Chapter 1
Instrument Description

1.1 Overview

The Quattro Premier ™ XE (Figure 1-1) is a high-performance tandem quadrupole mass spectrometer designed for routine LC/MS/MS operation.

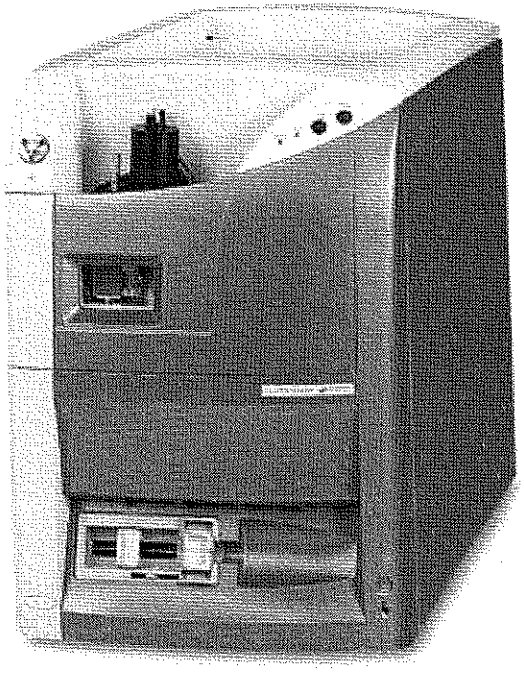

Figure 1-1 Quattro Premier XE Mass Spectrometer

The Quattro Premier XE may be coupled to either of two types of inlet:

- An HPLC system, to provide molecular weight information from an LC run or perform target analysis and quantification.
- A syringe pump, for analysis of precious, low-concentration compounds.

The sample is ionized at atmospheric pressure in the source. The ions enter the vacuum system through a sampling cone, then pass through the source travelling-wave (T-Wave™) ion guide into the first quadrupole, where they are filtered according to their mass-to-charge ratio (m/z) (Figure 1-2). The mass-separated ions pass into the T-Wave collision cell where they either undergo collision-induced decomposition (CID) or pass to the second quadrupole. Any fragment ions are then mass-analyzed by the second quadrupole. The transmitted ions are detected by a conversion dynode, phosphor, and photomultiplier detection system. The output signal is then amplified, digitized, and passed to the control system.

