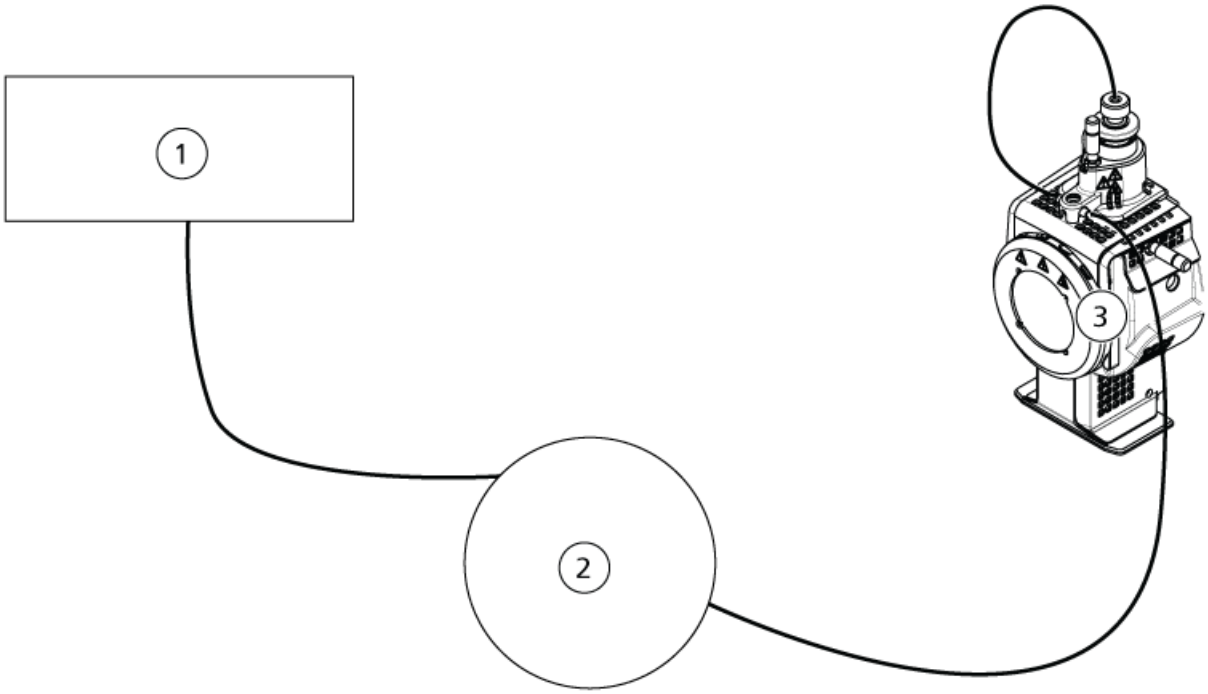
Prepare for the Test

WARNING! Electrical Shock Hazard. Avoid contact with the high voltages applied to the ion source during operation. Put the system in Standby mode before adjusting the sample tubing or other equipment near the ion source.

- When installing a new ion source, make sure that the mass spectrometer is performing to specifications with the existing ion source.
- Install the ion source on the mass spectrometer.
- Make sure that the ion source is fully optimized. Refer to the appropriate ion source *Operator Guide*.
- Refer to all applicable Safety Data Sheets for any necessary precautions before handling chemical solutions or solvents.
- Make sure that the users are sufficiently trained on mass spectrometer operation and safety procedures.
- Install the probe to be tested.
- Connect the grounding union on the ion source to a pump, through a manual injector equipped with a 5 µL loop, or to an autosampler.

Refer to Figure 1-1.

Figure 1-1 LC Pump Configuration



Item	Description
1	Pump for the flow inlet
2	Injector or autosampler
3	Ion source

Test the TurboIonSpray® Probe

WARNING! Hot Surface Hazard. Let the ion source cool for at least 90 minutes before starting any maintenance procedures. Surfaces of the ion source become hot during operation.

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 0.5 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the method parameters as shown in Table 1-1.

Table 1-1 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	MRM
Q1	609.3
Q3	195.1
Scan Time (seconds)	0.200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	30 (or as optimized)
Temperature (TEM)	700 (or as optimized)
Ion Source Gas 1 (GS1)	60 (or as optimized)
Ion Source Gas 2 (GS2)	70 (or as optimized)
IonSpray Voltage (IS)	4500 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized

4. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

5. Click **Acquire** to begin collecting data.
6. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

7. Print the results.
8. Average the three intensities of the ions and then record the result in the Data Log.
9. Confirm that the average intensity is acceptable. Refer to Data Log: IonDrive™ Turbo V Ion Source.

   If the result is not acceptable, refer to Troubleshooting Tips.
10. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the APCI Probe

WARNING! Hot Surface Hazard. Let the ion source cool for at least 90 minutes before starting any maintenance procedures. Surfaces of the ion source become hot during operation.

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 1 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the method parameters as shown in Table 1-2.

Table 1-2 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	MRM
Q1	609.3

Table 1-2 Method Parameters (continued)

Parameter	Value
Q3	195.1
Scan Time (seconds)	0.200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	30 (or as optimized)
CAD Gas	9 (or as optimized)
Nebulizer Current (NC)	3 (or as optimized)
Temperature (TEM)	425
Ion Source Gas 1 (GS1)	70 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized

4. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

5. Click **Acquire** to begin collecting data.
6. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

7. Print the results.

8. Average the three intensities of the ions and then record the result in the Data Log.
9. Confirm that the average intensity is acceptable. Refer to Data Log: IonDrive™ Turbo V Ion Source.

   If the result is not acceptable, refer to Troubleshooting Tips.
10. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Turbo V™ Ion Source Tests 2

Run these tests in any of the following situations:

- When a new ion source is installed.
- After major maintenance to the ion source.
- Whenever the performance of the ion source must be assessed, either before starting a project or as part of a standard operating procedure.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of toxic or injurious materials used with the ion source.

WARNING! Puncture Hazard, Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Discontinue use of the ion source if the ion source window is cracked or broken and then contact a SCIEX Field Service Employee (FSE). Any toxic or injurious materials introduced into the equipment will be present in the source exhaust output. Dispose of sharps following established laboratory safety procedures.

WARNING! Toxic Chemical Hazard. Wear personal protective equipment, including a laboratory coat, gloves, and safety glasses, to avoid skin or eye exposure.

WARNING! Ionizing Radiation Hazard, Biohazard, Electrical Shock Hazard, or Toxic Chemical Hazard. In the event of a chemical spill, review product Safety Data Sheets for specific instructions. Make sure that the system is in Standby mode before cleaning a spill near the ion source. Use appropriate personal protective equipment and absorbent wipes to contain the spill and dispose of it following local regulations.

Required Materials

- Mobile phase solvent: 70:30 acetonitrile:water solution
- Test Solution:
  - For 4500, 5500, 6500, and 6500+ systems, use the pre-diluted 0.0167 pmol/µL reserpine solution included in the SCIEX Standard Chemical Kit (PN 4406127).
  - For 3200 and 3500 systems, use the pre-diluted 0.167 pmol/µL reserpine solution included in the SCIEX Standard Chemical Kit (PN 4406127).
  - For TripleTOF® systems, prepare the test solution from the 0.167 pmol/µL reserpine solution and the standard diluent provided in the SCIEX TripleTOF® System Chemical Kit (PN 4456736)

  A vortex mixer is required.
- HPLC pump (for mobile phase)
- Manual injector (8125 Rheodyne or equivalent) with a 5 µL loop or an autosampler set up for 5 µL injections
- PEEK tubing 1/16-inch outside diameter (o.d.), 0.005-inch inside diameter (i.d.)
- Ion source with a probe installed
- Syringe 250 µL to 1000 µL
- Powder-free gloves (nitrile or neoprene is recommended)
- Safety glasses
- Lab coat

Note: All test solutions must be kept refrigerated. If they are left out of the refrigerator for longer than 48 hours, then discard them and use new solutions.

CAUTION: Potential Wrong Result. Do not use expired solutions.

Prepare for the Test

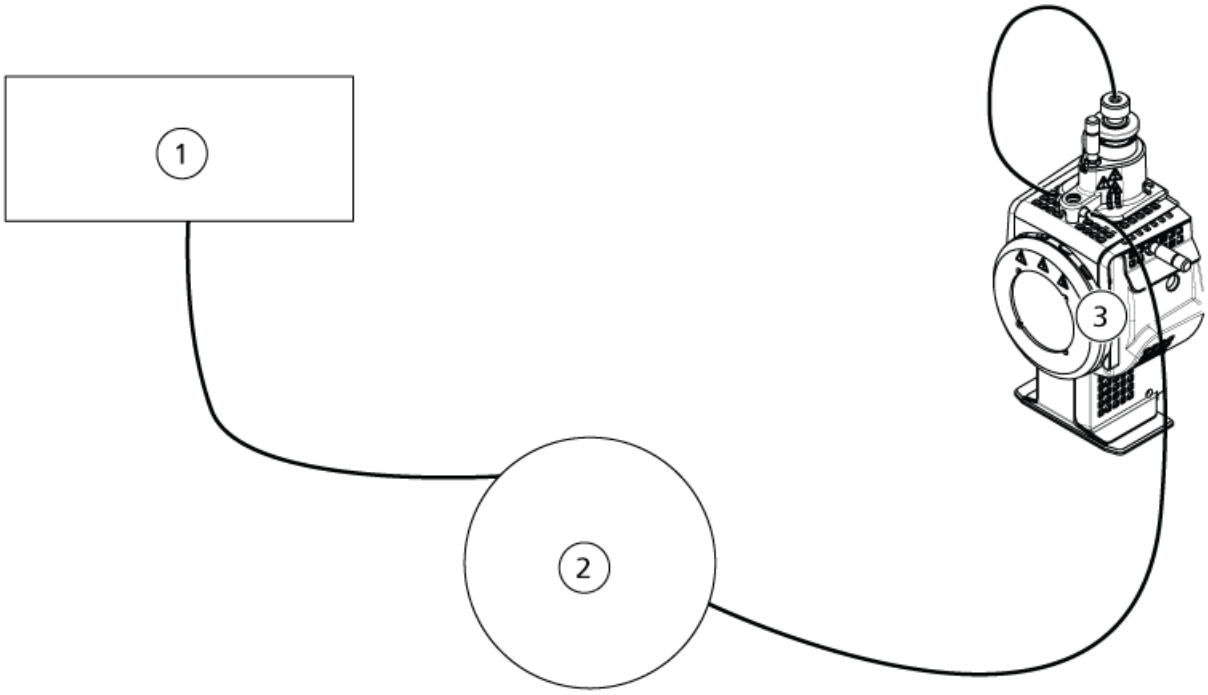
WARNING! Electrical Shock Hazard. Avoid contact with the high voltages applied to the ion source during operation. Put the system in Standby mode before adjusting the sample tubing or other equipment near the ion source.

- When installing a new ion source, make sure that the mass spectrometer is performing to specifications with the existing ion source.
- Install the ion source on the mass spectrometer.

- Make sure that the ion source is fully optimized. Refer to the appropriate ion source *Operator Guide*.
- Refer to all applicable Safety Data Sheets for any necessary precautions before handling chemical solutions or solvents.
- Install the probe to be tested.
- Connect the grounding union on the ion source to a pump, through a manual injector equipped with a 5 µL loop, or to an autosampler.

Refer to Figure 2-1.

Figure 2-1 LC Pump Configuration



Item	Description
1	Pump for the flow inlet
2	Injector or autosampler
3	Ion source

Test the Ion Source on Triple Quadrupole and QTRAP® Systems

Test the TurboIonSpray® Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 0.2 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the method parameters as shown in Table 2-1.

Table 2-1 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	MRM
Q1	609.3 (or as optimized)
Q3	195.1 (or as optimized)
Scan Time (seconds)	0.200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20 (or as optimized)
Temperature (TEM)	700 (or as optimized)
Ion Source Gas 1 (GS1)	60 (or as optimized)
Ion Source Gas 2 (GS2)	70 (or as optimized)
IonSpray™ Voltage (IS)	4500 (or as optimized)

Table 2-1 Method Parameters (continued)

Parameter	Value
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized

4. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

5. Perform several 5 µL injections of the reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, TEM, GS1, GS2, and IS
6. Click **Acquire** to begin collecting data.
7. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

8. Print the results.
9. Average the three intensities of the ions and then record the result in the Data Log.
10. Confirm that the average intensity is acceptable. Refer to Data Log: Turbo V™ Ion Source.

    If the result is not acceptable, then refer to Troubleshooting Tips.
11. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the APCI Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 1 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the method parameters as shown in Table 2-2.

Table 2-2 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	MRM
Q1	609.3 (or as optimized)
Q3	195.1 (or as optimized)
Scan Time (seconds)	0.200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20 (or as optimized)
CAD Gas	9 (or as optimized)
Nebulizer Current (NC)	3 (or as optimized)
Temperature (TEM)	425
Ion Source Gas 1 (GS1)	70 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)

Table 2-2 Method Parameters (continued)

Parameter	Value
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized

4. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

5. Perform several 5 µL injections of the reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, GS1, and NC
6. Click **Acquire** to begin collecting data.
7. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

8. Print the results.
9. Average the three intensities of the ions and then record the result in the Data Log.
10. Confirm that the average intensity is acceptable. Refer to Data Log: Turbo V™ Ion Source.

    If the result is not acceptable, then refer to Troubleshooting Tips.
11. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the Ion Source on TripleTOF® Systems

Note: Specifications are not available for the TripleTOF® 4600 system. The recommended ion source for TripleTOF® systems is the DuoSpray™ ion source.

Prepare the Test Solution

1. Combine 100 µL of the 0.167 pmol/µL reserpine solution and 900 µL of the standard diluent.
2. Mix using a vortex mixer for 30 seconds.

   This step produces the 0.0167 pmol/µL reserpine solution.

Test the TurboIonSpray® Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 0.2 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the method parameters as shown in Table 2-3.

Table 2-3 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	Product Ion
High Sensitivity (5600/5600+ and 6600 systems only)	On
Product Of	609.2807
TOF Masses (Da)	150 to 650

Table 2-3 Method Parameters (continued)

Parameter	Value
Accumulation time (seconds)	0.200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20
Temperature (TEM)	700
Ion Source Gas 1 (GS1)	50
Ion Source Gas 2 (GS2)	50
IonSpray Voltage Floating (ISVF)	5000
Compound Parameters	
Declustering Potential (DP)	100
Collision Energy (CE)	45
Resolution Parameters	
Q1 Resolution	Unit

4. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

5. Perform several 5 µL injections of the 0.0167 pmol/µL reserpine solution while optimizing the following for maximum signal intensity and stability:

   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, TEM, GS1, GS2, and ISVF

6. Click **Acquire** to begin collecting data.
7. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

8. Print the results.
9. Average the three intensities of the ions and then record the result in the Data Log.
10. Confirm that the average intensity is acceptable. Refer to Data Log: Turbo V™ Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.
11. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the APCI Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 1 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the method parameters as shown in Table 2-4.

Table 2-4 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	Product Ion
High Sensitivity (5600/5600+ and 6600 systems only)	On
Product Of	609.2807
TOF Masses (Da)	150 to 650
Accumulation time (seconds)	0.200

Table 2-4 Method Parameters (continued)

Parameter	Value
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20 (or as optimized)
Temperature (TEM)	425
Ion Source Gas 1 (GS1)	70 (or as optimized)
Nebulizer Current (NC)	3 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100
Collision Energy (CE)	45
Resolution Parameters	
Q1 Resolution	Unit

4. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

5. Perform several 5 µL injections of the reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, GS1, and NC
6. Click **Acquire** to begin collecting data.
7. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

8. Print the results.
9. Average the three intensities of the ions and then record the result in the Data Log.
10. Confirm that the average intensity is acceptable. Refer to Data Log: Turbo V™ Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.
11. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

DuoSpray™ Ion Source Tests 3

Run these tests in any of the following situations:

- When a new ion source is installed.
- After major maintenance to the ion source.
- Whenever the performance of the ion source must be assessed, either before starting a project or as part of a standard operating procedure.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of toxic or injurious materials used with the ion source.

WARNING! Puncture Hazard, Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Discontinue use of the ion source if the ion source window is cracked or broken and then contact a SCIEX Field Service Employee (FSE). Any toxic or injurious materials introduced into the equipment will be present in the source exhaust output. Dispose of sharps following established laboratory safety procedures.

WARNING! Toxic Chemical Hazard. Wear personal protective equipment, including a laboratory coat, gloves, and safety glasses, to avoid skin or eye exposure.

WARNING! Ionizing Radiation Hazard, Biohazard, Electrical Shock Hazard, or Toxic Chemical Hazard. In the event of a chemical spill, review product Safety Data Sheets for specific instructions. Make sure that the system is in Standby mode before cleaning a spill near the ion source. Use appropriate personal protective equipment and absorbent wipes to contain the spill and dispose of it following local regulations.

Required Materials

- Mobile phase solvent: 70:30 acetonitrile:water solution
- Test Solution:
  - For 4500, 5500, 6500, and 6500+ systems, use the pre-diluted 0.0167 pmol/µL reserpine solution included in the SCIEX Standard Chemical Kit (PN 4406127).
  - For 3200 and 3500 systems, use the pre-diluted 0.167 pmol/µL reserpine solution included in the SCIEX Standard Chemical Kit (PN 4406127).
  - For TripleTOF® systems, prepare the test solution from the 0.167 pmol/µL reserpine solution and the standard diluent provided in the SCIEX TripleTOF® System Chemical Kit (PN 4456736)

  A vortex mixer is required.
- HPLC pump (for mobile phase)
- Manual injector (8125 Rheodyne or equivalent) with a 5 µL loop or an autosampler set up for 5 µL injections
- PEEK tubing 1/16-inch outside diameter (o.d.), 0.005-inch inside diameter (i.d.)
- Ion source with a probe installed
- Syringe 250 µL to 1000 µL
- Powder-free gloves (nitrile or neoprene is recommended)
- Safety glasses
- Lab coat

Note: All test solutions must be kept refrigerated. If they are left out of the refrigerator for longer than 48 hours, then discard them and use new solutions.

CAUTION: Potential Wrong Result. Do not use expired solutions.

Prepare for the Test

WARNING! Electrical Shock Hazard. Avoid contact with the high voltages applied to the ion source during operation. Put the system in Standby mode before adjusting the sample tubing or other equipment near the ion source.

- When installing a new ion source, make sure that the mass spectrometer is performing to specifications with the existing ion source.
- Install the ion source on the mass spectrometer.

- Make sure that the ion source is fully optimized. Refer to the appropriate ion source *Operator Guide*.
- Refer to all applicable Safety Data Sheets for any necessary precautions before handling chemical solutions or solvents.
- Connect the grounding union on the ion source to a pump, through a manual injector equipped with a 5 µL loop, or to an autosampler.

Refer to Figure 3-1 and Figure 3-2.

