

Hardware Guide



AB SCIEX QTRAP® 5500 System

D1000079384 E
May 2010

AB SCIEX

This document is provided to customers who have purchased AB SCIEX equipment to use in the operation of such AB SCIEX equipment. This document is copyright protected and any reproduction of this document or any part of this document is strictly prohibited, except as AB SCIEX may authorize in writing.

Equipment that may be described in this document is protected under one or more patents filed in the United States, Canada, and other countries. Additional patents are pending.

Software that may be described in this document is furnished under a license agreement. It is against the law to copy, modify, or distribute the software on any medium, except as specifically allowed in the license agreement. Furthermore, the license agreement may prohibit the software from being disassembled, reverse engineered, or decompiled for any purpose.

Portions of this document may make reference to other manufacturers and/or their products, which may contain parts whose names are registered as trademarks and/or function as trademarks of their respective owners. Any such usage is intended only to designate those manufacturers' products as supplied by AB SCIEX for incorporation into its equipment and does not imply any right and/or license to use or permit others to use such manufacturers' and/or their product names as trademarks.

AB SCIEX makes no warranties or representations as to the fitness of this equipment for any particular purpose and assumes no responsibility or contingent liability, including indirect or consequential damages, for any use to which the purchaser may put the equipment described herein, or for any adverse circumstances arising therefrom.

For research use only. Not for use in diagnostic procedures.

CE



The trademarks mentioned herein are the property of AB Sciex Pte. Ltd. or their respective owners. AB SCIEX™ is being used under license.

System Information

1

The AB SCIEX QTRAP® 5500 System is designed for the qualitative and quantitative analysis of chemical species. The system includes a mass spectrometer, a Turbo V™ ion source, a computer, and the Analyst® software.



WARNING! Risk of personal injury or instrument damage. If you need to move the system, contact an FSE to assist you.



Note: Before you operate the instrument, make sure you have read the *Safety Practices* guide.

Figure 1-1 *Front View* shows a system with a syringe pump, Turbo V ion source, a diverter valve, and the optional NanoSpray® ion source monitors.

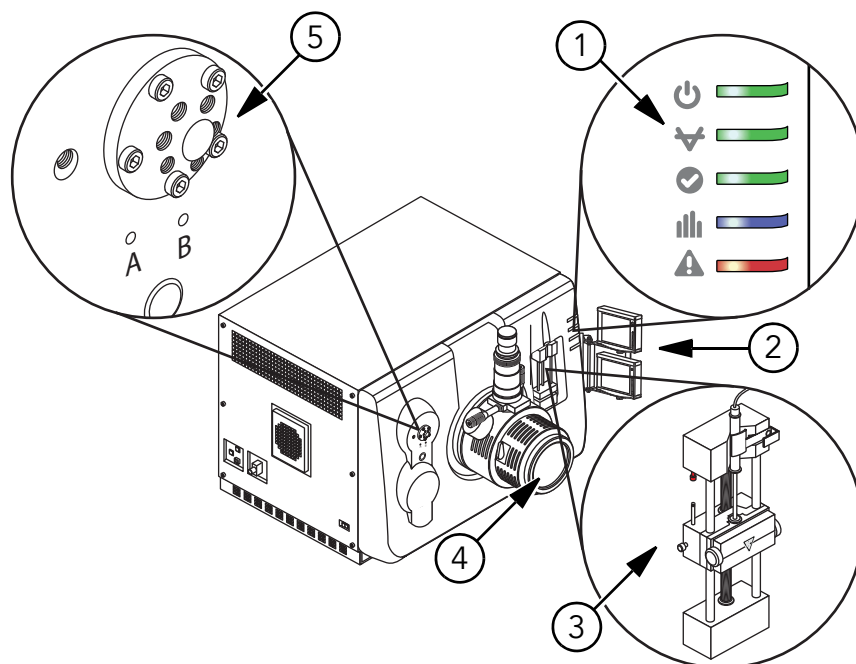


Figure 1-1 Front View

Item	Description	For more information see...
1	Instrument panel symbols	Table 1-1 on page 5.
2	Nanospray® ion source monitors (optional)	<i>NanoSpray® Ion Source Operator's Guide</i> located on the CD that comes with the ion source.