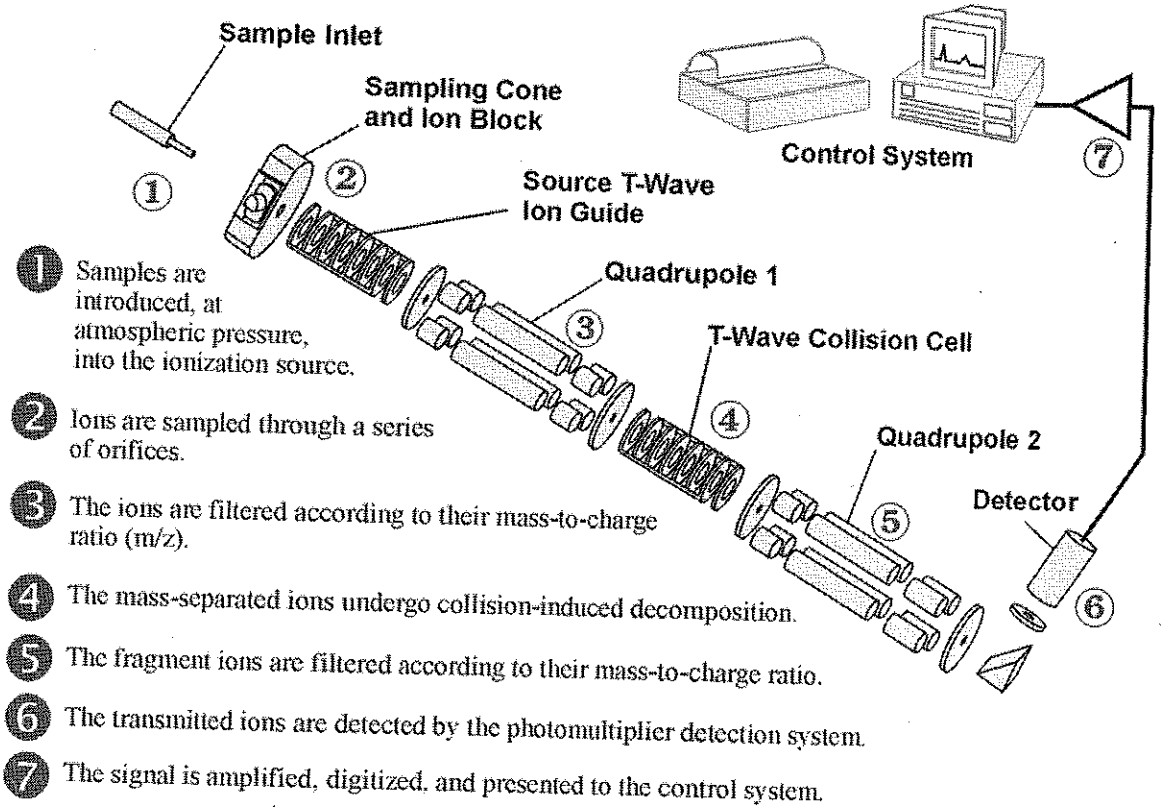

Figure 1-2 Quattro Premier XE Schematic

1.2 Sample Inlet

An HPLC system or infusion pump delivers sample to a ZSpray™ Ionization Source.

The ionization technique (see Section F.1) is selected by installing the appropriate probe. An ESI (electrospray ionization) probe is supplied as standard. An APCI (atmospheric pressure chemical ionization) is available as an option. Recognition pins on the probe identify the ionization method to the system. The source can also be operated as an ESCi™ multi-mode ionization source to combine ESI and APCI operation in a single run (see Chapter 4). In this case the ESI probe is used together with an APCI corona discharge pin, which is supplied as standard.

1.3 Vacuum System

An external backing pump and internal turbomolecular pumps generate vacuum in the instrument. The backing pump may be a rotary pump or, optionally, an oil-free scroll pump.

The control system monitors the turbomolecular pump speeds and continuously monitors the vacuum using an integral Pirani gauge. The Pirani gauge stops instrument operation if a vacuum loss is detected.

A vacuum isolation valve allows routine source maintenance to be performed without breaking the vacuum.

1.4 MassLynx Control System

The Quattro Premier XE is controlled by the PC-based MassLynx™ software. MassLynx also controls the HPLC system, autosampler, and divert/injector valve, if applicable. A second PC, embedded in the Quattro Premier XE, processes the acquired data. Communication between the MassLynx PC and the embedded PC is via a network link.

Analog inputs allow data acquisition from conventional LC detectors like an ultraviolet (UV) detector or evaporative light scattering detector (ELSD). Data from selected UV photo diode array detectors (for example, the Waters 996 PDA detector) can also be acquired.

The MassLynx software allows the following processes:

- Configuring the Quattro Premier XE.
- Creating inlet and MS methods that define operating parameters for a run.
- Tuning and calibrating the Quattro Premier XE.
- Running samples.
- Monitoring the run.
- Acquiring data.

See the *MassLynx User's Guide* and *MassLynx Help* for more information on installing and using the MassLynx software.

1.5 Front Panel Controls, Indicators, and Connections

Figure 1-3 shows a general view of the front of the instrument with the access door open.

1.5.1 Power Switch

Warning: *The power switch does not isolate the instrument from the mains power supply. To do this, disconnect the power supply cord (see Section 1.6.13) from the rear of the instrument.*

The instrument's power switch is located on the lower-right side corner of the front panel.

Note: *As the power switch does not isolate the instrument from the mains power supply, fans may be heard running, even when the instrument is off.*

1.5.2 Embedded PC Reset Switch

The embedded PC reset switch resets the embedded PC and instrument's electronics. This switch is accessed through a hole in the instrument's front panel and can be operated by means of a short length of PEEK™ tubing, or similar object.

If the instrument is in Operate, the embedded PC reset switch switches it into Standby in a controlled manner, even if communication with the MassLynx PC is lost. This may cause the backing pump to momentarily start or stop.