Figure 3-1 LC Pump Configuration: TurboIonSpray® Probe

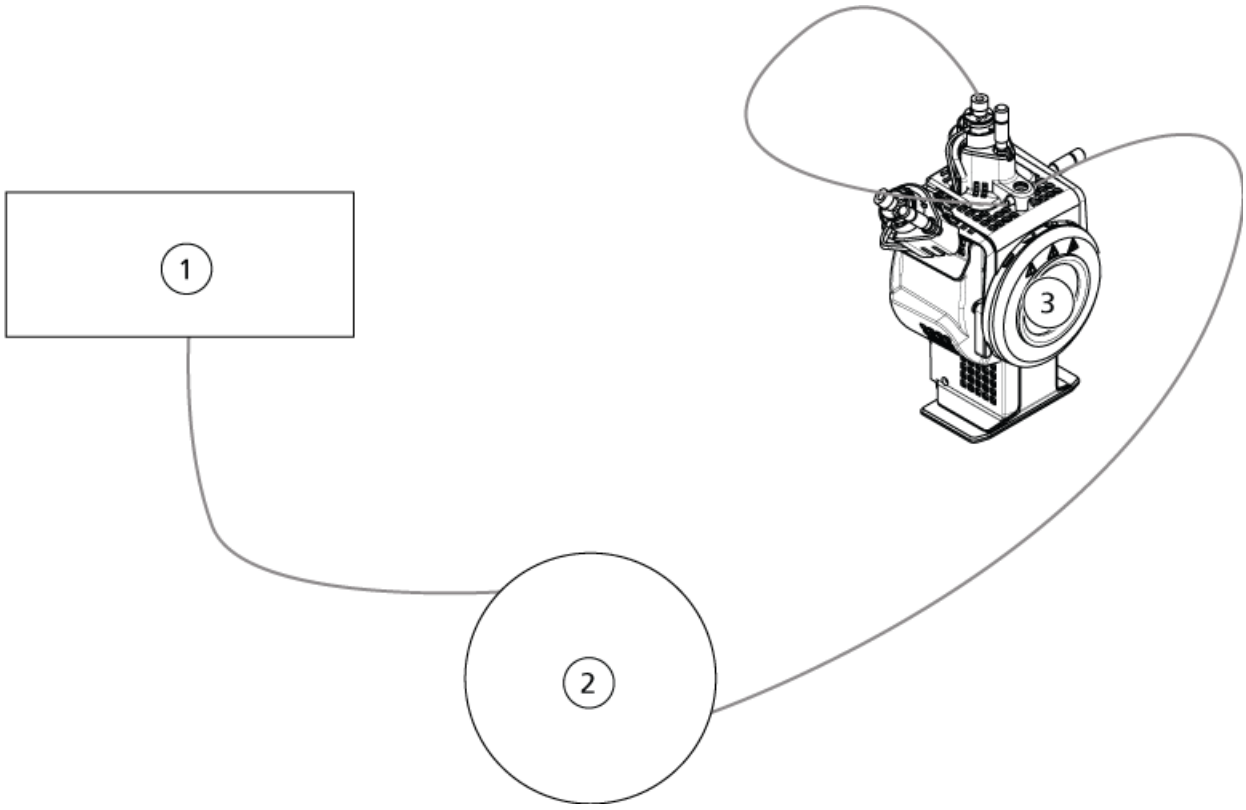
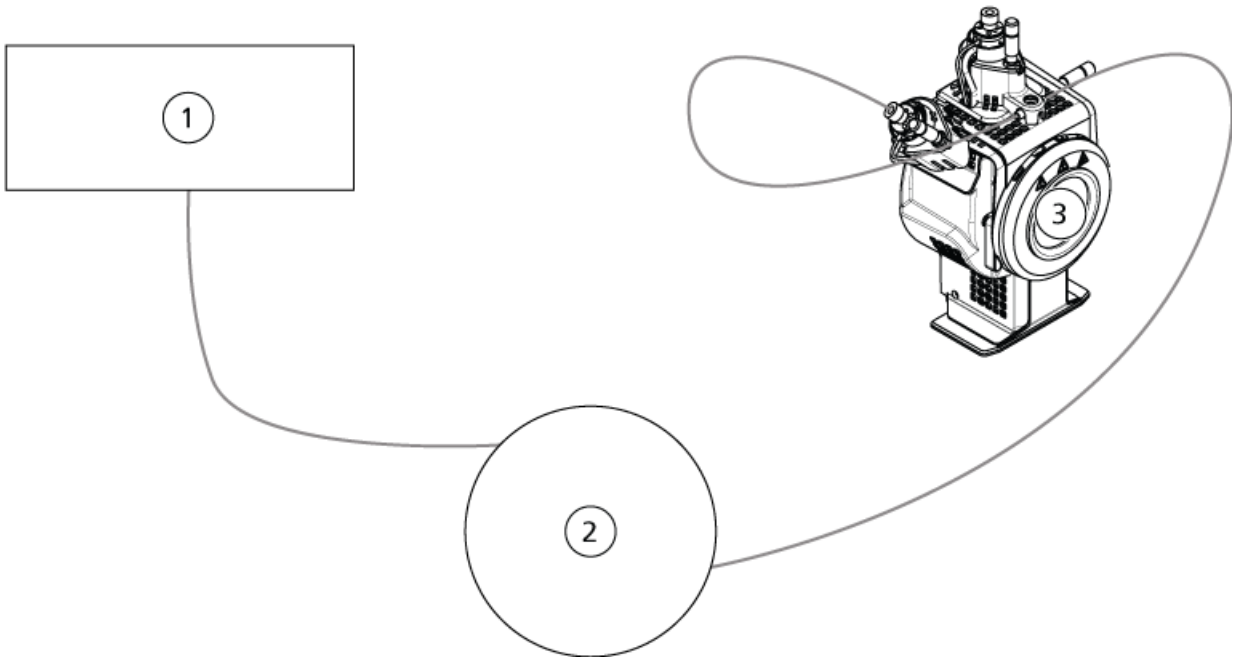


Figure 3-2 Pump Configuration: APCI Probe



Item	Description
1	LC pump
2	Injector or autosampler
3	Ion source

Test the Ion Source on TripleTOF® Systems

Prepare the Test Solution

1. Combine 100 µL of the 0.167 pmol/µL reserpine solution and 900 µL of the standard diluent.
2. Mix using a vortex mixer for 30 seconds.

   This step produces the 0.0167 pmol/µL reserpine solution.

Test the TurboIonSpray® Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 0.2 mL/min of the mobile phase.
2. In the Analyst® TF software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Adjust the probe positions as shown in the Table 3-1.

Table 3-1 Probe Positions

Probe	Vertical Position	Horizontal Position	Electrode Tip Extension
APCI	5	—	0.5 mm
TurboIonSpray	5	5	0.5 mm

4. Open a previously optimized method or set the method parameters as shown in Table 3-2.

Table 3-2 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	Product Ion
High Sensitivity (5600/5600+ and 6600 systems only)	On
Product Of	609.2807
TOF Masses (Da)	150 to 650
Accumulation time (seconds)	0.200
Duration (minutes)	10

Table 3-2 Method Parameters (continued)

Parameter	Value
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20
Temperature (TEM)	650
Ion Source Gas 1 (GS1)	50
Ion Source Gas 2 (GS2)	70
IonSpray Voltage Floating (ISVF)	5500
Compound Parameters	
Declustering Potential (DP)	100
Collision Energy (CE)	45
Resolution Parameters	
Q1 Resolution	Unit

5. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

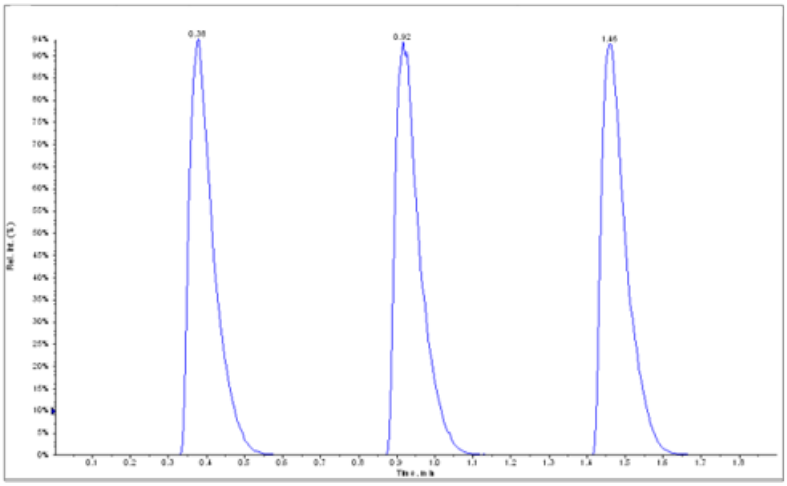
6. Perform several 5 µL injections of the 0.0167 pmol/µL reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, TEM, GS1, GS2, and ISVF
7. Click **Acquire** to begin collecting data.
8. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

9. After the acquisition, for each injection, generate an XIC of the 50 mDa window centered on m/z 195.0652 (or the observed mass, as calibrated). Record the intensity (peak height) for each injection.
10. Print the results.

    The results should be similar to the following figure.

Figure 3-3 XIC for the 50 mDa Window Around the Centroid Mass of m/z 195



11. Average the three intensities of the ions and then record the result in the Data Log.
12. Confirm that the average intensity is acceptable. Refer to Data Log: DuoSpray™ Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.
13. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the APCI Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 1 mL/min of the mobile phase.

2. In the Analyst® TF software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Adjust the probe positions as shown in the Table 3-3.

Table 3-3 Probe Positions

Probe	Vertical Position	Horizontal Position	Electrode Tip Extension
APCI	5	—	0.5 mm
TurboIonSpray	5	5	0.5 mm

4. Open a previously optimized method or set the method parameters as shown in Table 3-4.

Table 3-4 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	Product Ion
High Sensitivity (5600/5600+ and 6600 systems only)	On
Product Of	609.2807
TOF Masses (Da)	150 to 650
Accumulation time (seconds)	0.200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20
Temperature (TEM)	650
Ion Source Gas 2 (GS2)	70
IonSpray Voltage Floating (ISVF)	5500
Compound Parameters	
Declustering Potential (DP)	100
Collision Energy (CE)	45

Table 3-4 Method Parameters (continued)

Parameter	Value
Resolution Parameters	
Q1 Resolution	Unit

5. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

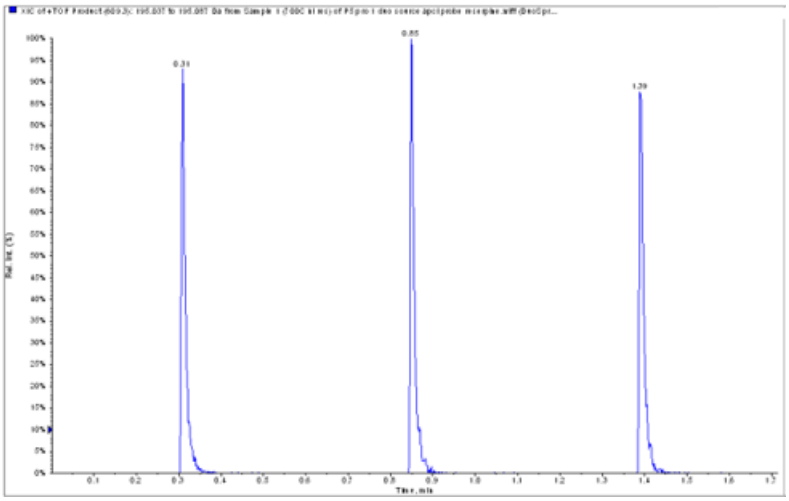
6. Perform several 5 µL injections of the 0.0167 pmol/µL reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical position of the probe
   - The electrode tip extension
   - CUR, TEM, GS2, and ISVF
7. Click **Acquire** to begin collecting data.
8. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

9. After the acquisition, for each injection, generate an XIC of the 50 mDa window centered on m/z 195.0652 (or the observed mass, as calibrated). Record the intensity (peak height) for each injection.
10. Print the results.

    The results should be similar to the following figure.

Figure 3-4 XIC for the 50 mDa Window Around the Centroid Mass of m/z 195



11. Confirm that the average intensity is acceptable. Refer to Data Log: DuoSpray™ Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.

12. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the Ion Source on Triple Quadrupole and QTRAP® Systems

Test the TurboIonSpray® Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 0.2 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. On the **Source/Gas** tab, select **TIS** from the list

4. Adjust the probe positions as shown in the Table 3-5.

Table 3-5 Probe Positions

Probe	Vertical Position	Horizontal Position	Electrode Tip Extension
APCI	5	—	0.5 mm
TurboIonSpray	5	5	0.5 mm

5. Open a previously optimized method or set the method parameters as shown in Table 3-6.

Table 3-6 Method Parameters

Parameter	Value
MS Parameters	Product Ion
Scan Mode	MRM
Q1	609.3
Q3	195.1
Scan Time (ms)	200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20 (or as optimized)
IonSpray Voltage (IS)	4500 (or as optimized)
Temperature (TEM)	700 (or as optimized)
Ion Source Gas 1 (GS1)	60 (or as optimized)
Ion Source Gas 2 (GS2)	70 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized

6. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

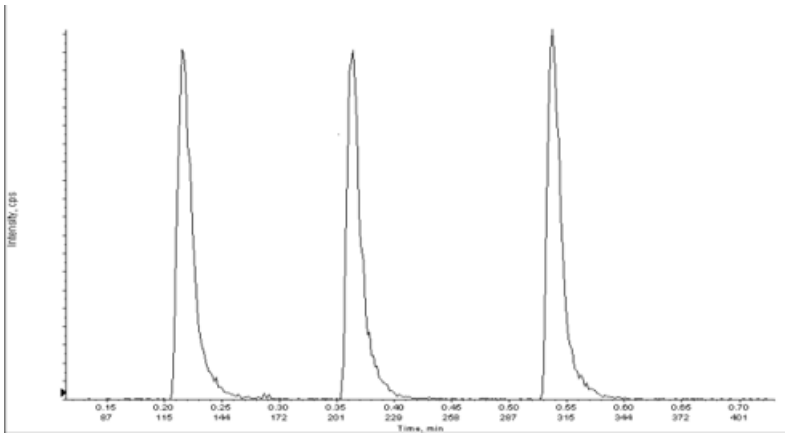
7. Perform several 5 µL injections of the reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, TEM, GS1, GS2, and IS
8. Click **Acquire** to begin collecting data.
9. Perform three 5 µL injections of the 10 pg/µL test solution while monitoring the 50 mDa window around the centroid mass of m/z 195.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

10. Print the results.

    The results should be similar to the following figure.

Figure 3-5 Reserpine



11. Average the three intensities of the ions and then record the result in the Data Log.
12. Confirm that the average intensity is acceptable. Refer to Data Log: DuoSpray™ Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.
13. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

Test the APCI Probe

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

CAUTION: Potential System Damage. Do not introduce any solvent flow until after the ion source has reached the correct temperature.

Refer to the ion source *Operator Guide* for information about installing or optimizing the ion source.

1. Configure the HPLC pump to deliver 1 mL/min of the mobile phase.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Adjust the probe positions as shown in the Table 3-7.

Table 3-7 Probe Positions

Probe	Vertical Position	Horizontal Position	Electrode Tip Extension
APCI	5	—	0.5 mm
TurboIonSpray	5	5	0.5 mm

4. Open a previously optimized method or set the method parameters as shown in Table 3-8.

Table 3-8 Method Parameters

Parameter	Value
MS Parameters	
Scan Mode	MRM
Q1	609.3
Q3	195.1

Table 3-8 Method Parameters (continued)

Parameter	Value
Scan Time (ms)	200
Duration (minutes)	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20 (or as optimized)
Nebulizer Current (NC)	3 (or as optimized)
Temperature (TEM)	350 (or as optimized)
Ion Source Gas 2 (GS2)	70 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized

5. Click **Start** to run the method.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Make sure that the electrode protrudes beyond the tip of the probe, to prevent hazardous vapors from escaping from the source. The electrode must not be recessed within the probe.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

6. Perform several 5 µL injections of the reserpine solution while optimizing the following for maximum signal intensity and stability:
   - The vertical and horizontal position of the probe
   - The electrode tip extension
   - CUR, GS1, and NC
7. Click **Acquire** to begin collecting data.
8. Perform three 5 µL injections of the reserpine solution.

Tip! We recommend that the 5 µL loop be overfilled with 30 µL to 40 µL of the solution.

9. After the acquisition, for each injection, generate an XIC of the 50 mDa window centered on m/z 195.0652 (or the observed mass, as calibrated). Record the intensity (peak height) for each injection.
10. Print the results.
11. Confirm that the average intensity is acceptable. Refer to Data Log: DuoSpray™ Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.
12. After completing the tests, stop the LC pump, set **TEM** to 0, and then let the probe cool.

NanoSpray® Ion Source Tests 4

Run these tests in any of the following situations:

- When a new ion source is installed.
- After major maintenance to the ion source.
- Whenever the performance of the ion source must be assessed, either before starting a project or as part of a standard operating procedure.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of toxic or injurious materials used with the ion source.

WARNING! Electrical Shock Hazard. Never operate the NanoSpray® ion source without the illuminator, camera, stop, and covers properly installed. Never touch the curtain plate or allow the emitter tip to contact the curtain plate. If the mass spectrometer is operational and the ion source is installed, then high voltage is present on the curtain plate, even if the X-Y-Z positioning unit is moved away from the interface.

WARNING! Toxic Chemical Hazard. Wear personal protective equipment, including a laboratory coat, gloves, and safety glasses, to avoid skin or eye exposure.

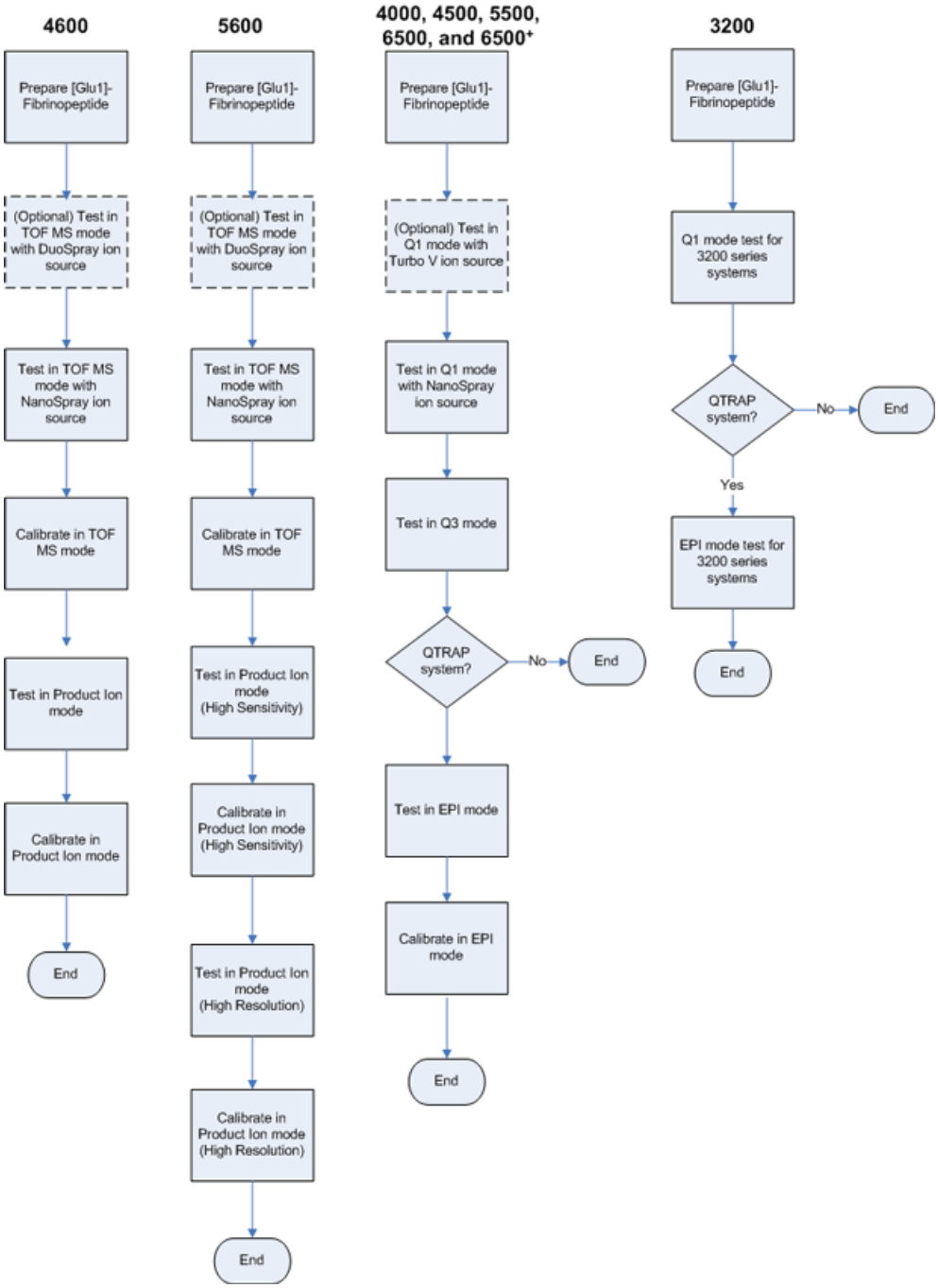
WARNING! Ionizing Radiation Hazard, Biohazard, Electrical Shock Hazard, or Toxic Chemical Hazard. In the event of a chemical spill, review product Safety Data Sheets for specific instructions. Make sure that the system is in Standby mode before cleaning a spill near the ion source. Use appropriate personal protective equipment and absorbent wipes to contain the spill and dispose of it following local regulations.

