Source Parameters and Voltages

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Depending on the ion source installed on the mass spectrometer, different source-dependent parameters will be available to optimize.

TurboIonSpray® Probe Parameters

Table C-1 shows the recommended operating conditions for the TurboIonSpray® probe at three different flow rates. For each flow rate, the Curtain Gas™ flow should be as high as possible. The solvent composition used for optimization was 50:50 water:acetonitrile. These conditions represent a starting point from which to optimize the TurboIonSpray probe. By an iterative process, you can optimize the parameters using flow injection analysis until you achieve the best signal or signal-to-noise for the compound of interest.

Table C-1 Parameter Optimization for TurboIonSpray® Probe

Parameter	Typical values			Operational range
LC flow	5 µL/min to 50 µL/min	200 µL/min	1000 µL/min	5 µL/min to 3000 µL/min
Gas 1 (nebulizer gas)	20 psi to 40 psi	40 psi to 60 psi	40 psi to 60 psi	0 psi to 90 psi
Gas 2 (heater gas)	0 psi	50 psi	50 psi	0 psi to 90 psi
Curtain Gas™ supply	20 psi	20 psi	20 psi	10 to 50 psi
Temperature*	0°C to 200°C	425°C to 650°C	550°C to 750°C	Up to 750°C
DP**	Positive: 70 V Negative: –70 V	Positive: 70 V Negative: –70 V	Positive: 70 V Negative: –70 V	Positive: 0 V to 400 V Negative: –400 V to 0 V
Probe Y-axis position	7 to 10	2 to 5	0 to 2	0 to 13
Probe X-axis position	4 to 6	4 to 6	4 to 6	0 to 10

* Optimum temperature values depend on the compound and mobile phase composition (higher aqueous content requires higher temperature). 0 means no temperature is applied.

** DP value depends on the compound.

Note: The lower the number in the Scale Position column, the farther away from the orifice the probe is positioned.

APCI Probe Parameters

Table C-2 Parameter Optimization for the APCI Probe

Parameter	Nominal value	Operational range
LC Flow	1000 µL/min	200 µL/min to 2000 µL/min
Gas 2	30 psi	0 psi to 90 psi
Curtain Gas™ supply	20 psi	10 psi to 50 psi
Temperature*	400 °C	100°C to 750°C
Nebulizer Current	Positive: 3 Negative: –3	Positive: 0 to 5 Negative: –5 to 0
DP	Positive: 60 V Negative: –60 V	Positive: 0 V to 300 V Negative: –300 V to 0 V
Probe vertical y-axis position	4 mm	Scale 0 mm to 13 mm
* Temperature value depends on the compound.		

Parameter Descriptions

Source-Dependent Parameters

Table C-3 Source-Dependent Parameters

ID	Name	Values	Description
GS1	Ion Source Gas 1	Range: 0 to 90 psi Typical: 20 to 60 psi	Controls the nebulizer gas for the TurboIonSpray® probe and the auxiliary gas for the APCI probe. Nebulizer gas helps generate small droplets of sample flow and affects spray stability and sensitivity.
GS2	Ion Source Gas 2	Range: 0 to 90 psi Typical: 30 to 70 psi	Controls the heater gas for the TurboIonSpray probe. Heater gas evaporates the spray droplets. The best sensitivity is achieved when the combination of temperature (TEM) and turbo-gas (GS2) flow rate causes the LC solvent to reach a point at which it is nearly all vaporized. To optimize GS2, increase the flow until you obtain the best signal or signal-to-noise ratio. If you see a significant increase in background noise, reduce the value. Too high a gas flow can produce a noisy or unstable signal.

Table C-3 Source-Dependent Parameters (cont'd)

ID	Name	Values	Description
CUR	Curtain Gas™ flow	Range: 0 psi to 50 psi Typical: 20 psi	Controls the flow of gas to the Curtain Gas interface. The Curtain Gas interface is located between the curtain plate and the orifice. It prevents ambient air and solvent droplets from entering and contaminating the ion optics, while permitting direction of sample ions into the vacuum chamber by the electrical fields generated between the vacuum interface and the spray needle. Contamination of the ion entrance optics thus reduces Q0 transmission, stability, and sensitivity, and increases background noise. Maintain the Curtain Gas flow as high as possible without losing sensitivity.
TEM	Temperature	Range: 0 to 750 Typical: 600	Controls the heat applied to the sample to vaporize it. The optimal temperature is the lowest temperature at which the sample is vaporized completely. Optimize in increments of 50°C.