When the embedded PC reboots, it will take a short time to re-establish communication with the MassLynx PC.

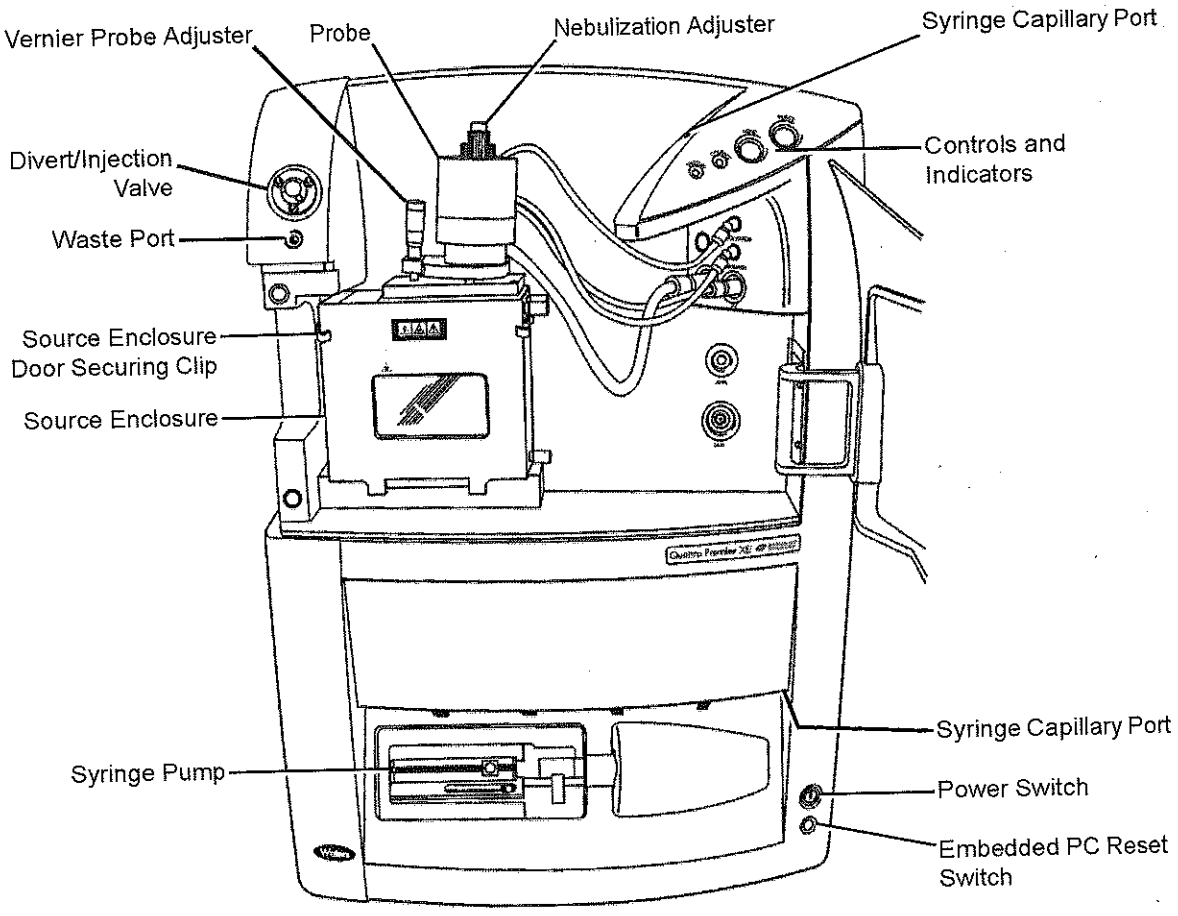

Figure 1-3 Front View with the Access Door Open

After the switch is operated, the high voltages will be switched off and the turbomolecular pumps will gradually slow down.

If the reset switch is operated when the MassLynx PC is offline, and the turbomolecular pump speed falls below 50% of full speed, the vent solenoid will open and admit air into the analyzer. The backing pump will be switched off a few seconds later.

If the instrument is vented fully, it must be evacuated again by selecting Options > Pump in the MassLynx Tune window (see Appendix C).