Figure 1-1 Front View (cont'd)

Item	Description	For more information see...
3	Syringe pump	To use the integrated syringe pump on page 7.
4	Turbo V™ ion source	Turbo V™ Ion Source Operator's Guide located on the CD that comes with the ion source.
5	Diverter valve	If the optional DuoSpray™ ion source is installed, then the diverter valve is replaced with the DuoSpray valve. The diverter valve is installed below the DuoSpray valve. See Diverter Valve on page 10 . For information about the DuoSpray ion source, see the <i>DuoSpray™ Ion Source Operator's Guide</i> located on the CD that comes with the ion source.

Figure 1-2 *Rear and Side Views on page 4* shows the location of the instrument connections, including the locations of the reset and vent buttons and the instrument switch.

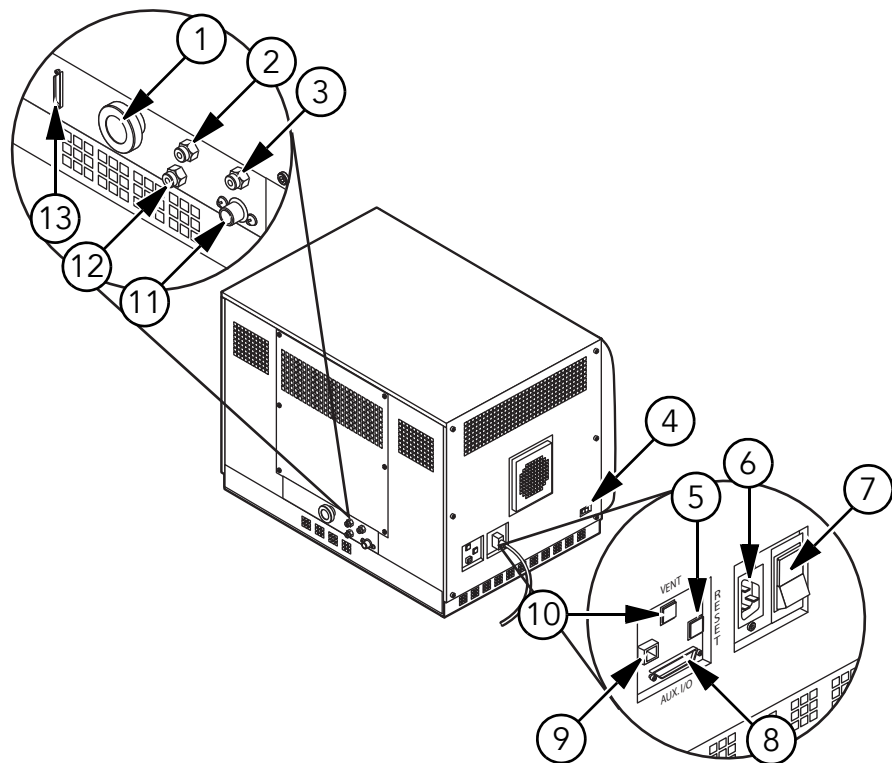


Figure 1-2 Rear and Side Views

Item	Description	For more information...
1	Roughing pump vacuum connection	Contact your FSE.
2	Nitrogen gas supply (Curtain Gas™ supply, CAD gas)	Contact your FSE.
3	Source exhaust supply	Contact your FSE.
4	Source communication connection	Contact your FSE.


Figure 1-2 Rear and Side Views (cont'd)

Item	Description	For more information...
5	Instrument reset button	See To reset the system on page 6 .
6	Mains supply connection	See To turn on the system on page 5 or To shut down the system on page 6 .
7	Instrument switch (Up = On; Down = Off)	See To turn on the system on page 5 or To shut down the system on page 6 .
8	Aux I/O connection	See the <i>Peripheral Devices Setup Guide</i> .
9	Ethernet connection (connects the instrument and the computer)	Contact your FSE.
10	Instrument vent (shutdown) button	See To turn on the system on page 5 or To shut down the system on page 6 .
11	Source exhaust waste (to waste bottle)	Contact your FSE.
12	Air supply (Gas1/Gas2)	Contact your FSE.
13	Roughing pump communication connection	Contact your FSE.

Instrument Panel Symbols

Table 1-1 shows the instrument status LEDs.

Table 1-1 Instrument Panel Symbols

Instrument LEDs	Colour	Name	Description
	Green	Power	Lit when the instrument is powered up.
	Green	Vacuum	Lit when the proper vacuum has been achieved; and flashing if the vacuum is not at the proper vacuum (during pumpdown and venting.)
	Green	Ready	Lit when the instrument is in the Ready state. Instrument must be in the Ready state to operate.
	Blue	Scanning	Flashing when the instrument is acquiring data.
	Red	Fault	Lit when the instrument encounters a system fault.