Prepare for the Test

WARNING! Electrical Shock Hazard. Avoid contact with the high voltages applied to the ion source during operation. Put the system in Standby mode before adjusting the sample tubing or other equipment near the ion source.

- When installing a new ion source, make sure that the mass spectrometer is performing to specifications with the existing ion source.
- Install the ion source on the mass spectrometer.
- Make sure that the ion source is fully optimized. Refer to the appropriate ion source *Operator Guide*.
- Refer to all applicable Safety Data Sheets for any necessary precautions before handling chemical solutions or solvents.

Figure 4-1 Test Workflow



Prepare the [Glu^1]-Fibrinopeptide B Dilution

Required Material
• [Glu1]-Fibrinopeptide B, included in the LC/MS Peptide Calibration Kit (PN 4465867) • Standard diluent, included in the LC/MS Peptide Calibration Kit • Powder-free gloves (nitrile or neoprene is recommended) • Safety glasses • Lab coat

For the list of masses for [Glu^1]-Fibrinopeptide B, refer to Masses for [Glu^1]-Fibrinopeptide B.

Note: Always prepare the dilution just before running the test.

Note: The [Glu^1]-Fibrinopeptide B might become lodged in the rubber septum of the vial. Gently tap or shake it down before opening the vial. Then, partially remove the septum to reveal a slot. Add the dilution solvent through the slot. Then push the septum back into place and mix well to dissolve.

CAUTION: Potential Wrong Result. Do not use expired solutions.

1. Add 900 µL of Standard diluent (0.1% formic acid, 10% acetonitrile) to the glass amber vial containing 0.1 mg [Glu^1]-Fibrinopeptide B.
2. Cover the vial tightly, shake it, and then vortex it for at least 2 minutes, to make sure that the peptide is fully dissolved.

   Note: Peptide concentration may vary depending on the total peptide content and peptide purity of the standard solution. Refer to the Certificate of Analysis provided by the vendor. At 100% purity, 0.1 mg [Glu^1]-Fibrinopeptide B dissolved as described in the preceding steps produces a stock solution with a concentration of approximately 66.67 pmol/µL.

3. Aliquot the stock solution in 50 µL volumes into clean tubes. Freeze unused aliquots at –20°C for future use.
4. Put 50 µL of the stock solution into a clean tube and then add 450 µL of standard diluent.
5. Vortex the tube for 30 seconds.

   This is a 1:10 dilution, providing 500 µL of a 6.7 pmol/µL solution.
6. Put 50 µL of the 6.7 pmol/µL solution into another clean tube.
7. Add 450 µL of standard diluent.

8. Vortex the tube for 30 seconds.

   This is a 1:10 dilution, providing 500 µL of the 667 fmol/µL solution.

9. Put 50 µL of the 667 fmol/µL solution into another clean tube.
10. Add 450 µL of standard diluent.
11. Vortex the tube for 30 seconds.

    This is a 1:10 dilution, providing 500 µL of the final 66.7 fmol/µL solution, to be used for the infusion test.

Test the Ion Source on TripleTOF® Systems

WARNING! Electrical Shock Hazard. Never operate the NanoSpray® ion source without the illuminator, camera, stop, and covers properly installed. Never touch the curtain plate or allow the emitter tip to contact the curtain plate. If the mass spectrometer is operational and the ion source is installed, then high voltage is present on the curtain plate, even if the X-Y-Z positioning unit is moved away from the interface.

WARNING! Hot Surface Hazard. Do not touch the high voltage rail or emitter tip.

Refer to Figure 4-1 for an overview of the required tasks.

For TripleTOF® 4600 systems, perform these tasks:

- Prepare the [Glu[1]]-Fibrinopeptide B Dilution
- Test and Calibrate in TOF MS Mode
- Test and Calibrate in Product Ion Mode

For TripleTOF® 5600/5600+ and 6600 systems, perform these tasks:

- Prepare the [Glu[1]]-Fibrinopeptide B Dilution
- Test and Calibrate in TOF MS Mode
- Test and Calibrate in Product Ion Mode (High Sensitivity) (5600/5600+ and 6600 Systems Only)
- Test and Calibrate in Product Ion Mode. This test is performed in High Resolution mode.

Required Materials
• [Glu1]-Fibrinopeptide B Dilution. Refer to Prepare the [Glu[1]]-Fibrinopeptide B Dilution. • 100 µL syringe (1.46 mm i.d.) or equivalent for infusion with the NanoSpray® ion source • (Optional) 1 mL syringe (4.61 mm i.d.) or equivalent for infusion with the DuoSpray™ ion source • Powder-free gloves (nitrile or neoprene is recommended) • Safety glasses • Lab coat

Test and Calibrate in TOF MS Mode

(Optional) Perform the TOF MS Test with the DuoSpray™ Ion Source

This procedure confirms the integrity of the dilution.

Note: Before filling the syringe with the [Glu[1]]-Fibrinopeptide B solution, wash it three times with the wash solution. Then connect the syringe to the proper tubing and wash it again before connecting it to the union on the high-voltage rail. Then, flush the tubing with the [Glu[1]]-Fibrinopeptide B solution.

1. Install the DuoSpray™ ion source on the mass spectrometer. Refer to the *DuoSpray™ Ion Source Operator Guide*.
2. Using the 1 mL syringe, infuse the [Glu[1]]-Fibrinopeptide B solution at a flow rate of 5 µL/min.
3. In the Analyst® TF software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
4. Open a previously optimized method or set the method parameters as shown in Table 4-1.

Table 4-1 Parameters for the TOF MS Test with the DuoSpray™ Ion Source

Parameter	Value
MS Parameters	
Scan type	TOF MS
Accumulation time (sec)	
Polarity	Positive
TOF masses (Da)	400 to 1800
Duration (min)	0.5

Table 4-1 Parameters for the TOF MS Test with the DuoSpray™ Ion Source (continued)

Parameter	Value
Advanced MS Parameters	
MCA	Off
Auto Adjust with mass	On
Q1 Transmission Window	Default (with Auto-adjust)
Pulsar Frequency	Default (with Auto-adjust)
Time bins to sum	4
Settling time	Default
Pause between mass ranges	Default
Source/Gas Parameters	
Ion Source Gas 1 (GS1)	20
Curtain Gas™ flow (CUR)	20
Temperature (TEM) (°C)	0
IonSpray Voltage Floating (ISVF)	5500
Compound Parameters	
Declustering Potential (DP)	100
Syringe Pump Method Parameters	
Flow rate (µL/min)	5
Syringe Size	1 mL (4.61 mm i.d.)

5. Save the new method.

Tip! Save the methods used for the NanoSpray® ion source tests in a separate folder, named NanoSpray Installation <date>.

6. Click **Acquire** to acquire 30 seconds of data.
7. Highlight 30 seconds in the **TIC of +TOF MS** window in the lower left pane, and then double-click to display an averaged spectrum.
8. Right-click in the averaged spectrum, which appears in the bottom pane, and then click **List Data**. Then record the centroid intensity and resolution.

9. Confirm that the centroid intensity and resolution are acceptable. Refer to Data Log: NanoSpray® Ion Source.

   Guideline: The centroid intensity and resolution achieved with the DuoSpray™ ion source should meet the specifications given for the NanoSpray® ion source. If they do not, prepare a new dilution.

Perform the TOF MS Test with the NanoSpray® Ion Source

Note: Before filling the syringe with the [Glu[1]]-Fibrinopeptide B solution, wash it three times with the wash solution. Then connect the syringe to the proper tubing and wash it again before connecting it to the union on the high-voltage rail. Then, flush the tubing with the [Glu[1]]-Fibrinopeptide B solution.

1. Install the NanoSpray® ion source on the mass spectrometer. Refer to the *NanoSpray® Ion Source Operator Guide*.
2. Prepare the NanoSpray III head. Refer to the *NanoSpray® Ion Source Operator Guide*.
3. Using the 100 µL syringe, infuse the [Glu[1]]-Fibrinopeptide B solution at a flow rate of 0.5 µL/min.
4. In the Analyst® TF software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
5. If the optional procedure, (Optional) Perform the TOF MS Test with the DuoSpray™ Ion Source , is performed, open the method and then and set the parameters as shown in Table 4-2. If the procedure is not performed, then create a method using these parameters.

Table 4-2 TOF MS Method Parameters with the NanoSpray® Ion Source

Parameter	Value
MS Parameters	
Scan type	TOF MS
Accumulation time (sec)	1.0
Polarity	Positive
TOF masses (Da)	400 to 1800
Duration (min)	0.5
Advanced MS Parameters	
MCA	Off
Auto Adjust with mass	On
Q1 Transmission Window	Default (with Auto-adjust)
Pulsar Frequency	Default (with Auto-adjust)
Time bins to sum	4

Table 4-2 TOF MS Method Parameters with the NanoSpray® Ion Source (continued)

Parameter	Value
Settling time	Default
Pause between mass ranges	Default
Source/Gas Parameters	
Ion Source Gas 1 (GS1)	3
Curtain Gas™ flow (CUR)	25
Interface Heater Temperature (IHT) (°C)	75
IonSpray Voltage Floating (ISVF)	2100
Compound Parameters	
Declustering Potential (DP)	100
Syringe Pump Method Parameters	
Flow rate (µL/min)	0.5
Syringe Size	100 Gastight (1.46 mm)

6. Click **Start** to run the method.

CAUTION: Potential System Damage. Do not allow the emitter tip to contact the curtain plate. Use the fine Z-axis adjustment knob to adjust the sprayer position, to avoid damage to the emitter tip.

CAUTION: Potential System Contamination. Do not insert the end of the emitter tip into the curtain plate aperture. Make sure that the emitter tip is at least 2 mm to 5 mm outside the aperture. Spraying too close to the aperture can cause contamination of the mass spectrometer.

7. Adjust the position of the sprayer head relative to the curtain plate aperture to optimize signal intensity. Record the XYZ values for future use.
8. Adjust **ISVF** in 100 V increments to achieve the best signal and signal-to-noise ratio.

Note: If the IonSpray™ voltage is too high, then a corona discharge can occur. It is visible as a blue glow at the tip of the probe. A corona discharge results in decreased sensitivity and stability of the signal.

9. Increase **GS1** until the signal starts to decrease and then reduce **GS1** until the signal reaches its maximum value.

   GS1 usually optimizes between 3 and 10. If **GS1** is outside this range, then the tip protrusion is incorrect (1 to 2 mm) or the tip may need to be replaced.

   Note: The GS1 parameter might optimize at zero.

10. Increase **CUR** until the signal starts to decrease, and then reduce **CUR** until the signal reaches its maximum value.

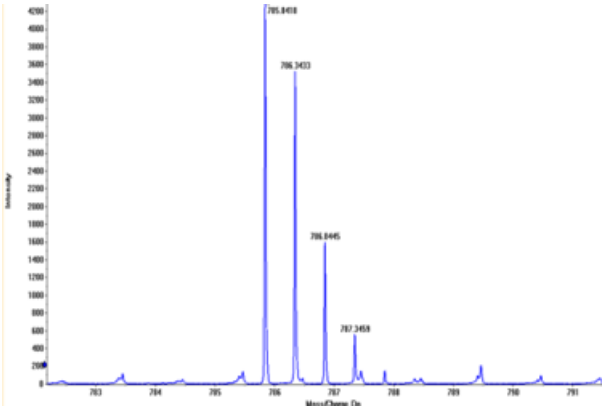
    Note: To prevent contamination, use the highest value for CUR possible without sacrificing sensitivity. Do not set CUR lower than 20. This helps to prevent penetration of the Curtain Gas™ flow, which can produce a noisy signal; prevent contamination of the aperture; and increase the overall signal-to-noise ratio.

11. If you moved the sprayer head to optimize signal intensity, adjust the position of the illuminator as necessary.
12. Save the new method.

    Tip! Save the methods used for the NanoSpray® ion source tests in a separate folder, named NanoSpray Installation <date>.

13. Run the method for at least 20 minutes. Monitor the spray stability. If the spray is stable, only minimal fluctuations are visible in the TIC.
14. After the spray is optimized and has stabilized, click **Acquire** and acquire 30 seconds of data.
15. Highlight 30 seconds in the **TIC of +TOF MS** window in the lower left pane, and then double-click to display an averaged spectrum.
16. Right-click in the averaged spectrum, which appears in the bottom pane, and then click **List Data**. Record the centroid intensity and the resolution.
17. Confirm that the centroid intensity and resolution are acceptable. Refer to Figure 4-2 and Data Log: NanoSpray® Ion Source.

Figure 4-2 Sample Spectra: TOF MS Scan for GluFibrinopeptide B, TripleTOF 5600 system



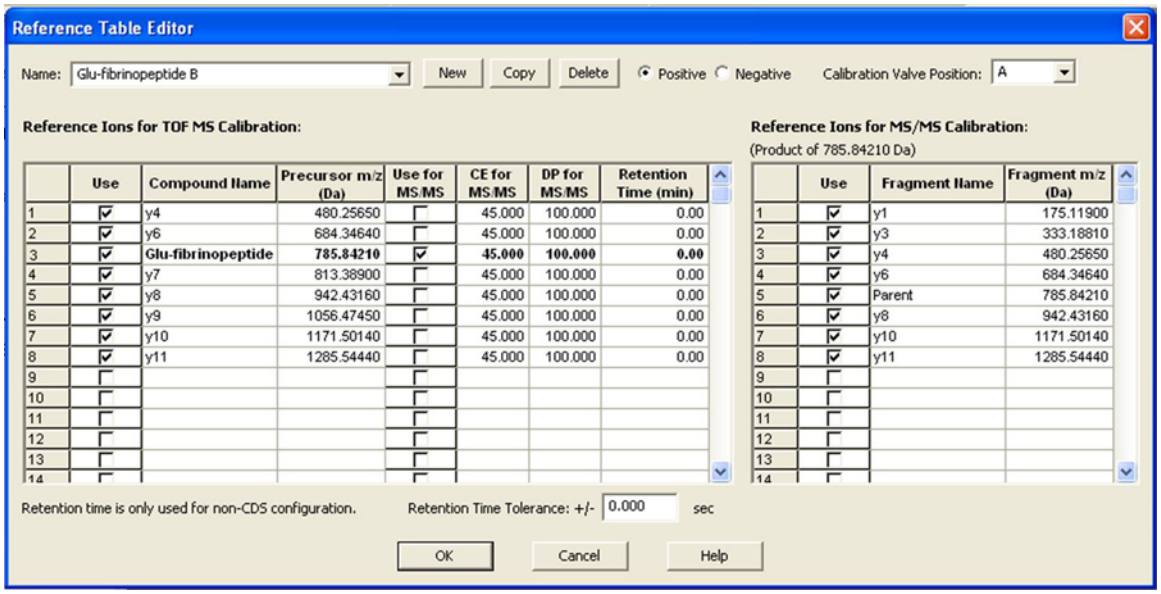
If the results are not acceptable, then refer to Troubleshooting Tips.

18. Print a copy of the results and record the centroid intensity and resolution in the Data Log.

Update the Calibration Reference Table for [Glu[1]]-Fibrinopeptide B

1. In the Analyst® TF software, in **Tune and Calibrate** mode, click **Tools > Settings > Tuning Options.**
2. On the **Calibration** tab, click **Reference**.
3. In the **Reference Table Editor**, in the **Name** field, select **Glu-fibrinopeptide B.**
4. In the table of **Reference Ions for TOF MS Calibration** (on the left side) add the masses shown in Figure 4-3. For the list of masses for [Glu[1]]-fibrinopeptide B, refer to Masses for [Glu[1]]-Fibrinopeptide B.

Figure 4-3 Reference Table Editor: Reference Ions for TOF MS Calibration



5. Click **OK**.
6. In the **Tuning Options** dialog, click **OK**.

Calibrate in TOF MS Mode

1. In **Manual Tune** mode, make sure that the parameters are set to the values specified in Table 4-2.
2. On the **Compound** tab, set **Collision Energy (CE)** to **35** V.
3. When the spray is stable, click **Acquire** and acquire 30 seconds of scan data.
4. In the **TIC of +TOF MS** window (at the lower left), highlight 30 seconds of TIC signal to average and then double-click.
5. In the new window that appears (at the bottom of the Analyst® software window), right-click and click **Re-Calibrate TOF**.
6. In the **TOF Calibration** dialog, in the **Reference Table** list, select **Glu-fibrinopeptide B**.
7. Make sure that the proper experimental masses have been identified in the infusion spectrum and that they match the reference table theoretical masses.
8. Check the **Average Error** value displayed to the right of the **Calculate New Calibrations** button.
9. Click **Calculate New Calibrations** and make sure that the **Average Error** value drops to less than 2 ppm.
10. Under **Calibration Values**, click **Calibrate Spectrum**.

11. Under **Save Current Calibration**, select **Set as Instrument Default** and **Overwrite Current File**.
12. Click **Entire File**.
13. Click **Close**.

Test and Calibrate in Product Ion Mode (High Sensitivity) (5600/5600+ and 6600 Systems Only)

Perform the Product Ion mode (High Sensitivity) Test (5600/5600+ and 6600 Systems Only)

1. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
2. Open a previously optimized method or set the method parameters as shown in Table 4-3.

Table 4-3 Product Ion Method Parameters

Parameter	Value
MS Parameters	
Scan type	Product Ion
Product of	785.8
Accumulation time (sec)	1.0
Polarity	Positive
TOF masses (Da)	100 to 1800
High sensitivity	On
Duration (min)	0.5
Advanced MS Parameters	
MCA	Off
Auto Adjust with mass	On
Q1 Transmission windows	Default (with Auto-adjust)
Pulsar Frequency	Default (with Auto-adjust)
Time Bins to Sum	4
Settling time	Default
Pause between mass	Default

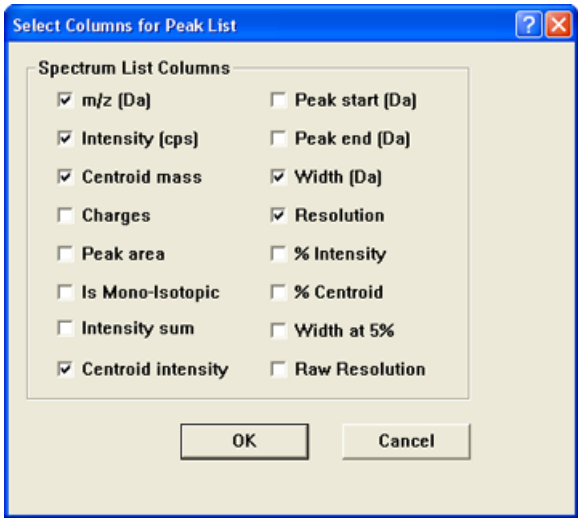
Table 4-3 Product Ion Method Parameters (continued)

Parameter	Value
Source/Gas Parameters	
Ion Source Gas 1 (GS1)	as optimized
Curtain Gas™ flow (CUR)	as optimized
Interface Heater Temperature (IHT) (°C)	75
IonSpray Voltage Floating (ISVF)	as optimized
Compound Parameters	
Collision Energy (CE) (V)	45 (or as optimized)
Resolution Parameters	
Q1 resolution	Unit

Note: CE normally optimizes between 40 V and 48 V. If CE is not in this range, then the CAD gas value may be set too low. If the intensity of the precursor ion at m/z 785.9 is not 10% or less of the original intensity, then the interaction of CE and CAD gas is incorrect. Contact SCIEX technical support for more information.