Table C-3 Source-Dependent Parameters (cont'd)

ID	Name	Values	Description
TEM	Temperature (cont'd)	Range: 0 to 750 Typical: 600	**TurboIonSpray probe:** Controls the temperature of the heater gas in the TurboIonSpray probe. Heater gas evaporates the solvent to produce gas phase sample ions. The best sensitivity is achieved when the combination of temperature (TEM) and heater gas (GS2) flow rate causes the LC solvent to reach a point at which it is nearly all vaporized. As the organic content of the solvent increases, the optimal probe temperature should decrease. With solvents consisting of 100% methanol or acetonitrile, the probe performance may optimize as low as 300°C. Aqueous solvents consisting of 100% water at flows of approximately 1000 µL/min require a maximum probe temperature of 750°C. If the temperature is set too low, then vaporization is incomplete and large, visible droplets are expelled into the ion source housing. If the temperature is set too high, solvent may vaporize prematurely at the TurboIonSpray probe tip, especially if the probe is set too low (5 mm to 13 mm).
			APCI probe: Controls the temperature of the temperature of the APCI probe. As the organic content of the solvent increases, the optimal probe temperature should decrease. With solvents consisting of 100% methanol or acetonitrile the probe performance may optimize at temperatures as low as 400°C at flow rates of 1000 µL/min. Aqueous solvents consisting of 100% water set at flows of approximately 2000 µL/min require a minimum probe temperature of 700°C. If the temperature is set too low, then vaporization is incomplete and large, visible droplets are expelled into the ion source housing. If the temperature is set too high, thermal degradation of the sample occurs.

Table C-3 Source-Dependent Parameters (cont'd)

ID	Name	Values	Description
NC	Nebulizer, or Needle, Current	Range: –5 to 5 Typical: Positive: 2 Negative: –2	The NC parameter controls the current applied to the corona discharge needle in the APCI probe. The discharge ionizes solvent molecules, which in turn ionize the sample molecules. For the APCI probe the current applied to the corona discharge needle (NC) usually optimizes over a broad range (about 1 μA to 5 μA). To optimize, start at a value of 1 and increase until you achieve the best signal or signal-to-noise ratio. If, on increasing the current, you observe no changes in signal, leave the current at the lowest setting that provides the best sensitivity (for example, 2 μA).
IS	IonSpray™ Voltage or IonSpray™ Voltage Floating	Range: –4500 V to 5500 V Typical: Positive: 5000 V Negative: –4000 V	The IS parameter controls the voltage applied to the needle that ionizes the sample in the ion source. It depends on the polarity, and affects the stability of the spray and the sensitivity.
ihe	Interface Heater	Range: off; on Typical: on	This parameter is always on for 5600 and 5500 series mass spectrometers. The ihe parameter switches the interface heater on and off. Heating the interface helps maximize the ion signal and prevents contamination of the ion optics. Unless the compound you are analyzing is extremely fragile, we recommend that you heat the interface. With the Turbo V™ ion source, the interface plate is heated to 100°C.

Probe Position

The position of the probe can affect the sensitivity of the analysis. For more information on how to optimize the position of the probe, see Optimizing the TurboIonSpray® Probe on page 23 and Optimizing the APCI Probe on page 27. For information on optimizing the mass spectrometer, *see the Analyst® Software Getting Started Guide.*

Solvent Composition

The standard concentration of ammonium formate or ammonium acetate is from 2 mmol/L to 10 mmol/L for positive ions and 2 mmol/L to 50 mmol/L for negative ions. The concentration of organic acids is 0.1% to 0.5% by volume for the TurboIonSpray probe and 0.1% to 2.0% by volume for the APCI probe.

Commonly used solvents are:

- Acetonitrile
- Methanol

- Propanol
- Water

Commonly used modifiers are:

- Acetic acid
- Formic acid
- Ammonium formate
- Ammonium acetate

The following modifiers are not commonly used because they complicate the spectrum with their ion mixtures and cluster combinations. They may also suppress the strength of the target compound ion signal:

- Triethyl amine (TEA)
- Sodium phosphate
- Trifluoroacetic acid (TFA)
- Sodium dodecyl sulfate

Declustering Potential

Optimal declustering potential voltage should be set high enough to reduce the chemical noise, but low enough to avoid fragmentation. The fragmentation energy of a compound is a function of its structure and molecular weight. In general, lower molecular weight compounds require less energy—lower declustering potential—to induce fragmentation.

In general, the higher the declustering potential voltage the greater the energy imparted to the ions entering the analyzing region of the mass spectrometer. The energy helps to decluster the ions and to reduce the chemical noise in the spectrum, resulting in an increase in signal-to-noise, or sensitivity. Increasing the voltage beyond optimal conditions can induce fragmentation before the ions enter the mass filters, resulting in a decrease in sensitivity. In some instances, fragmentation is a valuable tool that provides additional structural information.