If the turbomolecular pump speed is above 50% of full speed when the embedded PC has booted-up, the embedded PC cancels the vent sequence, and the instrument evacuates again.

Note: *On certain early instruments, the embedded PC will not cancel the vent sequence after it has booted-up. You must select Options > Pump on the Tune window to stop the instrument being vented.*

1.5.3 Cone Gas, Desolvation Gas, and Nebulizer Gas Connections

The PTFE gas lines for the probe desolvation gas and nebulizer gas are connected to the front of the instrument by push-in fittings (Figure 1-4). The connection for the cone gas is inside the source; it also uses PTFE tubing.

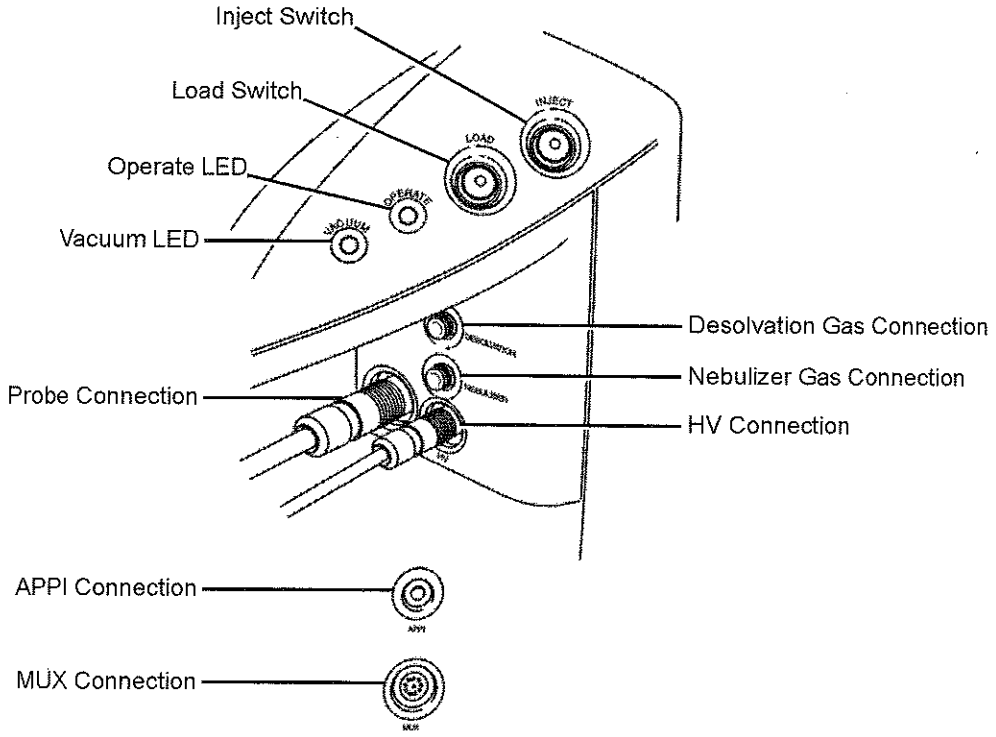

Figure 1-4 Front Panel Connections, Controls, and Indicators

1.5.4 Electrical Connections

The electrical connection for the ESI desolvation heater or APCI probe heater is via the Probe multi-way connector.

The high voltage connection for the ESI probe is via the front panel HV connection.

The APPI connection is used by the optional Combined APPI and APCI Source (see the *Waters Micromass Quattro Premier XE Combined APPI and APCI Source Operator's Guide* for details).

The MUX connection is used by the optional MUX-technology™ Interface (see the *Waters Micromass Quattro Premier XE MUX-technology Interface Operator's Guide* for details).

The high voltage connection for the corona discharge pin is inside the source.

1.5.5 Status Display

The Vacuum and Operate status light-emitting diodes (LEDs) are at the top-right corner of the instrument's front panel (see Figure 1-4).

The instrument's status is indicated as shown in Tables 1-1 and 1-2.