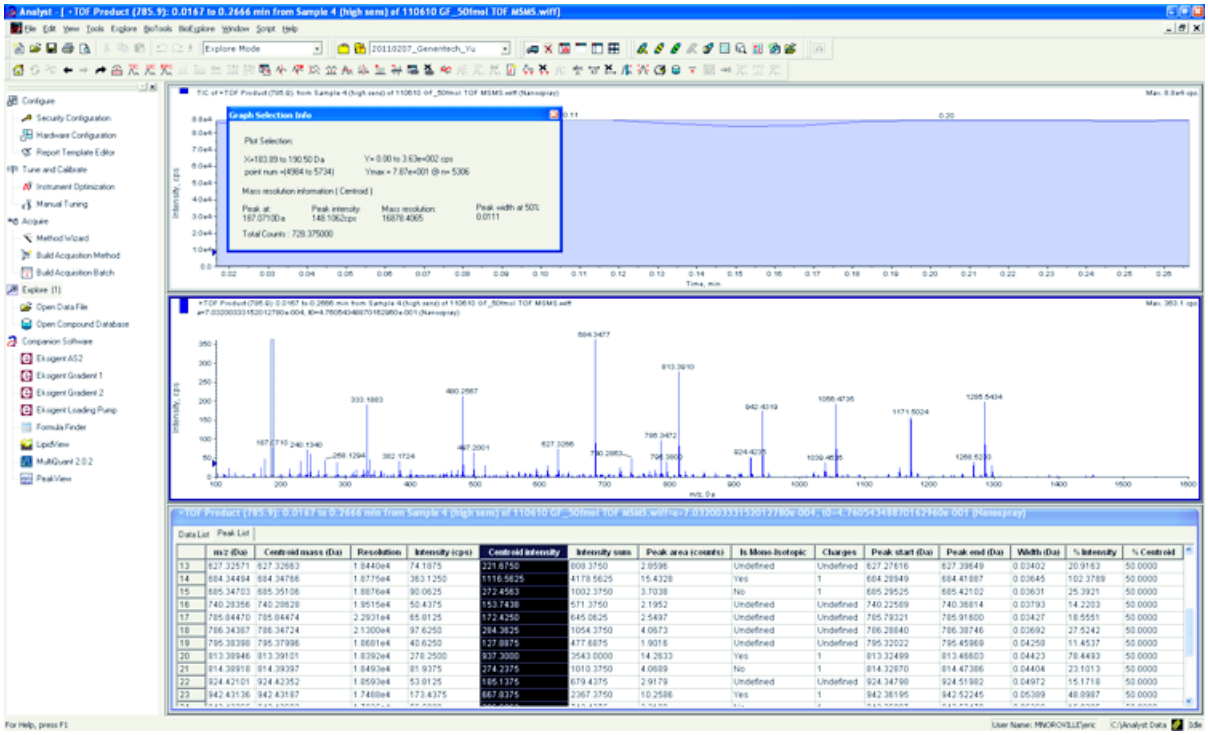
3. Save the new method.
4. When the spray is stable, click **Acquire** to acquire at least 30 seconds of scans.
5. Highlight 30 seconds in the **TIC of +TOF Product** window in the lower left pane, and then double-click to display an averaged spectrum.
6. Right-click in the averaged spectrum, which appears in the bottom pane, and then click **List Data**.
7. Click the **Peak List** tab.
8. Right-click the column header row, and click **Column Options**.

Figure 4-4 Select Columns for Peak List Dialog



9. Select the m/z (Da), Intensity, Centroid mass, Centroid Intensity, Width (Da), and Resolution check boxes.
10. Click **OK**.
11. Confirm that the centroid intensity and resolution are acceptable. Refer to Figure 4-5 and Data Log: NanoSpray® Ion Source.

Figure 4-5 Sample Spectra: Product Ion High Sensitivity Test



If the result is not acceptable, refer to Troubleshooting Tips.

12. Print a copy of the results and record the centroid intensity and resolution in the Data Log.

Calibrate in Product Ion Mode (High Sensitivity)

1. In **Manual Tune** mode, make sure that the parameters are set to the values specified in Table 4-3.
2. When the spray is stable, click **Acquire** and acquire at least 30 seconds of scan data.
3. In the **TIC of +TOF Product** window (at the lower left), highlight 30 seconds of TIC signal to average and then double-click.
4. In the new window that appears (at the bottom of the Analyst® window), right-click and click **Re-Calibrate TOF**.
5. In the **TOF Calibration** dialog, in the **Reference Table** list, select **Glu-fibrinopeptide B**.
6. Make sure that the proper experimental masses have been identified in the infusion spectrum and that they match the reference table theoretical masses.
7. Select the **Average Error** value shown to the right of the **Calculate New Calibrations** button.

8. Click **Calculate New Calibrations** and make sure that the **Average Error** value drops to less than 2 ppm.
9. Under **Calibration Values**, click **Calibrate Spectrum**.
10. Under **Save Current Calibration**, select **Set as Instrument Default** and **Overwrite Current File**.
11. Click **Entire File**.
12. Click **Close**.

Test and Calibrate in Product Ion Mode

For SCIEXTripleTOF® 5600/5600+ and 6600 systems, this test is performed in High Resolution mode.

Perform the Product Ion Test

1. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
2. Open a previously optimized method or set the method parameters as shown in Table 4-4.

Table 4-4 Product Ion Method Parameters

Parameter	Value
MS Parameters	
Scan type	Product Ion
Product of	785.8
Accumulation time (sec)	1.0
Polarity	Positive
TOF masses (Da)	100 to 1800
High resolution (5600/5600+ and 6600 systems only)	On
Duration (min)	0.5
Advanced MS Parameters	
MCA	Off
Auto Adjust with mass	On
Q1 Transmission windows	Default (with Auto-adjust)
Pulsar Frequency	Default (with Auto-adjust)

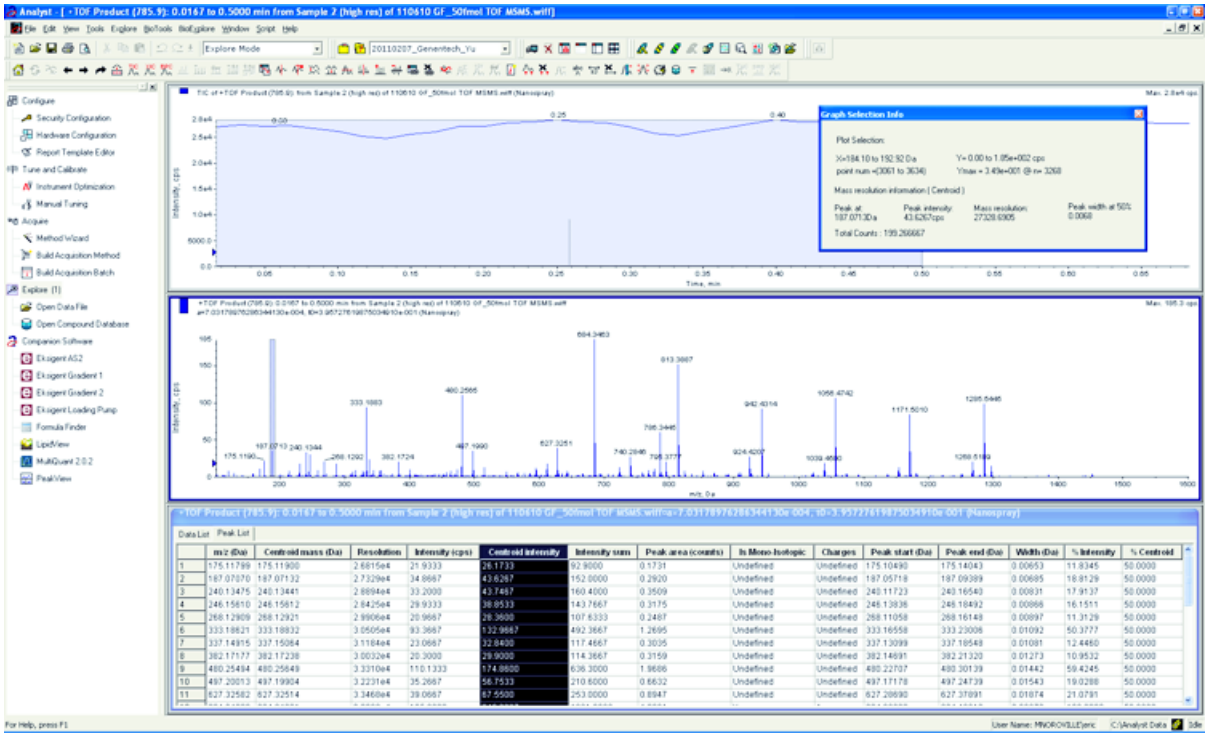
Table 4-4 Product Ion Method Parameters (continued)

Parameter	Value
Time Bins to Sum	4
Settling time	Default
Pause between mass	Default
Source/Gas Parameters	
Ion Source Gas 1 (GS1)	as optimized
Curtain Gas™ flow (CUR)	as optimized
Interface Heater Temperature (IHT) (°C)	75
IonSpray Voltage Floating (ISVF)	as optimized
Compound Parameters	
Collision Energy (CE) (V)	45 (or as optimized)
Resolution Parameters	
Q1 resolution	Unit

Note: CE normally optimizes between 40 V and 48 V. If CE is not in this range, then the CAD gas value may be set too low. If the intensity of the precursor ion at m/z 785.9 is not 10% or less of the original intensity, then the interaction of CE and CAD gas is incorrect. Contact SCIEX technical support for more information.

3. Save the new method.
4. When the spray is stable, click **Acquire** to acquire at least 30 seconds of scans.
5. Highlight 30 seconds in the **TIC of +TOF Product** window in the lower left pane, and then double-click to display an averaged spectrum.
6. Right-click in the averaged spectrum, which appears in the bottom pane, and then click **List Data**.
7. Click the **Peak List** tab.
8. Confirm that the centroid intensity and resolution are acceptable. Refer to Figure 4-6 and Data Log: NanoSpray® Ion Source.

Figure 4-6 Sample Spectra: Product Ion Test, TripleTOF 5600 System



If the results are not acceptable, refer to Troubleshooting Tips.

9. Print a copy of the results and record the centroid intensity and resolution in the data log.

Calibrate in Product Ion Mode

For SCIEX TripleTOF® 5600/5600+ and 6600 systems, this procedure calibrates High Resolution mode.

1. In **Manual Tune** mode, make sure that the parameters are set to the values specified in Table 4-4.
2. When the spray is stable, click **Acquire** and acquire at least 30 seconds of scan data.
3. In the **TIC of +TOF Product** window (at the lower left), highlight 30 seconds of TIC signal to average and then double-click.
4. In the new window that appears (at the bottom of the Analyst® window), right-click and click **Re-Calibrate TOF**.
5. In the **TOF Calibration** dialog, in the **Reference Table** list, select **Glu-fibrinopeptide B**.
6. Make sure that the proper experimental masses have been identified in the infusion spectrum and that they match the reference table theoretical masses.
7. Check the **Average Error** value displayed to the right of the **Calculate New Calibrations** button.

8. Click **Calculate New Calibrations** and make sure that the **Average Error** value drops to less than 2 ppm.
9. Under **Calibration Values**, click **Calibrate Spectrum**.
10. Under **Save Current Calibration**, click **Entire File**.
11. Click **Close**.

Wrap-Up

Note: The SCIEX Field Service Employee (FSE) must e-mail the results of the NanoSpray® acceptance test run after installation to servicedata@sciex.com.

1. Flush the tip and the infusion line thoroughly.
2. Make a copy of the completed data log and test results and provide the customer with the originals.

Test the Ion Source on Triple Quadrupole and QTRAP® Systems

WARNING! Hot Surface Hazard. Do not touch the high voltage rail or emitter tip.

WARNING! Electrical Shock Hazard. Never operate the NanoSpray® ion source without the illuminator, camera, stop, and covers properly installed. Never touch the curtain plate or allow the emitter tip to contact the curtain plate. If the mass spectrometer is operational and the ion source is installed, then high voltage is present on the curtain plate, even if the X-Y-Z positioning unit is moved away from the interface.

Refer to Figure 4-1 for an overview of the required tasks.

For triple quadrupole systems, except 3200 series systems, do these tasks:

- Prepare the [Glu[1]]-Fibrinopeptide B Dilution
- Test in Q1 Mode
- Test in Q3 Mode

For QTRAP® systems, except 3200 QTRAP® systems, perform these tests:

- Prepare the [Glu[1]]-Fibrinopeptide B Dilution
- Test in Q1 Mode

- Test in Q3 Mode

For API 3200™ and 3200 QTRAP® systems, refer to Test the Ion Source on 3200 Series Systems.

Required Materials
• [Glu[1]]-Fibrinopeptide B, included in the LC/MS Peptide Calibration Kit (PN 4465867) • Standard diluent • 100 µL syringe (1.46 mm i.d.) or equivalent for infusion with the NanoSpray® ion source • (Optional) 1 mL syringe (4.61 mm i.d.) or equivalent for infusion with the Turbo V™ ion source • Powder-free gloves (nitrile or neoprene is recommended) • Safety glasses • Lab coat

Test in Q1 Mode

(Optional) Perform the Q1 Test with the Turbo V™ Ion Source

This procedure confirms the integrity of the dilution.

Note: Before filling the syringe with the [Glu[1]]-Fibrinopeptide B solution, wash it three times with the wash solution. Then connect the syringe to the proper tubing and wash it again before connecting it to the union on the high-voltage rail. Then, flush the tubing with the [Glu[1]]-Fibrinopeptide B solution.

1. Install the Turbo V™ ion source on the mass spectrometer. Refer to the *Turbo V™ Ion Source Operator Guide*.
2. Using the 1 mL syringe, infuse the [Glu[1]]-Fibrinopeptide B solution at a flow rate of 5 µL/min.
3. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
4. Open a previously optimized method or set the method parameters as shown in Table 4-5.

Table 4-5 Parameters for the Q1 Test with the Turbo V™ Ion Source

Parameter	Value
MS Parameters	
Scan type	Q1 scan
Mass mode (6500 and 6500+ series systems)	Low mass
Polarity	Positive

Table 4-5 Parameters for the Q1 Test with the Turbo V™ Ion Source (continued)

Parameter	Value
Display masses (Da)	Center: 785.9 Width: 20
Scan Speed (Da/sec)	10
MCA	On
Cycles	10
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20
IonSpray Voltage (IS)	5500
Ion Source Gas 1 (GS1)	20
Interface Heater (IHT)	Not used
Compound Parameters	
Declustering Potential (DP)	100
Syringe Pump Method Parameters	
Flow rate (µL/min)	5
Syringe Size	1 mL (4.61 mm i.d.)

5. Save the method.

Tip! Save the methods used for the NanoSpray® ion source tests in a separate folder, named NanoSpray Installation <date>.

6. Click **Acquire** to acquire 30 seconds of data.
7. Record the intensity of the peak at m/z 785.8421.
8. Repeat step 6 to step 7 two more times.
9. Average the results of the three scans.
10. Compare the centroid intensity and resolution with the NanoSpray® ion source specifications shown in Data Log: NanoSpray® Ion Source.

Guideline: The centroid intensity and resolution achieved with the Turbo V ion source should meet the specifications given for the NanoSpray® ion source. If they do not, prepare a new dilution.

Perform the Q1 Test with the NanoSpray® Ion Source

Note: Before filling the syringe with the [Glu[1]]-Fibrinopeptide B solution, wash it three times with the wash solution. Then connect the syringe to the proper tubing and wash it again before connecting it to the union on the high-voltage rail. Then, flush the tubing with the [Glu[1]]-Fibrinopeptide B solution.

1. Install the NanoSpray® ion source on the mass spectrometer. Refer to the *NanoSpray® Ion Source Operator Guide*.
2. Prepare the NanoSpray® III head. Refer to the *NanoSpray® Ion Source Operator Guide*.
3. Using the 100 µL syringe, infuse the [Glu[1]]-Fibrinopeptide B solution at a flow rate of 0.5 µL/min.
4. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
5. If the optional procedure is performed, (Optional) Perform the Q1 Test with the Turbo V™ Ion Source, then open the method created, and set the parameters as specified in Table 4-5. If the procedure was not performed, then create a method using these parameters.

Table 4-6 Method Parameters with the NanoSpray® Ion Source

Parameter	Value
MS Parameters	
Scan type	Q1 scan
Mass mode (6500 and 6500+ series systems)	Low mass
Polarity	Positive
Mass Range	400 to 1000
Scan Speed (Da/sec) (4500, 5500, 6500, and 6500+ series systems)	2000
Scan Time (sec) (4000 series systems)	3
MCA	Off
Cycles	**Note**: The number of cycles if fixed for the specific instrument analyzed. Refer to the parameters above. 500 (4000 series systems) 50 (4500, 5500, 6500, and 6500+ series systems)
Source/Gas Parameters	

Table 4-6 Method Parameters with the NanoSpray® Ion Source (continued)

Parameter	Value
CAD Gas	Low (4000 series systems) Medium (or as optimized) (4500, 5500, 6500, and 6500+ series systems)
IonSpray Voltage (IS)	2100
Ion Source Gas 1 (GS1)	10
Interface Heater Temperature (IHT) (°C)	75
Compound Parameters	
Declustering Potential (DP)	70 (4000 series systems) 100 (4500, 5500, 6500, and 6500+ series systems)
Syringe Pump Method Parameters	
Flow rate (µL/min)	0.5
Syringe Size (µL)	100 Gastight (1.46 mm)

6. Click **Start** to run the method.

CAUTION: Potential System Damage. Do not allow the emitter tip to contact the curtain plate. Use the fine Z-axis adjustment knob to adjust the sprayer position, to avoid damage to the emitter tip.

CAUTION: Potential System Contamination. Do not insert the end of the emitter tip into the curtain plate aperture. Make sure that the emitter tip is at least 2 mm to 5 mm outside the aperture. Spraying too close to the aperture can cause contamination of the mass spectrometer.

7. Adjust the position of the sprayer head relative to the curtain plate aperture to optimize signal intensity. Record the XYZ values for future use.
8. Adjust IS in 100 V increments to achieve the best signal and signal-to-noise ratio.

Note: If the IonSpray™ voltage is too high, then a corona discharge can occur. It is visible as a blue glow at the tip of the probe. A corona discharge results in decreased sensitivity and stability of the signal.

9. Increase GS1 until the signal starts to decrease and then reduce GS1 until the signal reaches its maximum value.

Note: The GS1 parameter might optimize at zero.