After the instrument is turned on, all five LEDs illuminate. The power LED remains lit. The other four LEDs flash for two seconds and then turn off. The vacuum LED starts flashing. After the proper vacuum has been achieved this LED remains lit.

Shutting Down, Turning On, and Resetting the System

Use the following procedures if you need to shut down or turn on the system. Resetting restarts the system without shutting down the roughing pump.

To turn on the system

1. Make sure that the mains supply cable is plugged in to the instrument.

2. Turn on the instrument switch.



Note: If the switch is already on, turn it off and then on.

The instrument starts, and then the roughing pump starts up after approximately 30 seconds. When the Vacuum light is lit, the instrument is in Standby mode.

3. Turn on the computer, if it was turned off, and then start the Analyst® software.
4. Click **View > Sample Queue** and then click the Ready icon.

To reset the system

- Press and hold the Reset button for 5 seconds.
You will hear a click when the relay activates. After approximately three minutes, the mass spectrometer should reach operating pressure.

To shut down the system

1. Complete or stop any ongoing scans. For more information, see the *Getting Started Guide* for the Analyst software.
2. Shut off the sample flow to the instrument.

CAUTION! Potential Instrument Damage: Shut off the sample flow before you shut down the instrument.

3. In the Analyst software, deactivate the hardware profile, if active, and then close the application software.
4. Press and hold the Vent button for one second.
The turbo pump will spin down gradually. The roughing pump is controlled by the instrument and will continue to run for approximately 15 minutes.
5. After the roughing pump shuts down (in about 15 minutes), turn off the instrument switch.
6. Unplug the mains supply cable from the bulkhead on the left side of the instrument.

Using the Integrated Syringe Pump

Use the following procedure to set up and use the syringe pump. Make sure the syringe pump is seated properly to avoid damaging the syringe. For more information about creating and editing hardware profiles, see the *Getting Started Guide*.

To configure the integrated syringe pump in the hardware profile

1. On the Navigation bar, in **Configure** mode, double-click **Hardware Configuration**.
2. Create or edit the hardware profile containing your instrument.
3. On the Configuration tab ([Figure 1-3 Configuration tab on page 7](#)), select **Use integrated syringe pump** and then click **OK**.

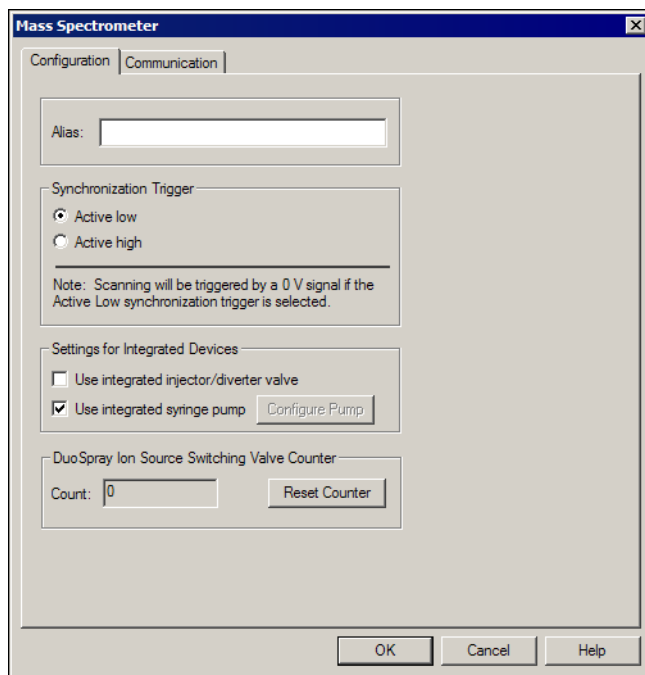


Figure 1-3 Configuration tab

4. Activate the hardware profile.

To use the integrated syringe pump

1. Press the button on the right side of the syringe pump to lower the base and then insert the syringe as shown in [Figure 1-4 Lowering the syringe](#).

Make sure that the end of the syringe is flush against the base and that the shaft of the syringe rests in the cutout.

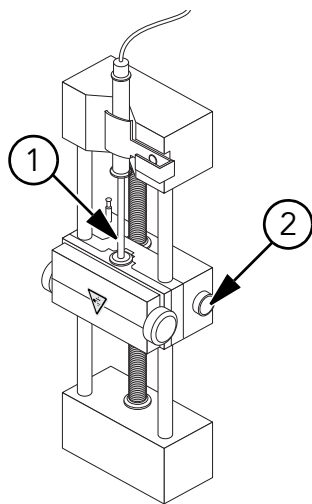


Figure 1-4 Lowering the syringe

Item	Description
1	Syringe plunger.
2	Release button. Press to raise or lower the base.