Table 1-1 Vacuum LED Display

State	Vacuum LED Indication
Pumping	Flashing green
Pumped, below trip level	Steady green
Pumped, above trip level	Steady amber
Venting, if the turbomolecular pump speeds are above 50% of full speed	Flashing red
Venting, if the turbomolecular pump speeds are below 50% of full speed	Flashing amber, for approximately 10 seconds before the vented state is achieved
Vented	Steady red

Table 1-2 Operate LED Display

State	Operate LED Indication
Standby	No indication
Operate, above trip level	Steady amber
Operate, below trip level	Steady green
RF error	Flashing red
Tripped out of Operate due to low nitrogen gas supply pressure	Flashing amber

Note: *To return the instrument to Operate, you must:*

1. *Re-establish the nitrogen supply.*
2. *In the Tune window, click Press for Standby.*
3. *In the Tune window, click Press for Operate.*

Note: *Any combination of LED indications not covered by Tables 1-1 and 1-2 indicates an instrument fault. Contact Waters for advice (see Section 8.6).*

1.5.6 Divert/Injection Valve

Warning: *The liquids passing through the divert/injection valve may be biohazardous and/or toxic. Always wear nitrile gloves when working with the divert/injection valve.*

Warning: *To avoid high-pressure liquid jet spray, wear safety goggles when working with the divert/injection valve.*

The divert/injection valve (Figure 1-5) is at the top-left corner of the instrument front panel (see Figure 1-3). It is an electrically driven Rheodyne® injector, which can be used in several ways, depending on the plumbing arrangement:

- As an injection valve (with the needle port and sample loop fitted).
- As a divert valve (to switch the flow of solvent during an LC run.)
- As a switching valve (for example, to switch between an LC system and a syringe pump containing calibrant).

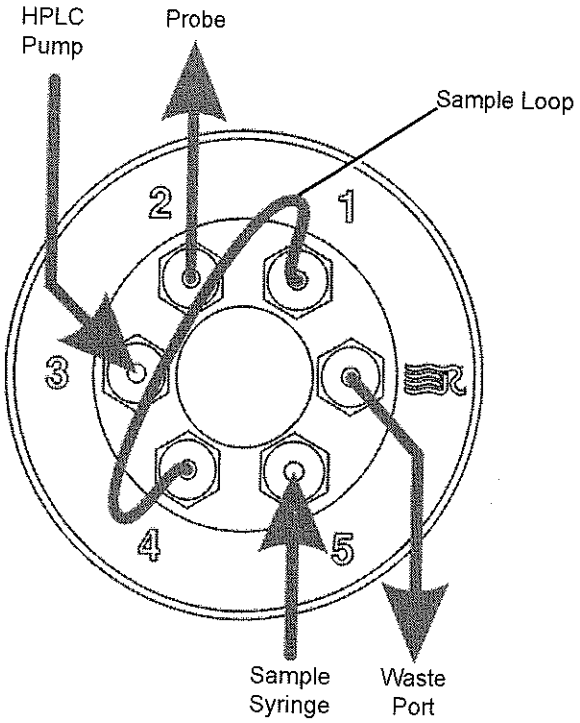

Figure 1-5 Divert/Injection Valve

The valve is controlled by MassLynx. The two switches, Load and Inject, at the top-right corner of the instrument front panel (see Figure 1-4), allow you to control the valve directly when making loop injections at the instrument.

For details of using the valve as a divert valve, see "Setting Solvent Delays" on page 74.

1.6 Rear Panel Connections

The rear panel connections are shown in Figure 1-6.