10. Increase CUR until the signal starts to decrease, and then reduce CUR until the signal reaches its maximum value.

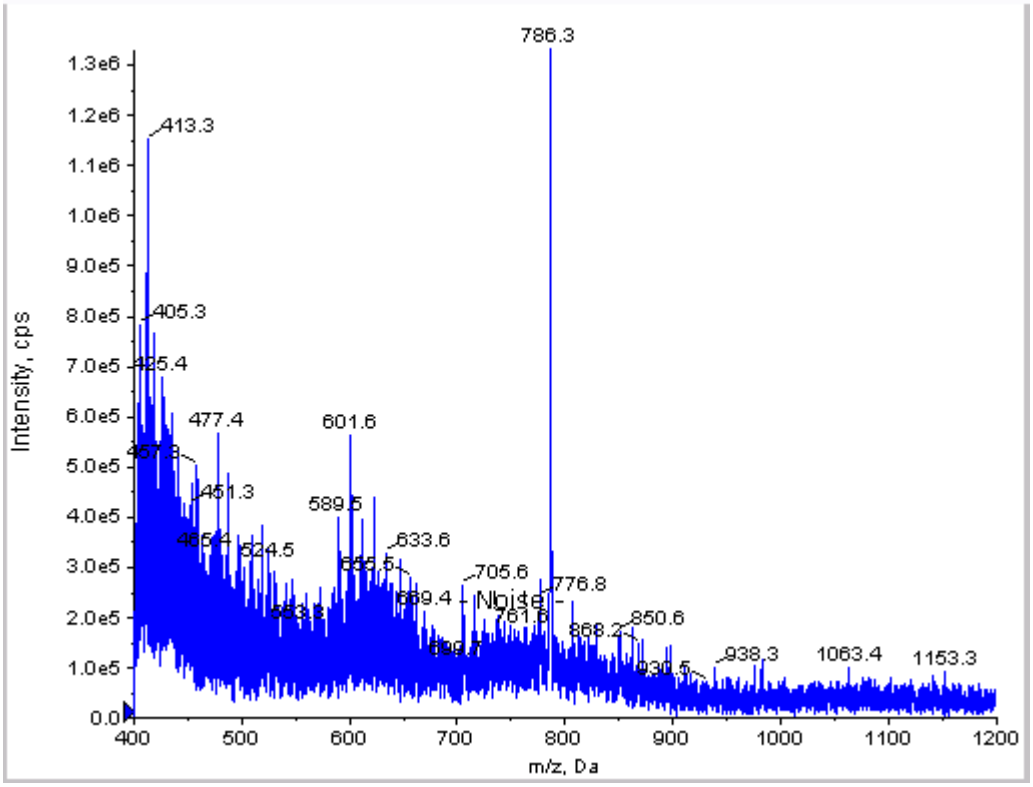
Note: To prevent contamination, use the highest value for CUR possible without sacrificing sensitivity. Do not set CUR lower than 20. This helps to prevent penetration of the Curtain Gas™ flow, which can produce a noisy signal; prevent contamination of the aperture; and increase the overall signal-to-noise ratio.

11. If you moved the sprayer head to optimize signal intensity, adjust the position of the illuminator as necessary.
12. Save the new method.

Tip! Save the methods used for the NanoSpray® ion source tests in a separate folder, named NanoSpray Installation <date>.

13. Monitor the spray stability for 5 minutes. If the spray is stable, only minimal fluctuations are visible in the TIC.

Figure 4-7 Sample Spectra: Q1 Mode Test on a 4000 QTRAP® System



14. After the spray has stabilized, change **Scan Speed** to **10**.
15. Select **Center/Width**, and then type **785.9** in the **Center** column and **20** in the **Width** column.
16. Turn **MCA** on.
17. Click **Acquire** to begin collecting data.
18. Record the intensity of the peak at m/z 785.9.
19. Repeat step 17 to step 18 two more times.
20. Average the three intensities.
21. Confirm that the average intensity is acceptable. Refer to Data Log: NanoSpray® Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.
22. Print a copy of the results and record the intensity in the data log.

Test in Q3 Mode

Note: Before filling the syringe with the [Glu[1]]-Fibrinopeptide B solution, wash it three times with the wash solution. Then connect the syringe to the proper tubing and wash it again before connecting it to the union on the high-voltage rail. Then, flush the tubing with the [Glu[1]]-Fibrinopeptide B solution.

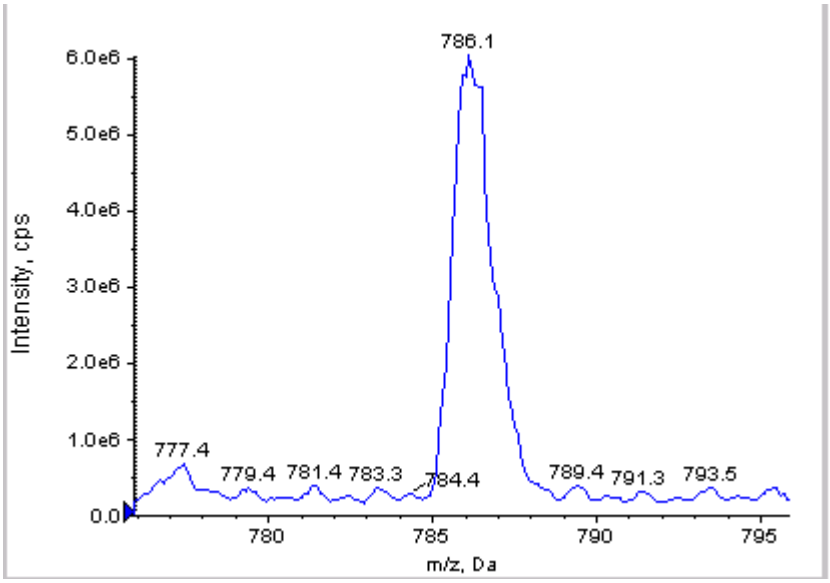
1. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
2. Open the method used for the Q1 test.
3. Open a previously optimized method or set the method parameters as shown in Table 4-7.

Table 4-7 Q3 Method Parameters

Parameter	Value
MS Parameters	
Scan type	Q3 scan
Mass mode (6500 and 6500+ series systems)	Low mass
Display masses (Da)	Center: 785.9 Width: 20
Scan Speed (Da/sec)	10
MCA	Off
Cycles	10
Compound Parameters	
Collision Cell Exit Potential (CXP) (V)	15 (or as optimized) (4000 series systems) 30 (or as optimized) (4500, 5500, 6500, and 6500+ series systems)

4. Save the new method.
5. Click **Start** to run the method.
6. When the spray is stable, turn MCA on.
7. Click **Acquire** to begin collecting data.
8. Record the intensity of the peak at m/z 785.9.
9. Repeat step 7 to step 8 two more times.

Figure 4-8 Sample Spectra: Q3 Mode Test on a QTRAP® 5500 System



10. Print the results.
11. Average the three intensities of the ions and then record the result in the Data Log.
12. Confirm that the average intensity is acceptable. Refer to Data Log: NanoSpray® Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.

Test and Calibrate in EPI Mode (QTRAP® Systems Only)

Perform the EPI Mode Test

1. Using the 100 µL syringe, infuse the [Glu1]-Fibrinopeptide B solution at a flow rate of 0.5 µL/min.
2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open a previously optimized method or set the parameters as shown in Table 4-8.

Table 4-8 EPI Method Parameters

Parameter	Value
MS Parameters	
Scan type	EPI Scan
Mass mode (6500 and 6500+ series systems)	Low mass

Table 4-8 EPI Method Parameters (continued)

Parameter	Value
Polarity	Positive
Mass Range (Da)	100 to 1500 (4000 series systems) 100 to 1000 (4500, 5500, 6500, and 6500+ series systems)
Scan speed (Da/sec)	4000 (4000 series systems) 10 000 (4500, 5500, 6500, and 6500+ series systems)
Precursors of	785.9
MCA	On
Scans to sum	1
Cycles	10 (4000 series systems) 50 (4500, 5500, 6500, and 6500+ series systems)
Advanced MS Parameters	
Fixed LIT Fill Time (ms)	50 (4000 series systems) 10 (4500, 5500, 6500, and 6500+ series systems)
Compound Parameters	
Collision Energy (CE) (V)	45 (or as optimized)
Declustering Potential (DP)	70 (or as optimized)
Syringe Pump Method Parameters	
Flow rate (µL/min)	0.5
Syringe Size (µL)	100 Gastight (1.46 mm)

Note: CE normally optimizes between 40 V and 48 V. If CE is not in this range, then the CAD gas value may be set too low. If the intensity of the precursor ion at m/z 785.9 is not 10% or less of the original intensity, then the interaction of CE and CAD gas is incorrect. Contact SCIEX technical support for more information.

4. Click **Start** to run the method.
5. Optimize CE to maximize the intensity for the fragments at *m/z* 480.3, 813.4, 942.4, and 1171.7.
6. Save the new method.
7. When the spray is stable, click **Acquire** and acquire data.

8. Record the intensities of the fragments at *m/z* 480.3, 813.4, 942.4, and 1171.7.
9. Repeat step 7 to step 8 two more times.
10. Print the results.
11. Average the three intensities of the ions and then record the result in the Data Log.
12. Confirm that the average intensities are acceptable. Refer to Data Log: NanoSpray® Ion Source.

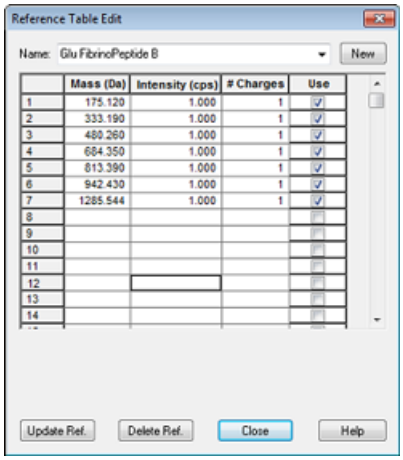
    If the results are not acceptable, refer to Troubleshooting Tips.

Create a Reference Table for Calibration

Before you can calibrate the mass spectrometer from a data spectrum, you must define the reference table for the calibrant being used. If a reference table for [Glu^1]-Fibrinopeptide B does not exist, follow these steps to create it.

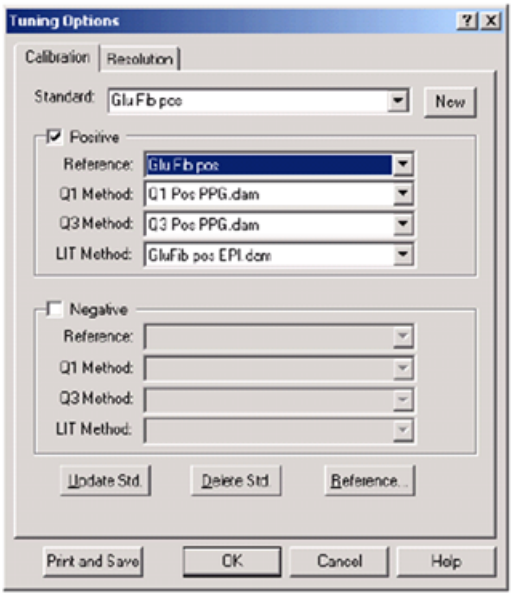
1. Click **Tools > Settings > Tuning Options.**
2. Click **Reference**.

Figure 4-9 Reference Table Editor



3. Create a reference table for [Glu1]-Fibrinopeptide B, with the entries shown in Figure 4-9. Be sure to enter the values for the lowest and highest mass fragments in the **Low Mass** and **High Mass** fields.
4. Click **Update Ref**.
5. Click **Close**.
6. Click **New**.

Figure 4-10 Tuning Options Dialog



7. In the **Standard** field, type **GluFib pos**.
8. Select the **Positive** check box.
9. In the **Q1 Method** field, select the method used for Q1 calibration.
10. In the **Q3 Method** field, select the method used for Q3 calibration.
11. In the **LIT Method** field, select the method created in Perform the EPI Mode Test.
12. Click **Update Std**.
13. Click **OK**.

Calibrate in EPI Mode

1. In **Manual Tune** mode, make sure that the parameters are set to the values specified in Table 4-8.
2. When the spray is stable, click **Acquire** and acquire at least 30 seconds of scan data.
3. Click the EPI spectrum pane.
4. Click the Calibrate button ( ).

Figure 4-11 LIT Mass Calibration Dialog for 4000 Series Systems

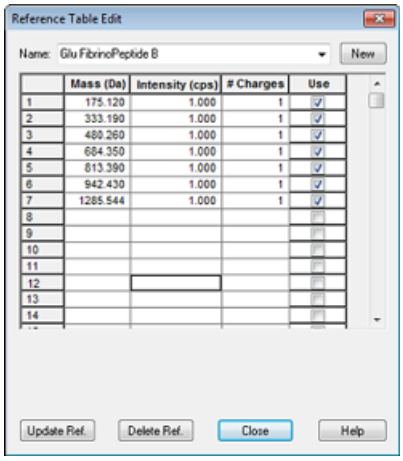
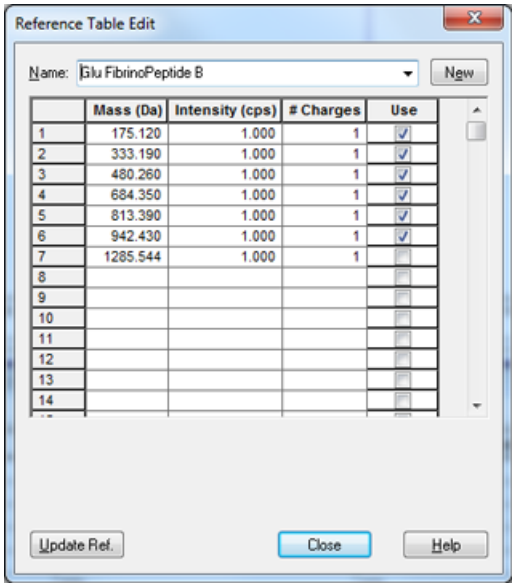


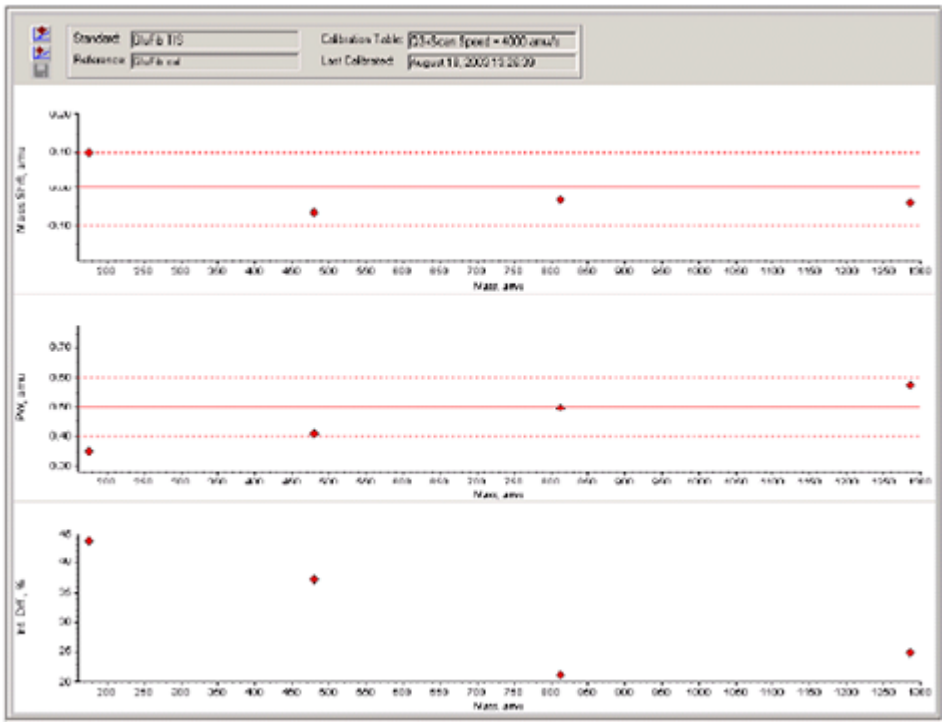
Figure 4-12 LIT Mass Calibration Dialog for 4500, 5500, 6500, and 6500+ Series Systems



5. In the **Standard** field, select the standard created in step 7 Create a Reference Table for Calibration (**GluFib pos**).
6. Click **Start**.

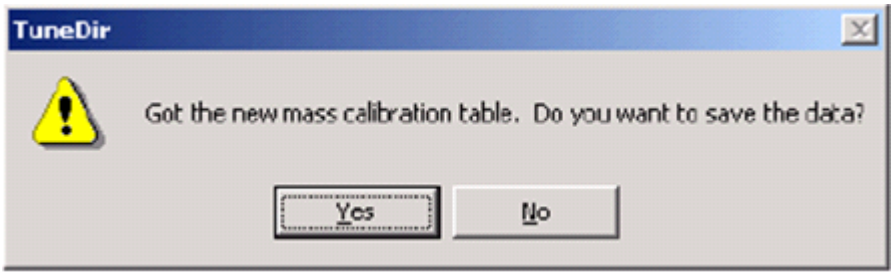
   The Mass Calibration Report pane opens. The top graph shows the mass shift in the calibration ions since the last calibration.

Figure 4-13 Mass Calibration Report



7. If the data spectra look good, and the mass shifts are within the specified range, click **Replace Calibration** ( ).

Figure 4-14 TuneDir Dialog

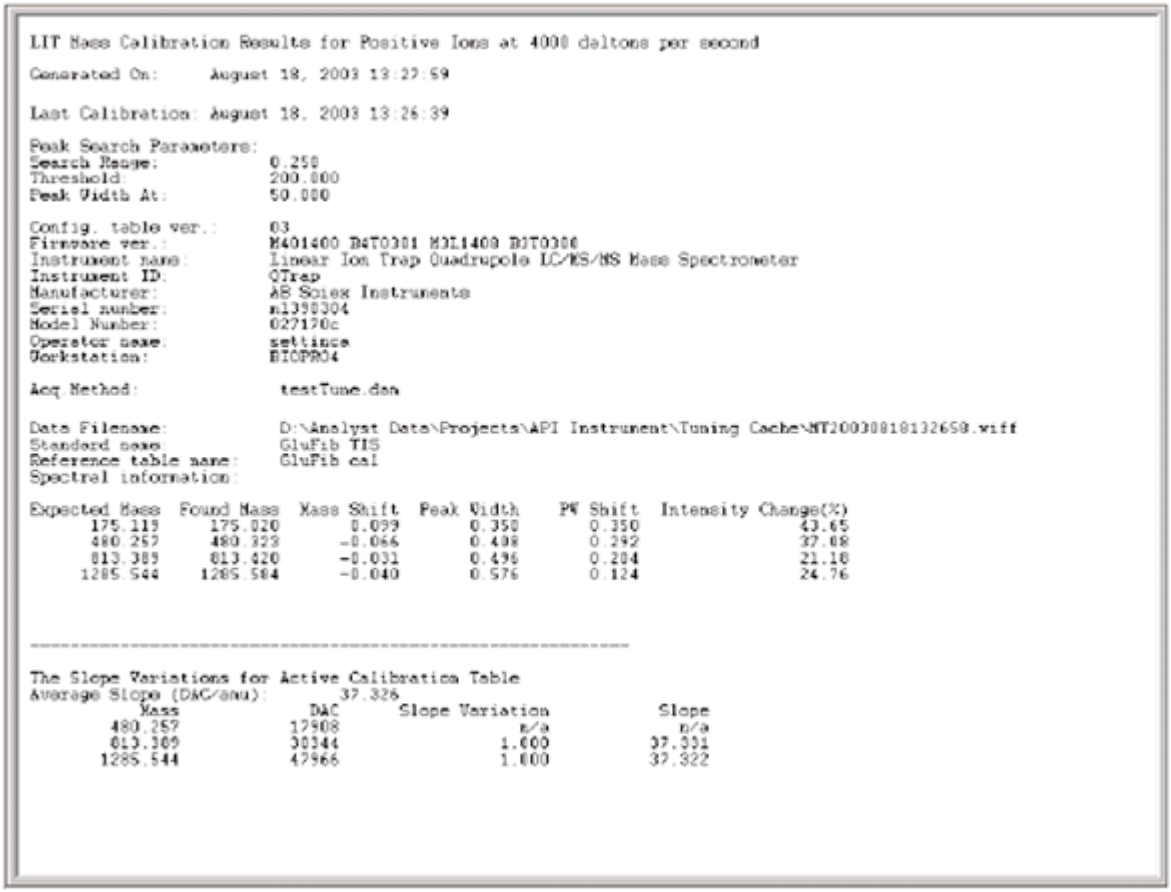


8. Click **Yes**.

   The values for the new calibration are shown at the bottom of the calibration summary report pane.