2. Adjust the post ([Figure 1-5 Safety stop](#)) so that it triggers the automatic syringe stop before the syringe plunger hits the glass syringe.

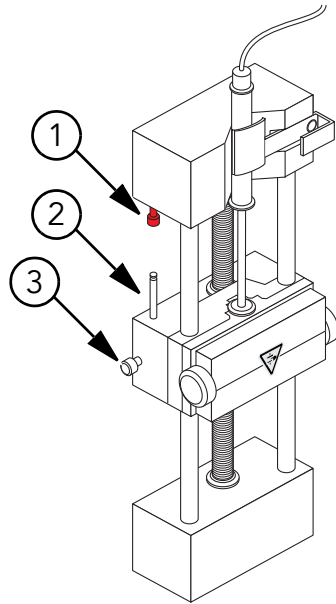


Figure 1-5 Safety stop

Item	Description
1	Automatic syringe stop. After the post hits the automatic syringe stop, the syringe pump stops.
2	Post. Adjust the height to prevent the syringe plunger from hitting the syringe during sample infusion.
3	Post lock screw. Tighten the screw after you have adjusted the height of the post.

3. Turn the side screws as shown in [Figure 1-6 Syringe pump on page 9](#) to secure the syringe.

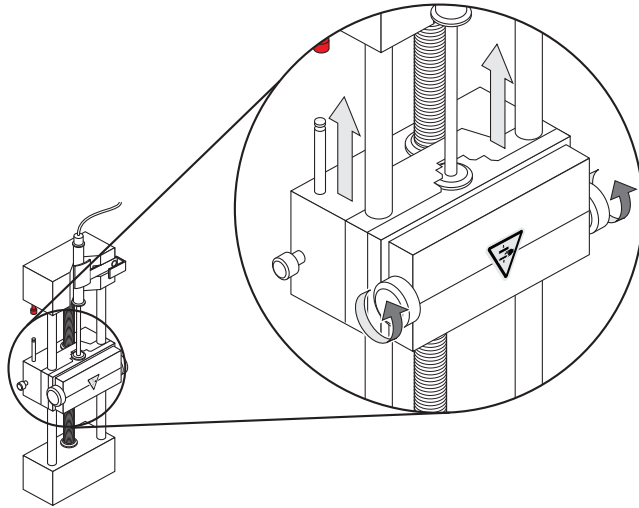


Figure 1-6 Syringe pump

4. On the instrument, press the button on the right side of the syringe pump ([Figure 1-7 Syringe pump LED](#)) to start the flow.

The light next to the button illuminates when the syringe pump is in use.



Tip! You can also start the syringe pump using the Analyst® software in Manual Tune.

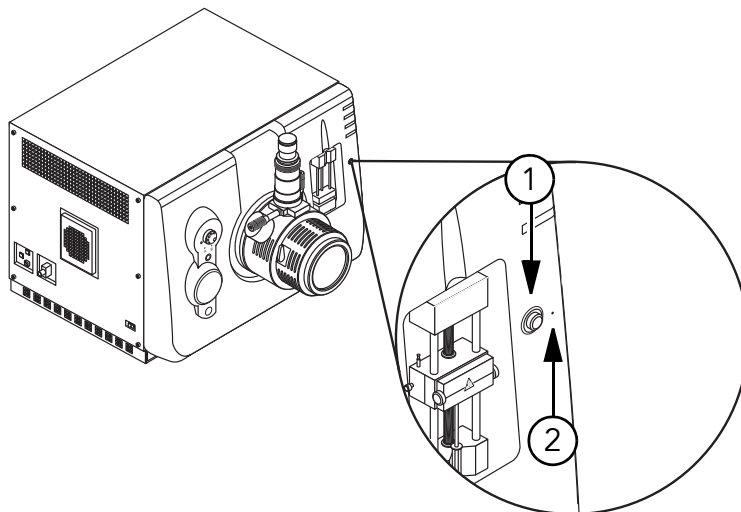


Figure 1-7 Syringe pump LED

Item	Description
1	Syringe pump on/off button
2	Syringe pump status LED

Diverter Valve

The diverter valve is a two position, 6 port valve. If you put the valve in Position A ([Figure 1-9 Diverter Valve Position A on page 11](#)), the sample flows through the external loop. When you switch the valve to Position B ([Figure 1-10 Diverter Valve Position B on page 12](#)), the sample is injected. For more information about creating and editing hardware profiles, see the *Getting Started Guide*.