Note: If the mass or intensity of one of the fragment ions changes drastically, determine why the change occurred before using this ion in calibration. Click **No** on the **TuneDir** dialog, and then review the calibration summary report. Find the mass in the **Found Mass** column, and observe the quality of the ion in the raw data spectrum. If the incorrect ion was chosen, widen or narrow the **Search Range** on the LIT Mass Calibration dialog. The software uses the centroid of the most intense peak in the search range for calibration.

Figure 4-15 LIT Mass Calibration Results Report



LIT Mass Calibration Results for Positive Ions at 4000 daltons per second

Generated On: August 18, 2009 13:27:59

Last Calibration: August 18, 2009 13:26:39

Peak Search Parameters:
Search Range: 0.250
Threshold: 200.000
Peak Width At: 50.000

Config. table ver.: 03
Firmware ver.: M401400 B4T0301 M3L1400 B3T0306
Instrument name: Linear Ion Trap Quadrupole LC/MS/MS Mass Spectrometer
Instrument ID: QTrap
Manufacturer: AB Sciex Instruments
Serial number: sn1390304
Model Number: 027170c
Operator name: settince
Workstation: BIOPRO4

Acq Method: testTune.dam

Data Filename: D:\Analyst Data\Projects\API Instrument\Tuning Cache\MT20090818132658.wiff
Standard name: GluFib TIS
Reference table name: GluFib cal
Spectral information:

Expected Mass	Found Mass	Mass Shift	Peak Width	PW Shift	Intensity Change(%)
175.119	175.020	0.099	0.350	0.350	43.65
480.259	480.323	-0.066	0.488	0.292	37.08
813.389	813.420	-0.031	0.496	0.284	21.18
1285.544	1285.584	-0.040	0.576	0.124	24.76

The Slope Variations for Active Calibration Table
Average Slope (DAC/amu): 37.326

Mass	DAC	Slope Variation	Slope
480.259	17908	n/a	n/a
813.389	30344	1.600	37.331
1285.544	47966	1.600	37.322

9. Calibrate for the other two scan speeds by changing the scan speed in the method, and then repeating this procedure.

Wrap-Up

Note: The SCIEX Field Service Employee (FSE) must e-mail the results of the NanoSpray® acceptance test run after installation to servicedata@sciex.com.

1. Flush the tip and the infusion line thoroughly.
2. Make a copy of the completed data log and test results and provide the customer with the originals.

Test the Ion Source on 3200 Series Systems

WARNING! Hot Surface Hazard. Do not touch the high voltage rail or emitter tip.

WARNING! Electrical Shock Hazard. Never operate the NanoSpray® ion source without the illuminator, camera, stop, and covers properly installed. Never touch the curtain plate or allow the emitter tip to contact the curtain plate. If the mass spectrometer is operational and the ion source is installed, then high voltage is present on the curtain plate, even if the X-Y-Z positioning unit is moved away from the interface.

For API 3200™ systems, perform this test:

- Test in Q1 and MS2 Modes

For 3200 QTRAP® systems, perform these tests:

- Test in Q1 and MS2 Modes
- Test in EPI Mode (3200 QTRAP® Systems Only)

Note: The NanoSpray® ion source is not supported on every 3200 series instrument. Contact a sales representative for more information.

Required Materials
• Renin 10 pmol/µL, included in the MS Chemical Kit2 Higher Concentration PPGs kit (PN 5512399) • Dilution solvent • 100 µL syringe (1.46 mm i.d.) or equivalent for infusion • Powder-free gloves (nitrile or neoprene is recommended) • Safety glasses • Lab coat

Prepare 2 mL of Renin Mixture (500 fmol/µL)

1. Measure 2 ml of dilution solvent (provided in the kit) into a vial.
2. Remove and discard 100 µL of the solvent.
3. Add 100 µL of renin 10 pmol/µL to the vial.
4. Mix.

Test in Q1 and MS2 Modes

1. Install the NanoSpray ion source on the mass spectrometer. Refer to the *NanoSpray® Ion Source Operator Guide*.
2. Prepare the NanoSpray III head. Refer to the *NanoSpray® Ion Source Operator Guide*.
3. Infuse the renin mixture at a flow rate of 0.5 µL/min.

CAUTION: Potential System Contamination. Do not insert the end of the emitter tip into the curtain plate aperture. Make sure that the emitter tip is at least 2 mm to 5 mm outside the aperture. Spraying too close to the aperture can cause contamination of the mass spectrometer.

4. Adjust GS1 until a stable spray is achieved. Start with a low value (2 or 3) and slowly increase it, until the spray is stable with no zero width noise spikes. It may take a few minutes for the spray to stabilize.
5. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
6. Open a previously optimized method or set the method parameters as shown in Table 4-9.

Table 4-9 Q1 Method Parameters

Parameter	Value
MS Method Parameters	
Scan type	Q1 MS (Q1)
Mass range	100 to 1200
Advanced MS Parameters	
Step size (Da)	0.1
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	20

Table 4-9 Q1 Method Parameters (continued)

Parameter	Value
IonSpray Voltage (IS)	2100
Ion Source Gas 1 (GSI)	3
Interface Heater Temperature (IHT) (°C)	75
Compound Parameters	
Declustering Potential (DP)	70 (or as optimized)

7. Run the method.

CAUTION: Potential System Damage. Do not allow the emitter tip to contact the curtain plate. Use the fine Z-axis adjustment knob to adjust the sprayer position, to avoid damage to the emitter tip.

CAUTION: Potential System Contamination. Do not insert the end of the emitter tip into the curtain plate aperture. Make sure that the emitter tip is at least 2 mm to 5 mm outside the aperture. Spraying too close to the aperture can cause contamination of the mass spectrometer.

8. Adjust the position of the sprayer head relative to the curtain plate aperture to optimize signal intensity. Record the XYZ values for future use.
9. Adjust IS in 100 V increments until you achieve the best signal and signal-to-noise ratio.

Note: If the IonSpray™ voltage is too high, then a corona discharge can occur. It is visible as a blue glow at the tip of the probe. A corona discharge results in decreased sensitivity and stability of the signal.

10. Increase GS2 until the signal starts to decrease and then reduce GS1 until the signal reaches its maximum value.

Note: The GS1 parameter might optimize at zero.

11. Increase CUR until the signal starts to decrease, and then reduce CUR until the signal reaches its maximum value.

Note: To prevent contamination, use the highest value for CUR possible without sacrificing sensitivity. Do not set CUR lower than 20. This helps to prevent penetration of the Curtain Gas™ flow, which can produce a noisy signal; prevent contamination of the aperture; and increase the overall signal-to-noise ratio.

12. Print a copy of the results and then save the optimized Q1 acquisition method.
13. Set the **Scan type** to **Product Ion (MS2)**, and set **Product Of** to **587**.
14. Set **CAD** to **Medium (6)**.
15. Adjust **CE** to optimize the intensity of the fragment ions at *m/z* 136 and 784.
16. Print a copy of the results and then save the optimized **Product Ion** method.
17. Verify that the intensity in MS2 mode meets the specifications in Data Log: NanoSpray® Ion Source.

    If the results are not acceptable, refer to Troubleshooting Tips.
18. Record the results in the Data Log.

Test in EPI Mode (3200 QTRAP® Systems Only)

1. Infuse the renin mixture at a flow rate of 0.5 µL/min.

CAUTION: Potential System Contamination. Do not insert the end of the emitter tip into the curtain plate aperture. Make sure that the emitter tip is at least 2 mm to 5 mm outside the aperture. Spraying too close to the aperture can cause contamination of the mass spectrometer.

2. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
3. Open the optimized Q1 method saved in step 12 Test in Q1 and MS2 Modes.
4. Set the method parameters as shown in Table 4-10.

Table 4-10 EPI Method Parameters

Parameter	Value
MS Parameters	
Scan type	EPI
Mass range (Da)	100 to 1200
Product Of (Da)	587.4
Duration (sec)	120

Table 4-10 EPI Method Parameters (continued)

Parameter	Value
Advanced MS Parameters	
Fixed LIT fill time (msec)	20
Q0 trapping	OFF
Q3 entry barrier	8
Source/Gas Parameters	
Curtain Gas™ flow (CUR)	As optimized
Collision Gas (CAD)	High
IonSpray Voltage (IS)	As optimized
Temperature (TEM) (°C)	150
Ion Source Gas 1 (GSI)	As optimized
Ion Source Gas 2 (GS2)	0
Interface Heater Temperature (IHT)	ON
Compound Parameters	
Declustering Potential (DP)	80
Collision Energy (CE) (V)	45 (or as optimized)
Collision Energy Spread (CES)	0
Resolution Parameters	
Q1 resolution	LOW

5. Run the method.
6. Adjust **CE** to optimize the intensity of the peaks at 136, 647, 784, and 1028.
7. Print a copy of the results and save the optimized EPI method.
8. Verify that the intensity meets the specifications in Data Log: NanoSpray® Ion Source.

   If the result is not acceptable, refer to Troubleshooting Tips.
9. Review the printed copy of the results and record the results in the Data Log.

Wrap-Up

Note: The SCIEX Field Service Employee (FSE) must e-mail the results of the NanoSpray® acceptance test run after installation to servicedata@sciex.com.

1. Flush the tip and the infusion line thoroughly.
2. Make a copy of the completed data log and test results and provide the customer with the originals.

PhotoSpray® Ion Source Tests 5

Run these tests in any of the following situations:

- When a new ion source is installed.
- After major maintenance to the ion source.
- Whenever the performance of the ion source must be assessed, either before starting a project or as part of a standard operating procedure.

WARNING! Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Use the ion source only if you have knowledge of and training in the proper use, containment, and evacuation of toxic or injurious materials used with the ion source.

WARNING! Puncture Hazard, Ionizing Radiation Hazard, Biohazard, or Toxic Chemical Hazard. Discontinue use of the ion source if the ion source window is cracked or broken and then contact a SCIEX Field Service Employee (FSE). Any toxic or injurious materials introduced into the equipment will be present in the source exhaust output. Dispose of sharps following established laboratory safety procedures.

WARNING! Toxic Chemical Hazard. Wear personal protective equipment, including a laboratory coat, gloves, and safety glasses, to avoid skin or eye exposure.

WARNING! Ionizing Radiation Hazard, Biohazard, Electrical Shock Hazard, or Toxic Chemical Hazard. In the event of a chemical spill, review product Safety Data Sheets for specific instructions. Make sure that the system is in Standby mode before cleaning a spill near the ion source. Use appropriate personal protective equipment and absorbent wipes to contain the spill and dispose of it following local regulations.

Required Materials
• MS-grade methanol • HPLC-grade deionized water • Mobile phase solvent: 70:30 acetonitrile:water solution • Dopant: toluene (HPLC grade) infused at 100 to 150 µL/min. The dopant should be infused using a separate HPLC pump. • Pre-diluted 0.0167 pmol/µL reserpine solution included in the SCIEX Standard Chemical Kit (PN 4406127) • HPLC pump (for mobile phase) • HPLC pump for dopant infusion. • Manual injector (8125 Rheodyne or equivalent) with a 5 µL loop or an autosampler set up for 5 µL injections • PEEK tubing 1/16-inch outside diameter (o.d.), 0.005-inch inside diameter (i.d.) • Syringe 250 µL to 1000 µL • Powder-free gloves (nitrile or neoprene is recommended) • Safety glasses • Lab coat

Note: All test solutions must be kept refrigerated. If they are left out of the refrigerator for longer than 48 hours, then discard them and use new solutions.

CAUTION: Potential Wrong Result. Do not use expired solutions.

Prepare for the Test

WARNING! Electrical Shock Hazard. Avoid contact with the high voltages applied to the ion source during operation. Put the system in Standby mode before adjusting the sample tubing or other equipment near the ion source.

- When installing a new ion source, make sure that the mass spectrometer is performing to specifications with the existing ion source.
- Install the ion source on the mass spectrometer.
- Make sure that the ion source is fully optimized. Refer to the appropriate ion source *Operator Guide*.
- Refer to all applicable Safety Data Sheets for any necessary precautions before handling chemical solutions or solvents.

Note: Regardless of the pump used, there is a significant back pressure on the dopant line.

Test the Ion Source

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

CAUTION: Potential System Damage. Do not introduce any solvent flow before verifying that the ion source has reached the correct temperature.

CAUTION: Potential System Damage. Optimize using the highest possible value for the Curtain Gas™ flow rate to avoid contaminating the mass spectrometer.

Note: The optimum ion transfer voltage is dependent upon the height of the UV lamp. There is only one optimum ion transfer voltage for a set UV lamp height and only one optimum UV lamp height for a given ion transfer voltage. If the user changes the UV lamp height, optimize the ion transfer voltage at each new height setting to converge on the best setting for UV lamp height and ion transfer voltage.

1. In the Analyst® software, in **Tune and Calibrate** mode, double-click **Manual Tune**.
2. Open a previously optimized method or set the parameters as shown in Table 5-1.

Table 5-1 Method Parameters

Parameter	Value
Probe Parameters	
Sample concentration	10 pg/µL
Mobile phase	70:30 ACN:H_2O
Flow rate (µL/min)	500
Injection volume (µL)	25 (overfill the loop)
Sample loop (µL)	5
Ionization mode	Positive
Probe vertical micrometer setting	2

Table 5-1 Method Parameters (continued)

Parameter	Value
Probe horizontal micrometer setting	5
UV Lamp vertical micrometer setting	5
Dopant	100 µL/min to 150 µL/min flow rate
MS Parameters	
Scan mode	MRM
Q1 mass (Da)	609.3 (or exact mass)
Q3 mass (Da)	195.1 (or exact mass)
Source/Gas Parameters	
Curtain Gas™ (CUR)	30 (or as optimized)
Collision Gas (CAD)	Medium
Ion Transfer Voltage (IS)	800 (or as optimized)
Temperature (TEM)	400 (or as optimized)
Ion Source Gas 1 (GS1)	60 (or as optimized)
Ion Source Gas 2 (GS2)	20 (or as optimized)
Compound Parameters	
Declustering Potential (DP)	100 (or as optimized)
Collision Energy (CE)	45 (or as optimized)
Collision Exit Potential (CXP)	As optimized
Resolution Parameters	
Resolution	Unit/Unit
The starting values obtained during instrument validation may differ from those in this table.	

3. Click **Acquire** to begin collecting data.
4. Introduce the 70:30 acetonitrile:water solution at a flow rate of 500 µL/min through the sample inlet.
5. Introduce the dopant at a flow rate of 75 µL/min through the dopant inlet.
6. Overfill the sample loop with the test solution.
7. Inject 10 pg/µL of reserpine test solution while monitoring the multiple creation monitoring (MRM) 609/195 transition.

8. Optimize the compound-specific parameters.
9. Optimize the probe and UV lamp positions.
10. Optimize the ion source parameters.
11. Print the results.
12. Review the printed copy of the results.
13. Confirm that the average intensity of the five injections is acceptable. Refer to Data Log: PhotoSpray® Ion Source.

    If the result is not acceptable, refer to Troubleshooting Tips.

Troubleshooting Tips 6

Symptom	Possible Cause	Corrective Action
No signal	1. No spray is being generated. 2. (NanoSpray® ion source) The ion source head position is incorrect.	1. Refer to the ion source *Operator Guide* to troubleshoot spray problems. 2. Use the X-Y-Z adjustment knobs to adjust the emitter tip position.
Unexpectedly wide LC peaks or tailing	(NanoSpray® ion source) The union has a dead volume.	• Make sure that all post-column tubing has an inside diameter less than or equal to 25 microns. • Check all connections to make sure that they are properly seated. • Flush all cuts. • Replace the emitter tip.
Low peak intensity	1. The source position, tip protrusion, or source parameter values are incorrect. 2. The syringe or sample line is leaking. 3. Q1 or Q3 is not calibrated. 4. The sample has degraded or has a low concentration. 5. There is a problem with the LC system.	1. Optimize the source. 2. Inspect for leaks. 3. Use the **Instrument Optimization** wizard to calibrate Q1 or Q3. 4. Check the sample concentration. Use either a fresh sample or a sample that has been frozen. 5. Troubleshoot the LC system.
Poor resolution	The instrument is not optimized.	Optimize the instrument.

Symptom	Possible Cause	Corrective Action
Poor sensitivity	1. The interface components (front end) are dirty. 2. Solvent vapor or other unknown compounds are present in the analyzer region. 3. The sample was not prepared correctly or the sample has degraded. 4. There are leaks at the sample inlet. 5. The ion source is faulty.	1. Clean the interface components and reposition the ion source. 2. Optimize the Curtain Gas™ flow. 3. Confirm that the sample was prepared correctly. 4. Verify that the fittings are tight and replace fittings if leaks continue. Do not overtighten the fittings. 5. Install and optimize an alternate ion source. If the problem persists, contact an FSE.
Low signal	1. The Declustering Potential (DP) is not optimized. 2. The electrode might be dirty or clogged.	1. Optimize declustering to achieve the best signal or signal-to-noise ratio. The optimum values may be different from those found using other ion sources. 2. Clean the electrode.
Low signal-to-noise ratio	1. The source position, tip protrusion, or source parameter values are incorrect. 2. The syringe or sample line is leaking. 3. The diluent is contaminated.	1. Optimize the source. 2. Check for leaks. 3. Use freshly prepared diluent, made with MS-grade reagents (0.1% formic acide and 10% acetonitrile).

Symptom	Possible Cause	Corrective Action
High background noise	1. The diluent is contaminated. 2. The syringe or sample line is dirty. 3. There is residue on the interface. 4. The temperature (TEM) is too high. 5. The heater gas flow rate (GS2) is too high. 6. The ion source is contaminated.	1. Use freshly prepared diluent made with MS-grade reagents (0.1% formic acid, 10% acetonitrile). 2. Clean or replace the syringe or sample line. 3. Clean the curtain plate and orifice plate (refer to the *Qualified Maintenance Person Guide* for the mass spectrometer). If necessary, bake the interface. If the problem is not resolved, clean Q0 or the QJet® ion guide. 4. Optimize the temperature. 5. Optimize the heater gas flow. 6. Clean or replace the ion source components and condition the source and the front end: a. Move the APCI or TIS probe to the furthest position from the aperture (vertically and horizontally). b. Infuse or inject 50:50 methanol:water with a pump flow of 1 mL/min. c. In the Analyst®/Analyst® TF software, set TEM to 650, GS1 to 60, and GS2 to 60. d. Set the Curtain Gas flow to 45 or 50. e. Run for a minimum of 2 hours or preferably overnight, for best results. 7. Adjust the emitter tip position.

Symptom	Possible Cause	Corrective Action
During testing, the ion source fails to meet specifications	The mass spectrometer has not passed the installation tests.	Perform installation tests on the mass spectrometer with the default source.
Temperature not reached or the temperature too high or unstable	The interface heater is faulty.	Open the **Mass Spectrometer Detailed Status** dialog. The **Source Temperature** field should contain the set temperature and the **Interface Heater Status** should be **Ready**. If not, then contact a Qualified Maintenance Person (QMP) or Field Service Employee (FSE) to replace the interface heater.

Data Log: IonDrive™ Turbo V Ion Source

A

System Information

Table A-1 Mass Spectrometer Information

Mass spectrometer serial number	

Ion Source Information

Component	Serial Number
Ion Source	
TurboIonSpray® probe	
APCI probe	

IonDrive Turbo V Ion Source Test Results

Note: TheIonDrive™ Turbo V ion source is supported by 6500 and 6500+ series of instruments and the and 6600 systems only.

Probe	Intensity (cps)	Intensity (cps)	Results (cps)
	6500	6500+	
TurboIonSpray® probe	1.25×10^6	1.9×10^6	
APCI probe	5.0×10^5	7.5×10^5	

Signoff

Organization			
FSE name		Date (yyyy-mm-dd)	
FSE signature			

Comments and Exceptions

Data Log: Turbo V™ Ion Source

B

System Information

Table B-1 Mass Spectrometer Information

Mass spectrometer serial number	

Ion Source Information

Component	Serial Number
Ion Source	
TurboIonSpray® probe	
APCI probe	

Turbo V Ion Source Test Results

Note: Specifications are not available for the TripleTOF® 4600 system. The recommended source for this system is the DuoSpray™ ion source.

Note: Tests for 6500 and 6500+ series systems are run in low mass mode.

Intensity (cps)								Results
3200	3500	4000	4500	5000 and 5500	5600 /5600+ and 6600	6500	6500+	
TurboIonSpray® Probe								
1.0×10^4	2.0×10^4	1.0×10^5	2.0×10^5	5.0×10^5	1.0×10^4	1.0×10^6	1.5×10^6	
APCI Probe								
5.0×10^3	1.0×10^4	5.0×10^4	1.0×10^5	2.5×10^5	5.0×10^3	5.0×10^5	7.5×10^5	

Signoff

Organization			
FSE name		Date (yyyy-mm-dd)	
FSE signature			

Comments and Exceptions

Data Log: DuoSpray™ Ion Source

C

System Information

Table C-1 Mass Spectrometer Information

Mass spectrometer serial number	

Ion Source Information

Component	Serial Number
Ion Source	
TurboIonSpray® probe	
APCI probe	

DuoSpray Ion Source Test Results

Note: Tests for 6500 and 6500+ series systems are run in low mass mode.

Intensity (cps)								Results
3200	4000	4500	4600	5000 and 5500	5600/5600+ and 6600	6500	6500+	
TurboIonSpray® Probe								
5.0×10^3	5.0×10^4	1.0×10^5	2.0×10^3	2.5×10^5	5.0×10^3	5.0×10^5	7.5×10^5	
APCI Probe								
2.5×10^3	2.5×10^4	5.0×10^4	1.0×10^3	1.25×10^5	2.5×10^3	2.5×10^5	3.8×10^5	

Signoff

Organization			
FSE name		Date (yyyy-mm-dd)	
FSE signature			

Comments and Exceptions

Data Log: NanoSpray® Ion Source

D

System Information

Table D-1 Mass Spectrometer Information

Mass spectrometer serial number	

Ion Source Information

Component	Serial Number
Ion Source	
TurboIonSpray® probe	
APCI probe	

NanoSpray Ion Source Test Results (TripleTOF Systems)

Note: The SCIEX Field Service Employee (FSE) must e-mail the results of the NanoSpray® acceptance test run after installation to servicedata@sciex.com.

Table D-2 TOF MS Test Results

Mass 786	Specification		Result
	4600	5600/5600+ and 6600	
Centroid intensity (peak height, cps)	≥ 1500	≥ 4000	
Resolution	≥ 25 000	≥ 30 000	
Printouts required: 785.8421			

Table D-3 Product Ion High Sensitivity Test Results (5600/5600+ and 6600 Systems Only)

Mass	Centroid Intensity (cps)		Resolution	
	Specification	Result	Specification	Result
187.0713	≥ 60		N/A	N/A
480.2565	≥ 212		≥ 15 000	
813.3890	≥ 375		≥ 15 000	
1056.4745	≥ 225		≥ 15 000	
Printouts required: 187.0713, 480.2565, 813.3890, and 1056.4745				

Table D-4 Product Ion Test Results

Mass	Centroid Intensity (cps)			Resolution		
	4600	5600/5600+ and 6600	Result	4600	5600/5600+ and 6600	Result
187.0713	≥ 8	≥ 20		N/A	N/A	N/A
480.2565	≥ 25	≥ 65		≥ 24 000	≥ 25 000	
813.3890	≥ 35	≥ 125		≥ 25 000	≥ 25 000	
1056.4745	≥ 25	≥ 65		≥ 25 000	≥ 25 000	

Note: For 5600/5600+ and 6600 systems, this test is run in High Resolution mode.

Printouts required: 187.0713, 480.2565, 813.3890, and 1056.4745

NanoSpray Ion Source Test Results (4000, 4500, 5500, 6500, and 6500+ Series Systems)

Note: The SCIEX Field Service Employee (FSE) must e-mail the results of the NanoSpray® acceptance test run after installation to servicedata@sciex.com.

Table D-5 Q1 Mode Test Results

Mass	Intensity (cps)					
	4000	4500	5500	6500	6500+	Result
786	1.0×10^5	2.5×10^5	5.0×10^5	1.0×10^6	1.5×10^6	

Table D-6 Q3 Mode Test Results

Mass	Intensity (cps)					
	4000	4500	5500	6500	6500+	Result
786	1.0×10^5	2.5×10^5	5.0×10^5	1.0×10^6	1.5×10^6	

Table D-7 EPI Mode Test Results (QTRAP® Systems Only)

Mass	Intensity (cps)					
	4000	4500	5500	6500	6500+	Result
	Intensity (cps)	Intensity (cps)	Intensity (cps)	Intensity (cps)	Intensity (cps)	
480.3	1.0×10^5	5.0×10^5	1.0×10^6	5.0×10^6	7.5×10^6	
813.4	1.0×10^5	5.0×10^5	1.0×10^6	5.0×10^6	7.5×10^6	
942.4	5.0×10^4	2.5×10^5	5.0×10^5	2.5×10^6	3.8×10^6	
1171.7	4.0×10^4	2.0×10^5	N/A	N/A	N/A	

NanoSpray Ion Source Test Results (3200 Series Systems)

Table D-8 MS2 Mode Test Results

Mass	Intensity (cps)	Results (cps)
136.1	≥1.6 × 105	
784.4	≥5000	

Table D-9 EPI Mode Test Results

Mass	Intensity (cps)	Results (cps)
136.1	1.0×10^5	
647.3	4.0×10^4	
784.4	8.0×10^4	
1028.5	1.0×10^4	

Signoff

Organization			
FSE name		Date (yyyy-mm-dd)	
FSE signature			

Comments and Exceptions

Data Log: PhotoSpray® Ion Source

E

System Information

Table E-1 Mass Spectrometer Information

Mass spectrometer serial number	

Ion Source Information

Component	Serial Number
Ion Source	
TurboIonSpray® probe	
APCI probe	

PhotoSpray Ion Source Test Results

Note: Tests for 6500 and 6500+ series systems are run in low mass mode.

Intensity (cps)						
3200	**4000**	**4500**	**5000 & 5500**	**6500**	**6500+**	**Results**
2.5×10^3	5.0×10^4	1.0×10^5	2.5×10^5	5.0×10^5	7.5×10^5	

Signoff

Organization			
FSE name		Date (yyyy-mm-dd)	
FSE signature			

Comments and Exceptions

TripleTOF® System Parameters F

The following table contains generic parameters for the TripleTOF® 4600, 5600/5600+, and 6600 systems.

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table F-1 TripleTOF® System Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	TOF MS	MS/MS	Q1	TOF MS	MS/MS
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	GS2	15 0 to 90	15 0 to 90	15 0 to 90	15 0 to 90	15 0 to 90	15 0 to 90
CUR	CUR	25 10 to 55	25 10 to 55	25 10 to 55	25 10 to 55	25 10 to 55	25 10 to 55
TEM [1,2,3,4,5]	TEM	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
ISVF[1,4] (ISVF = IS – OR)	IS	5000 0 to 5500	5000 0 to 5500	5000 0 to 5500	–4000 –4500 to 0	–4000 –4500 to 0	–4000 –4500 to 0
ISVF[6] (ISVF = IS – OR)	IS	1000 0 to 4000	1000 0 to 4000	1000 0 to 4000	–1000 –4000 to 0	–1000 –4000 to 0	–1000 –4000 to 0
NC[5]	NC	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0

1 DuoSpray™ ion source

2 Turbo V™ ion source

3 IonDrive™ Turbo V ion source, if applicable

4 TurboIonSpray® probe

5 APCI probe

6 NanoSpray® ion source

Table F-1 TripleTOF® System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	TOF MS	MS/MS	Q1	TOF MS	MS/MS
IHT[6]	IHT	150 0 to 225	150 0 to 225	150 0 to 225	150 0 to 225	150 0 to 225	150 0 to 225
OR (DP = OR – Q0)	DP	80 0 to 300	100 0 to 300	80 0 to 300	–80 –300 to 0	–80 –300 to 0	–80 –300 to 0
Q0	Q0	40 –300 to 300	N/A	N/A	–40 –300 to 300	N/A	N/A
Q0 (CE = Q0 – RO2)	CE	N/A	10 5 to 150	30 0 to 150	N/A	–10 –150 to –5	–30 –150 to 0
CES	CES	N/A	N/A	0 0 to 50	N/A	N/A	0 0 to 50
RO1 (IE1 = Q0 – RO1)	IE1	2 –300 to 300	2 –300 to 300	2 –300 to 300	–2 –300 to 300	–2 –300 to 300	–2 –300 to 300
IQ2	IQ2	0 –300 to 300	25 –300 to 300	0 –300 to 300	0 –300 to 300	–25 –300 to 300	0 –300 to 300
CAD	CAD	6 0 to 12	6 0 to 12	6 0 to 12	6 0 to 12	6 0 to 12	6 0 to 12
RO2	RO2	30 –57 to 57	30 –57 to 57	30 –57 to 57	–30 –57 to 57	–30 –57 to 57	–30 –57 to 57
IRD	IRD	30 6 to 1000	30 6 to 1000	30 6 to 1000	30 6 to 1000	30 6 to 1000	30 6 to 1000
IRW	IRW	15 5 to 1000	15 5 to 1000	15 5 to 1000	15 5 to 1000	15 5 to 1000	15 5 to 1000
LNR	LNR	–15000 –20000 to 20000	–15000 –20000 to 20000	–15000 –20000 to 20000	15000 –20000 to 20000	15000 –20000 to 20000	15000 –20000 to 20000

Table F-1 TripleTOF® System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	TOF MS	MS/MS	Q1	TOF MS	MS/MS
CEM	CEM	2300 0 to 3000	2200 0 to 3000	2200 0 to 3000	2200 0 to 3000	2200 0 to 3000	2200 0 to 3000
OFS	OFS	30 –100 to 100	30 –100 to 100	30 –100 to 100	–60 –100 to 100	–60 –100 to 100	–60 –100 to 100
MGV	MGV	–975 –2000 to 2000	–975 –2000 to 2000	–975 –2000 to 2000	975 –2000 to 2000	975 –2000 to 2000	975 –2000 to 2000
MPV	MPV	2600 –4000 to 4000	2600 –4000 to 4000	2600 –4000 to 4000	–2600 –4000 to 4000	–2600 –4000 to 4000	–2600 –4000 to 4000

6500 and 6500+ Series System Parameters

G

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table G-1 6500 and 6500+ Series System Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	20 20 to 55	20 20 to 55	20 20 to 55	20 20 to 55	20 20 to 55	20 20 to 55
CAD [7,8]	CAD[7,8]	0 N/A	6 N/A	Med Low, Medium, High	0 N/A	6 N/A	Med Low, Medium, High
CAD[9,10]	CAD[9,10]	0 N/A	6 N/A	9 0 to 12	0 N/A	6 N/A	9 0 to 12
IS[11,12,13]	IS[11,12,13]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
IS[14]	IS[14]	1500 0 to 2500	1500 0 to 2500	1500 0 to 2500	-1500 -2500 to 0	-1500 -2500 to 0	-1500 -2500 to 0
IS[15]	IS[15]	1000 0 to 4000	1000 0 to 4000	1000 0 to 4000	-1000 -4000 to 0	-1000 -4000 to 0	-1000 -4000 to 0

[7] QTRAP® 6500 or 6500+ system Low Mass (LM)

[8] QTRAP® 6500 or 6500+ system High Mass (HM)

[9] SCIEX Triple Quad™ 6500 or 6500+ system (LM)

[10] SCIEX Triple Quad™ 6500 or 6500+ system (LM)

[11] Turbo V™ ion source

[12] IonDrive™ Turbo V ion source

[13] TurboIonSpray® (TIS) probe

[14] PhotoSpray® ion source

[15] NanoSpray® ion source

Table G-1 6500 and 6500+ Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
NC[12,14,17,16]	NC[12,14,17,16]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[11,12,14,17,13,16]	TEM[11,12,14,17,13,16]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	100 0 to 300	100 0 to 300	100 0 to 300	–100 –300 to 0	–100 –300 to 0	–100 –300 to 0
Q0 (EP = –Q0)	EP	10 2 to 15	10 2 to 15	10 2 to 15	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2
ST (ST = Q0 + offset)	ST	Q0 + (-8) –12 to –5	Q0 + (-8) –12 to –5	Q0 + (-8) -12 to –5	Q0 + 8 5 to 12	Q0 + 8 5 to 12	Q0 + 8 5 to 12
RO1 (IE1 = Q0 – RO1)	IE1	1 0 to 3	N/A	1 0 to 3	–1 –3 to –0	N/A	–1 –3 to –0
IQ2 (IQ2 = Q0 + offset)	IQ2	Q0+ (–10) –30 to –8	Q0+ (–10) –30 to –8	Q0+ (–10) –30 to –8	Q0 + 10 8 to 30	Q0 + 10 8 to 30	Q0 + 10 8 to 30
RO2	RO2	–20 N/A	–20 N/A	N/A	20 N/A	20 N/A	N/A
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 180	N/A	N/A	–30 –180 to –5
ST3 (ST3 = RO2 + offset)	ST3	RO2 – 10 –30 to –5	N/A	N/A	RO2 + 10 5 to 30	N/A	N/A

[16]APCI probe

[17]DuoSpray™ ion source

Table G-1 6500 and 6500+ Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
ST3 (CXP = RO2 – ST3)	CXP	N/A	15 0 to 55	15 0 to 55	N/A	–15 –55 to 0	–15 –55 to 0
RO3	RO3	–50 N/A	N/A	N/A	50 N/A	N/A	N/A
RO3 (IE3 = RO2 – RO3)	IE3	N/A	1 0 to 5	1 0 to 5	N/A	–1 –5 to 0	–1 –5 to 0
CEM	CEM	1700 0 to 3300	1700 0 to 3300	1700 0 to 3300	1700 0 to 3300	1700 0 to 3300	1700 0 to 3300
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90
IHT[15]	IHT [15]	150	150	150	150	150	150
sdp[17]	sdp[17]	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2

Table G-2 6500 and 6500+ Series System Parameters for LIT Scan Types Only

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
CAD	CAD	High Low, Medium, High	High Low, Medium, High
AF2[18]	AF2	0.1 0 to 1	0.1 0 to 1
AF3	AF3	Mass-Speed Dependent 0 to 10	Mass-Speed Dependent 0 to 10

[18]MS/MS/MS only

Table G-2 6500 and 6500+ Series System Parameters for LIT Scan Types Only (continued)

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
EXB	EXB	Mass-Speed Dependent –165 to 0	Mass-Speed Dependent 0 to 165
CES	CES	0 0 to 87.5	0 0 to 87.5
ROS (Q0 - ROS)	CE	10 5 to 180	–10 –5 to –180

5500 Series System Parameters H

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table H-1 5500 Series System Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55
CAD	CAD	0 N/A	6 N/A	Med (9) 0 to 12	0 N/A	5 N/A	Med (9 0 to 12
IS[19,20]	IS[19,20]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
NC[21]	NC[21]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[20,21]	TEM[20,21]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	100 0 to 300	100 0 to 300	100 0 to 300	–100 –300 to 0	–100 –300 to 0	–100 –300 to 0
Q0 (EP = –Q0)	EP	10 2 to 15	10 2 to 15	10 2 to 15	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2

[19]Turbo V™ ion source

[20]TurboIonSpray® probe

[21]APCI probe

Table H-1 5500 Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
ST (ST = Q0 + offset)	ST	Q0 + (-8) –12 to –5	Q0 + (-8) –12 to –5	Q0 + (-8) -12 to –5	Q0 + 8 12 to 5	Q0 + 8 12 to 5	Q0 + 8 12 to 5
RO1 (IE1 = Q0 – RO1)	IE1	1 0 to 3	N/A	1 0 to 3	–1 –3 to –0	N/A	–1 –3 to –0
IQ2 (IQ2 = Q0 + offset)	IQ2	Q0+ (–10) –30 to –8	Q0+ (–10) –30 to –8	Q0+ (–10) –30 to –8	Q0 + 10 8 to 30	Q0 + 10 8 to 30	Q0 + 10 8 to 30
RO2	RO2	–20 N/A	–20 N/A	N/A	20 N/A	20 N/A	N/A
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 180	N/A	N/A	–30 –180 to –5
ST3 (ST3 = RO2 + offset)	ST3	RO2 – 10 –30 to –5	N/A	N/A	RO2 + 10 5 to 30	N/A	N/A
ST3 (CXP = RO2 – ST3)	CXP	N/A	15 0 to 55	15 0 to 55	N/A	–15 –55 to 0	–15 –55 to 0
RO3	RO3	–50 N/A	N/A	N/A	50 N/A	N/A	N/A
RO3 (IE3 = RO2 – RO3)	IE3	N/A	1 0 to 5	1 0 to 5	N/A	–1 –5 to 0	–1 –5 to 0
DF	DF	–200 –300 to 0	–200 –300 to 0	–200 –300 to 0	200 0 to 300	200 0 to 300	200 0 to 300
CEM	CEM	1800 0 to 3300	1800 0 to 3300	1800 0 to 3300	1800 0 to 3300	1800 0 to 3300	1800 0 to 3300

Table H-1 5500 Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90
IHT	IHT	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250
sdp[22]	sdp	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2

Table H-2 QTRAP® 5500 System Parameters for LIT Scan Types Only

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
CAD	CAD	High Low–High	High Low–High
AF2[23]	AF2	0.100 0 or 1	0.100 0 or 1
AF3	AF3	Mass-Speed Dependent 0 to 10	Mass-Speed Dependent 0 to 10
EXB	EXB	Mass-Speed Dependent –165 to 0	Mass-Speed Dependent 0 to 165
CES	CES	0 0 to 50	0 0 to 50
ROS (Q0 - ROS)	CE	10 5 to 180	–10 –5 to –180

[22]DuoSpray™ ion source (1=TurboIonSpray probe and 2=APCI probe)

[23]MS/MS/MS only

API 5000™ System Parameters

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table I-1 API 5000™ System Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	10 10 to 50	10 10 to 50	10 10 to 50	10 10 to 50	10 10 to 50	10 10 to 50
CAD	CAD	0 N/A	1 0 to 12	4 0 to 10	0 N/A	1 0 to 12	4 0 to 12
IS[24,25]	IS[24,25]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
NC[26]	NC[26]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[25,26]	TEM[25,26]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	120 0 to 400	120 0 to 400	120 0 to 400	–100 –400 to 0	–100 –400 to 0	–100 –400 to 0
Q0 (EP = –Q0)	EP	10 15 to 2	10 15 to 2	10 15 to 2	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–1) –0.5 to –2	Q0 + (–1) –0.5 to –2	Q0 + (–1) –0.5 to –2	Q0 + 1 0.5 to 2	Q0 + 1 0.5 to 2	Q0 + 1 0.5 to 2

[24]Turbo V™ ion source

[25]TurboIonSpray® probe

[26]APCI probe

Table I-1 API 5000™ System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
ST (ST = Q0 + offset)	ST	Q0 + (-7) –12 to –5	Q0 + (-7) –12 to –5	Q0 + (-7) -12 to –5	Q0 + 7 12 to 5	Q0 + 7 12 to 5	Q0 + 7 12 to 5
RO1 (IE1 = Q0 – RO1)	IE1	1 0.5 to 2	N/A	1 0.5 to 2	–1 –2 to –0.5	N/A	–1 –2 to –0.5
RO1 (IE1 = Q0 + offset)	RO1	N/A	Q0 + (–2) –0.5 to –2	N/A	N/A	Q0 + 2 0.5 to 2	N/A
IQ2 (IQ2 = Q0 + offset)	IQ2	Q0+ (–20) –100 to –8	Q0+ (–20) N/A	Q0+ (–20) N/A	Q0 + 20 100 to 8	Q0 + 20 N/A	Q0 + 20 N/A
RO2	RO2	–100 –200 to 200	–20 –145 to –2	N/A	100 –200 to 200	20 2 to 145	N/A
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 130	N/A	N/A	–30 –130 to –5
ST3	ST3	–120 –200 to 200	N/A	N/A	N/A	N/A	N/A
ST3 (CXP = RO2 – ST3)	CXP	N/A	20 0 to 55	15 0 to 55	N/A	–20 –55 to 0	–15 –55 to 0
RO3	RO3	–150 –200 to 200	N/A	N/A	100 –200 to 200	N/A	N/A
RO3 (IE3 = RO2 – RO3)	IE3	N/A	2 –0.5 to 5	2 –0.5 to 5	N/A	–1.5 –5 to 0	–1.5 –5 to 0