To configure the diverter valve in the hardware profile

1. On the Navigation bar, in **Configure** mode, double-click **Hardware Configuration**.
2. Create or edit the hardware profile containing your instrument.
3. On the Configuration tab ([Figure 1-8 Configuration tab](#)), select **Use integrated injector/diverter valve** and then click **OK**.

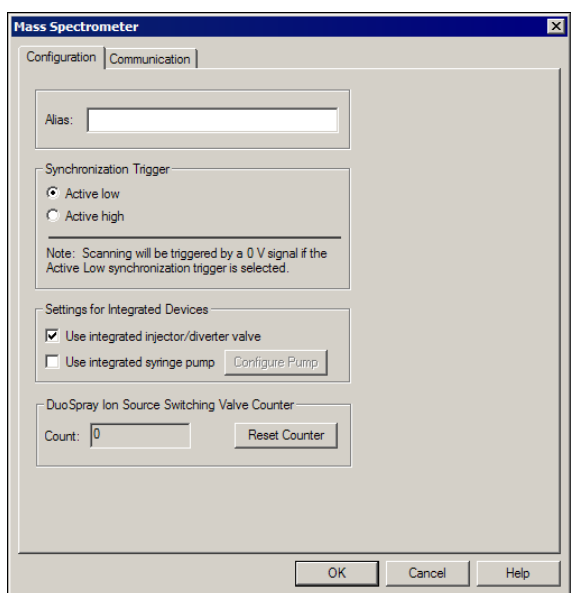
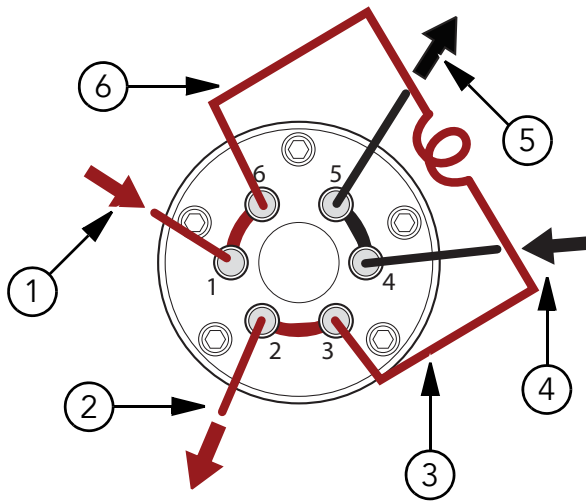


Figure 1-8 Configuration tab

4. Activate the hardware profile.

To plumb the diverter valve

- Use [Figure 1-9 Diverter Valve Position A on page 11](#) and [Figure 1-10 Diverter Valve Position B on page 12](#) to plumb the diverter valve.

**Figure 1-9** Diverter Valve Position A

Item	Description
1	Sample in
2	Waste out
3	Sample loop
4	Mobile phase in
5	To column
6	Sample loop

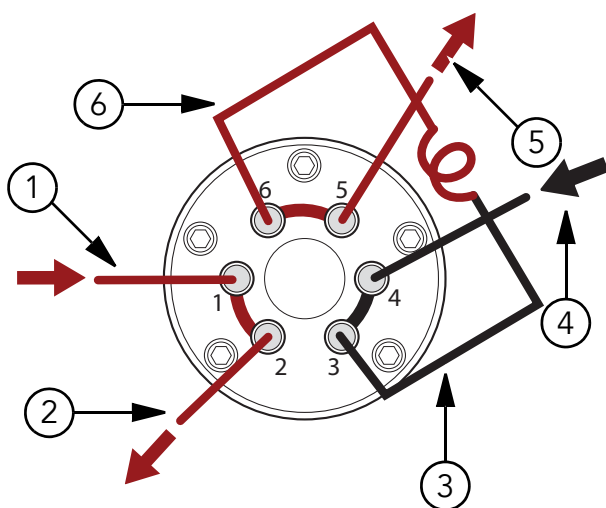


Figure 1-10 Diverter Valve Position B

Item	Sample in
1	Sample in
2	Waste out
3	Sample loop
4	Mobile phase in
5	To column
6	Sample loop

Instrument Safe Fluids

The following fluids can safely be used with the instrument:

- Methanol (0 to 100%)
- Acetonitrile (0 to 100%)
- Water
- Formic acid (0 to 1%)
- Ammonium acetate (0 to 1%)



Note: This list is not complete. If you are uncertain about a specific fluid, do not use the fluid until confirmation is received from AB SCIEX that it will not present a hazard.