Table I-1 API 5000™ System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
DF	DF	–200 –400 to 0	–200 –400 to 0	–200 –400 to 0	200 0 to 400	200 0 to 400	200 0 to 400
CEM	CEM	2000 500 to 3297	2000 500 to 3297	2000 500 to 3297	2000 500 to 3297	2000 500 to 3297	2000 500 to 3297
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	15 0 to 90	15 0 to 90	20 0 to 90
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90
ihe[27]	ihe	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1
IHT	IHT	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250
svp[28]	svp	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2

[27] 1=ON and 0=OFF

[28] DuoSpray™ ion source (1=TurboIonSpray® and 2=APCI probe)

4500 Series System Parameters J

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table J-1 4500 Series Instrument Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55
CAD	CAD	0 N/A	6 N/A	Medium (9) 0 to 12	0 N/A	6 N/A	Medium (9) 0 to 12
IS[29,30]	IS[29,30]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
NC[31]	NC[31]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[30,31]	TEM[30,31]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	100 0 to 300	100 0 to 300	100 0 to 300	–100 –300 to 0	–100 –300 to 0	–100 –300 to 0
Q0 (EP = –Q0)	EP	10 2 to 15	10 2 to 15	10 2 to 15	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2

[29]Turbo V™ ion source

[30]TurboIonSpray® probe

[31]APCI probe

Table J-1 4500 Series Instrument Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
ST (ST = Q0 + offset)	ST	Q0 + (-8) –12 to –5	Q0 + (-8) –12 to –5	Q0 + (-8) -12 to –5	Q0 + 8 12 to 5	Q0 + 8 12 to 5	Q0 + 8 12 to 5
RO1 (IE1 = Q0 – RO1)	IE1	1 0 to 3	N/A	1 0 to 3	–1 –3 to 0	N/A	–1 –3 to 0
IQ2 (ST = Q0 + offset)	IQ2	Q0 +(–10) –30 to –8	Q0 + (–11) –30 to –8	Q0 + (–10) –30 to –8	Q0 + 10 8 to 30	Q0 + 10 8 to 30	Q0 + 10 8 to 30
RO2	RO2	–20 N/A	–20 N/A	N/A	20 N/A	20 N/A	N/A
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 180	N/A	N/A	–30 –180 to –5
ST3 (ST3 = RO2 + offset)	ST3	RO2 – 10 –30 to –5	N/A	N/A	RO2 + 10 5 to 30	N/A	N/A
ST2 (CXP = RO2 - ST3)	CXP	N/A	15 0 to 55	15 0 to 55	N/A	–15 –55 to 0	–15 –55 to 0
RO3	RO3	–50 Fixed	N/A	N/A	50 Fixed	N/A	N/A
RO3 (IE3 = RO2 – RO3)	IE3	N/A	1 0 to 5	1 0 to 5	N/A	–1 –5 to 0	–1 –5 to 0
DF	DF	–200 –300 to 0	–200 –300 to 0	–200 –300 to 0	200 0 to 300	200 0 to 300	200 0 to 300
CEM	CEM	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90

Table J-1 4500 Series Instrument Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
IHT	IHT	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250
sdp[32]	sdp	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2

Table J-2 QTRAP®4500 System Parameters for LIT Scan Types Only

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
CAD	CAD	High Low–High	High Low–High
AF2[33]	AF2	0.100 0 or 0.2	0.100 0 or 0.2
AF3	AF3	Mass-Speed Dependent 0 to 10	Mass-Speed Dependent 0 to 10
EXB	EXB	Mass-Speed Dependent –165 to 0	Mass-Speed Dependent 0 to 165
CES	CES	0 0 to 50	0 0 to 50
ROS (Q0 - ROS)	CE	10 5 to 180	–10 –180 to –5

[32]DuoSpray™ ion source (1=TurboIonSpray probe and 2=APCI probe)

[33]MS/MS/MS only

4000 Series System Parameters K

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table K-1 4000 Series Instrument Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	20 10 to 50	20 10 to 50	20 10 to 50	20 10 to 50	20 10 to 50	20 10 to 50
CAD[34]	CAD	0 N/A	1 0 to 12	4 0 to 10	0 N/A	1 0 to 12	4 0 to 12
CAD[35]	CAD	0 N/A	1 0 to 12	6 0 to 10	0 N/A	1 0 to 12	6 0 to 12
IS[36,37]	IS[36,37]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
NC[38]	NC[38]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[37,38]	TEM[37, 38]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	20 0 to 400	20 0 to 400	20 0 to 400	–20 –400 to 0	–20 –400 to 0	–20 –400 to 0
Q0 (EP = –Q0)	EP	10 2 to 15	10 2 to 15	10 2 to 15	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2

[34]API 4000™ systems

[35]4000 QTRAP® systems

[36]Turbo V™ ion source

[37]TurboIonSpray® probe

[38]APCI probe

Table K-1 4000 Series Instrument Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–1) –0.5 to –2	Q0 + (–1) –0.5 to –2	Q0 + (–1) –0.5 to –2	Q0 + 1 0.5 to 2	Q0 + 1 0.5 to 2	Q0 + 1 0.5 to 2
ST (ST = Q0 + offset)	ST	Q0 + (–5) –7 to –4	Q0 + (–5) –7 to –4	Q0 + (–5) –7 to –4	Q0 + 5 4 to 7	Q0 + 5 4 to 7	Q0 + 5 4 to 7
RO1 (IE1 = Q0 – RO1)	IE1	1 0.5 to 2	N/A	1 0.5 to 2	–1 –2 to –0.5	N/A	–1 –2 to –0.5
RO1 (IE1 = Q0 + offset)	RO1	N/A	Q0 + (–1) –0.5 to –2	N/A	N/A	Q0 + 1 0.5 to 2	N/A
IQ2 (IQ2 = Q0 + offset)	IQ2	Q0+ (–8) N/A	Q0+ (–8) N/A	Q0+ (–8) N/A	Q0 + 8 N/A	Q0 + 8 N/A	Q0 + 8 N/A
RO2	RO2	–60 –145 to 20	–20 –145 to –20	N/A	60 60 to 100	20 20 to 145	N/A
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 130	N/A	N/A	–30 –130 to –5
ST3	ST3	–80 –80 to 200	N/A	N/A	80 80 to 200	N/A	N/A
ST3 (CXP = RO2 – ST3)	CXP	N/A	15 0 to 55	15 0 to 55	N/A	–15 –55 to 0	–15 –55 to 0
RO3	RO3	–62 –60 to 200	N/A	N/A	62 60 to 200	N/A	N/A

Table K-1 4000 Series Instrument Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
RO3 (IE3 = RO2 – RO3)	IE3	N/A	2 –0.5 to 5	2 –0.5 to 5	N/A	–1.5 –5 to 0	–1.5 –5 to 0
C2	C2	RO3 + 0 N/A	RO3 + 0 N/A	RO3 + 0 N/A	RO3 + 0 N/A	RO3 + 0 N/A	RO3 + 0 N/A
DF	DF	0 –400 to 0	0 –400 to 0	0 –400 to 0	0 0 to 400	0 0 to 400	0 0 to 400
CEM	CEM	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90
ihe[39]	ihe	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1
IHT	IHT	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250
svp[40]	svp	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2

[39] 1=ON and 0=OFF

[40] DuoSpray™ ion source (1=TurboIonSpray® probe and 2=APCI probe)

Table K-2 4000 QTRAP® System Parameters for LIT Scan Types Only

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
CAD	CAD	High Low–High	High Low–High
AF2[41]	AF2	100 0 to 200	100 0 to 200
AF3	AF3	Mass-Speed Dependent 0 to 5	Mass-Speed Dependent 0 to 5
EXB	EXB	Mass-Speed Dependent –200 to 0	Mass-Speed Dependent 0 to 200
CES	CES	0 –50 to 50	0 –50 to 50
ROS (Q0 - ROS)	CE	30 5 to 130	–30 –130 to –5

[41] MS/MS/MS only

SCIEX Triple Quad™ 3500 System Parameters

L

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table L-1 SCIEX Triple Quad™ 3500 System Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55
CAD	CAD	0 N/A	6 N/A	Medium (9) 0 to 12	0 N/A	6 N/A	Medium (9) 0 to 12
IS[42,43]	IS[42,42,43]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
NC[44]	NC[44]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[43,44]	TEM[43,44]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	100 0 to 300	100 0 to 300	100 0 to 300	–100 –300 to 0	–100 –300 to 0	–100 –300 to 0
Q0 (EP = –Q0)	EP	10 2 to 15	10 2 to 15	10 2 to 15	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + (–0.5) –0.1 to –2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2	Q0 + 0.5 0.1 to 2

[42]Turbo V™ ion source

[43]TurboIonSpray® probe

[44]APCI probe

Table L-1 SCIEX Triple Quad™ 3500 System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
ST (ST = Q0 + offset)	ST	Q0 + (-8) –12 to –5	Q0 + (-8) –12 to –5	Q0 + (-8) -12 to –5	Q0 + 8 12 to 5	Q0 + 8 12 to 5	Q0 + 8 12 to 5
RO1 (IE1 = Q0 – RO1)	IE1	1 0 to 3	N/A	1 0 to 3	–1 –3 to 0	N/A	–1 –3 to 0
IQ2 (ST = Q0 + offset)	IQ2	Q0 +(–10) –30 to –8	Q0 + (–11) –30 to –8	Q0 + (–10) –30 to –8	Q0 + 10 8 to 30	Q0 + 10 8 to 30	Q0 + 10 8 to 30
RO2	RO2	–20 N/A	–20 N/A	N/A	20 N/A	20 N/A	N/A
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 180	N/A	N/A	–30 –180 to –5
ST3 (ST3 = RO2 + offset)	ST3	RO2 – 10 –30 to –5	N/A	N/A	RO2 + 10 5 to 30	N/A	N/A
ST2 (CXP = RO2 - ST3)	CXP	N/A	15 0 to 55	15 0 to 55	N/A	–15 –55 to 0	–15 –55 to 0
RO3	RO3	–50 Fixed	N/A	N/A	50 Fixed	N/A	N/A
RO3 (IE3 = RO2 – RO3)	IE3	N/A	1 0 to 5	1 0 to 5	N/A	–1 –5 to 0	–1 –5 to 0
DF	DF	–200 –300 to 0	–200 –300 to 0	–200 –300 to 0	200 0 to 300	200 0 to 300	200 0 to 300
CEM	CEM	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300	2000 0 to 3300
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90

Table L-1 SCIEX Triple Quad™ 3500 System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90
IHT	IHT	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250

3200 Series System Parameters M

The first number under each scan type is the preset value. The range of numbers is the accessible range for each parameter.

Table M-1 3200 Series System Parameters

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR	CUR	20 10 to 50	20 10 to 50	20 10 to 50	20 10 to 50	20 10 to 50	20 10 to 50
CAD[45]	0 Fixed	2 Fixed	3 0 to 12	0 Fixed	2 Fixed	3 0 to 12	
CAD[46]	0 Fixed	2 Fixed	Medium Low, Medium, High	0 Fixed	2 Fixed	Medium Low, Medium, High	
IS[47]	IS[47]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4200 –4500 to 0	–4200 –4500 to 0	–4200 –4500 to 0
IS[48]	IS[48]	1000 0 to 5500	1000 0 to 5500	1000 0 to 5500	–1000 –4500 to 0	–1000 –4500 to 0	–1000 –4500 to 0
IS[49]	IS(4)	1500 0 to 2500	1500 0 to 2500	1500 0 to 2500	–1500 –2500 to 0	–1500 –2500 to 0	–1500 –2500 to 0
NC[50]	NC[50]	1 0 to 5	1 0 to 5	1 0 to 5	–1 –5 to 0	–1 –5 to 0	–1 –5 to 0

[45]API 3200™ systems

[46]3200 QTRAP® systems

[47]Turbo V™ ion source

[48]NanoSpray® ion source

[49]PhotoSpray® ion source

[50]DuoSpray™ ion source (1=TurboIonSpray® probe and 2=APCI probe)

Table M-1 3200 Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
NC[51]	NC[51]	1 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[47,50, 49]	TEM[48,50]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
OR (DP = OR)	DP	20 0 to 400	20 0 to 400	20 0 to 400	–20 –400 to 0	–20 –400 to 0	–20 –400 to 0
Q0 (EP = –Q0)	EP	10 1 to 12	10 1 to 12	10 1 to 12	–10 –12 to –1	–10 –12 to –1	–10 –12 to –1
IQ1 (IQ1 = Q0 + offset)	IQ1	Q0 + (–1) –2 to –1	Q0 + (–1) –2 to –1	Q0 + (–1) –2 to –1	Q0 + 1 1 to 2	Q0 + 1 1 to 2	Q0 + 1 1 to 2
ST (ST = Q0 + offset)	ST	Q0 + (–5) –8 to –2	Q0 + (–5) –8 to –2	Q0 + (–5) –8 to –2	Q0 + 5 2 to 8	Q0 + 5 2 to 8	Q0 + 5 2 to 8
RO1 (IE1 = Q0 – RO1)	IE1	1 0.5 to 2	N/A	1 0.5 to 2	–1 –2 to –0.5	N/A	–1 –2 to –0.5
RO1 (IE1 = Q0 + offset)	RO1	N/A	Q0 + (–2) –2 to –0.5	N/A	N/A	Q0 + 2 0.5 to 2	N/A
IQ2 (CEP = Q0 – IQ2)	CEP	Mass Dependent 0 to 188	N/A	Mass Dependent 0 to 188	Mass Dependent –188 to 0	N/A	Mass Dependent –188 to 0
IQ2 (IQ2 = RO2 + offset)	IQ2	N/A	RO2 + 0 0 to 2	N/A	N/A	RO2 + 0 –2 to 0	N/A

[51] APCI probe

[52] TurboIonSpray® probe

Table M-1 3200 Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
RO2 (CE = Q0 – RO2)	CE	N/A	N/A	30 5 to 130	N/A	N/A	–30 –130 to –5
RO2	RO2	–100 –150 to 20	–20 –130 to –5	N/A	100 20 to 150	20 5 to 130	N/A
IQ3 (CXP = RO2 – IQ3)	CXP	N/A	Mass Dependent 0 to 58	5 0 to 58	N/A	Mass Dependent –58 to 0	–5 –58 to 0
IQ3	IQ3	–125 –200 to –100	N/A	N/A	125 100 to 200	N/A	N/A
RO3 (IE3 = RO2 – RO3)	IE3	N/A	4 0.5 to 8	4 0.5 to 8	N/A	–4 –8 to 0.5	–4 –8 to 0.5
RO3	RO3	–150 –200 to –100	N/A	N/A	150 150 to 200	N/A	N/A
EX	EX	–200 N/A	–200 N/A	–200 N/A	200 N/A	200 N/A	200 N/A
DF	DF	–100 –400 to 0	–100 –400 to 0	–100 –400 to 0	100 0 to 400	100 0 to 400	100 0 to 400
CEM	CEM	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297	1800 500 to 3297
GS1	GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90

Table M-1 3200 Series System Parameters (continued)

Parameter ID	Access ID	Positive Ion Mode			Negative Ion Mode		
		Q1	Q3	MS/MS	Q1	Q3	MS/MS
ihe[53]	ihe	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1	1 0 or 1
C2	C2	0 N/A	0 N/A	0 N/A	0 N/A	0 N/A	0 N/A
XA3	XA3	0 N/A	0 N/A	0 N/A	0 N/A	0 N/A	0 N/A
XA2	XA2	0 N/A	0 N/A	0 N/A	0 N/A	0 N/A	0 N/A
IHT[48]	IHT	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250	40 0 to 250
svp[54]	svp	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2

Table M-2 3200 QTRAP® System Parameters for LIT Scan Types Only

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
CAD	CAD	High Low–Medium–High	High Low–High
FI2	CEP	Mass-Speed Dependent 0 to 188	Mass-Speed Dependent –188 to 0
ROS (Q0 – RO2)	CE	30 5 to 130	–30 –5 to –130
AF2[55]	AF2	100 0 to 200	100 0 to 200

[53] 1=ON and 0=OFF

[54] DuoSpray™ ion source (1=TurboIonSpray® probe and 2=APCI probe)

[55] MS/MS/MS only

Table M-2 3200 QTRAP® System Parameters for LIT Scan Types Only (continued)

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
AF3	AF3	Mass-Speed Dependent 0 to 5	Mass-Speed Dependent 0 to 5
EXB	EXB	Mass-Speed Dependent –200 to 0	Mass-Speed Dependent 0 to 200
DF	DF	–400 N/A	400 N/A
C2B	C2B	Mass-Speed Dependent –500 to 500	Mass-Speed Dependent –500 to 500
CES	CES	0 –50 to 50	0 –50 to 50

Masses for [Glu^1]-Fibrinopeptide B

N

Table N-1 [Glu1]-Fibrinopeptide B (Monoisotopic Molecular Weight, 1569.6696 Da)

Charge	$(M+nH)n^+$ Monoisotopic m/z
+1	1570.6768
+2	785.8421*
+3	524.2305*
+4	393.4247
+5	—
+6	—

* Indicates more commonly observed charged states.

Table N-2 contains the exact monoisotopic masses for the theoretical cleavages of [Glu1]-Fibrinopeptide B, as calculated for positive ion mode.

Table N-2 Theoretical Fragment Ions of [Glu1]-Fibrinopeptide B

b ions		y ions	
m/z	**Fragment**	***m/z***	**Fragment**
—	—	1570.6768	EGVNDNEEGFFSAR
130.0499	E	1441.6342	GVNDNEEGFFSAR
187.0713	EG	1384.6128	VNDNEEGFFSAR
286.1397	EGV	1285.5444	NDNEEGFFSAR
400.1827	EGVN	1171.5014	DNEEGFFSAR
515.2096	EGVND	1056.4745	NEEGFFSAR
629.2525	EGVNDN	942.4316	EEGFFSAR
758.2951	EGVNDNE	813.3890	EGFFSAR
887.3377	EGVNDNEE	684.3464	GFFSAR

Table N-2 Theoretical Fragment Ions of [Glu1]-Fibrinopeptide B (continued)

b ions		y ions	
944.3592	EGVNDNEEG	627.3249	FFSAR
1091.4276	EGVNDNEEGF	480.2565	FSAR
1238.4960	EGVNDNEEGFF	333.1881	SAR
1325.5281	EGVNDNEEGFFS	246.1561	AR
1396.5652	EGVNDNEEGFFSA	175.1190	R
1552.6663	EGVNDNEEGFFSAR	—	—

Prepare a Reserpine Dilution 60:1 (10 pg/µL) O

Follow this procedure to create the reserpine dilution from the reserpine 1 pmol/µL (PN 4405236).

1. Make the stock solution by adding 4.0 mL of dilution solvent to the vial.
2. Cap the vial and mix the contents gently or sonicate the vial to dissolve the material.

   This step produces a 1 pmol/µL solution of reserpine.
3. Put 1 mL of reserpine stock solution in a clean vial and add 5 mL of dilution solvent.
4. Combine 1 mL of the 6:1 dilution and 9 mL of dilution solvent.

   This step produces a 60:1 reserpine dilution.