Source/Gas Parameters

The parameters in [Table 1-2](#) are optimized for different LC conditions involving flow rate. For more information about the parameters, see the Analyst® software Help system.



Note: We recommend that you run the instrument with the Curtain Gas™ flow set to at least 20 to maintain good instrument performance.

Table 1-2 Source/Gas Parameters

Parameter	Value
Curtain Gas (CUR)	20
IonSpray Voltage (IS)	5000
Temperature (TEM)	700
Ion Source Gas (GS1)	60
Ion Source Gas 2 (GS2)	60

Turbo V™ Ion Source Settings

[Table 1-3](#) shows the recommended starting values for the X- and Y-axis parameters. For more information, see the *Turbo V™ Ion Source Operator's Guide*.

Table 1-3 Vertical and Horizontal Parameters

Parameter	Value
X-axis	5
Y-axis	5

Compound Parameters

In general, you can use the preset values for most of the parameters in [Table 1-4](#). For more information about the parameters, see the Analyst® software Help system.

Table 1-4 Compound Parameters

Parameter	Value
CAD Gas	Use the preset value and optimize for your compound.
DP (Declustering Potential)	Use the preset value and optimize for your compound.
EP (Entrance Potential)	Use the preset value.
CXP (Collision Cell Exit Potential)	Use the preset value and optimize for your compound.
CE (Collision Energy)	Use the preset value and optimize for your compound.
CES (Collision Energy Spread)	Use the preset value and optimize for your compound.
Fixed LIT Fill Time	Use the preset value.
DFT (Dynamic Fill Time)	Either select or deselect the feature based on your experiment. In the Tools > Settings > Method Options dialog box, the Dynamic Fill Time settings are optimized for the 10000 Da/s scan speed. These settings are also suitable for other LIT scan speeds.

Table 1-4 Compound Parameters (cont'd)

Parameter	Value
Q0 Trapping	Either select or deselect the feature based on your experiment. The recommended fixed fill time to use with Q0 trapping is 20 ms or greater.
MCS (Multi-Charge Separation) Barrier	Use the preset value.
Q3 Entry Barrier	Use the preset value.
Q3 Empty Time	Use the preset value.
MS/MS/MS Fragmentation Time	Use the preset value.
Q3 Cool Time	Use the preset value.
TDF CE (Time Delayed Fragmentation Collision Energy)	Use the preset value.
IE1 (Ion Energy 1) — <i>For experienced instrument operators only</i>	Do not adjust.
IE3 (Ion Energy 3) — <i>For experienced instrument operators only</i>	Do not adjust.

Related Documentation

The guides and tutorials for the instrument and the Analyst software are installed automatically with the software and are available from the Start menu: All Programs > AB SCIEX. A complete list of the available documentation can be found in the online Help. To view the Analyst software Help, press F1.

Technical Support

AB SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the instrument or any technical issues that may arise. For more information, visit the web site at <http://www.absciex.com>.

The following table contains generic parameters for the 5500 series of instruments. The first number under each scan type is the preset value; the range of numbers is the accessible range for each parameter.

Table 2-1 5500 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	Med (9) 0 to 12	0 n/a	6 n/a	Med (9) 0 to 12
IS ⁽¹⁾⁽²⁾	IS ⁽¹⁾⁽²⁾	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 ⁽³⁾	NC ⁽³⁾	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 ⁽²⁾⁽³⁾	TEM ⁽²⁾⁽³⁾	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

(1)IonSpray™ ion source (2)TurboIonSpray® ion source (3)Heated Nebulizer (4) 1=ON and 0=OFF (5)DuoSpray™ ion source, 1=TIS, and 2=HN

Table 2-1 5500 Series Instrument Parameters (cont'd)

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 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
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 ⁽⁵⁾	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

(1)IonSpray™ ion source (2)TurboIonSpray® ion source (3)Heated Nebulizer (4) 1=ON and 0=OFF (5)DuoSpray™ ion source, 1=TIS, and 2=HN

Table 2-2 AB SCIEX 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**	AF2	0.100 0 to 200	0.100 0 to 200

** MS/MS/MS only

Table 2-2 AB SCIEX QTRAP® 5500 System Parameters for LIT Scan Types Only (cont'd)

Parameter ID	Access ID	Positive Ion Mode	Negative Ion Mode
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
** MS/MS/MS only			