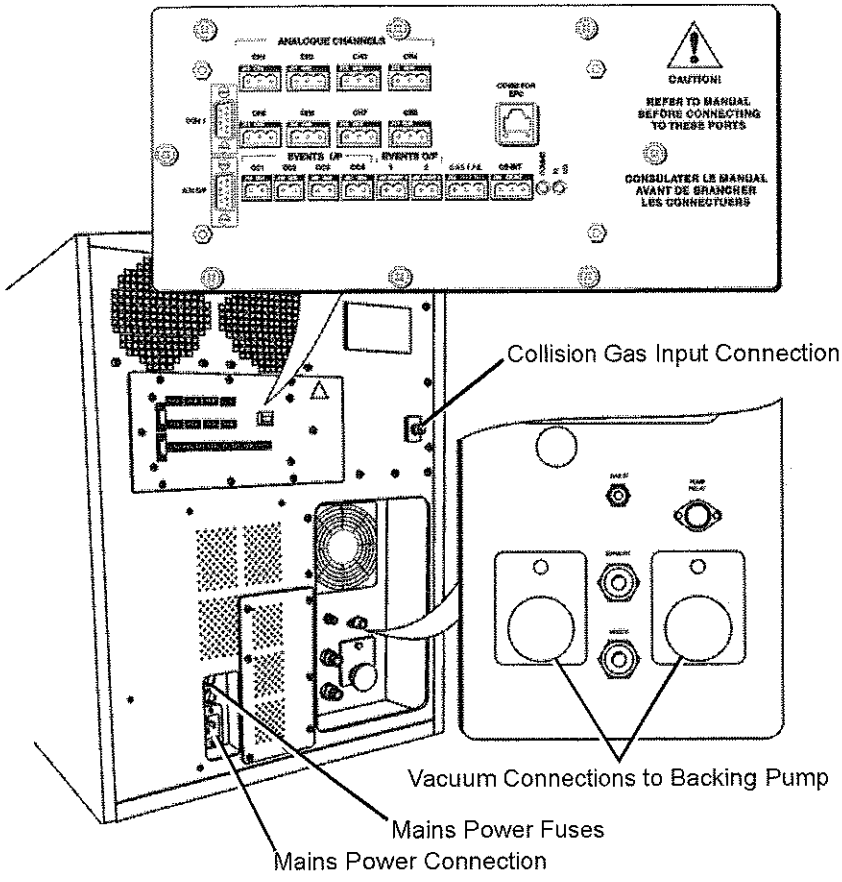

Figure 1-6 Rear Panel Connections

1.6.1 Analog Channels

Warning: *To avoid electric shock and damage to the instrument, do not apply more than 16 V to any of the Analogue Channels connections.*

Eight Analogue Channels inputs (CH1 to CH8) are available for acquiring simultaneous data such as a UV detector output (see "Acquiring Analog Data" on page 75 for further details).

Note: *Although eight inputs are available, the MassLynx software can only control four of the channels.*

Signals up to 2.5 V may be input. Analog data is processed by a 20-bit analog-to-digital converter. The maximum (overload) input is ±16 V.

If the input cable is a two-wire assembly, the negative pole of each channel may need to be grounded (earthed).

1.6.2 Contact Closure

Warning: *To avoid electric shock and damage to the instrument, do not apply more than 5 V to any of the Events I/P connections.*

Warning: *To avoid electric shock and damage to the instrument, do not apply more than 25 V to either of the Events O/P connections.*

Two types of contact closure are available:

- **In** – Four inputs, Events I/P CC1 to CC4, allow external devices to start acquisition. Each event input signal can be transistor-transistor logic or contact closure. The maximum voltage is 5 V.
- **Out** – Two outputs, Events O/P 1 and 2, allow the mass spectrometer to trigger an external event. The maximum rating is 25 V, 0.5 A.

1.6.3 Gas Fail

Warning: *To avoid electric shock and damage to the instrument, do not apply more than 25 V to the Gas Fail connection.*

If the nitrogen supply pressure falls below 4 bar (58 psi), or the instrument's power supply fails, a contact closure signal is generated. This signal can be used to stop solvent flowing into the source by connecting this Gas Fail connection to the Stop Flow of the HPLC system. If the nitrogen supply fails, any solvent from the LC will be automatically drained from the source enclosure. The maximum rating is 25 V, 0.5 A.

1.6.4 CE Int (Capillary Electrophoresis Interlock)

Warning: *To avoid electric shock and damage to the instrument, do not apply more than 25 V to the CE Int connection.*

This connector interfaces with a capillary electrophoresis power supply so that the instrument is safely interlocked against high voltages. The maximum rating is 25 V, 0.5 A.

1.6.5 Comm For EPC

This RJ45 connector links the instrument's embedded PC to the MassLynx PC using the network cable supplied.

1.6.6 Com1

This connection can be used by a Waters field service engineer to communicate with the embedded PC.

1.6.7 Aux O/P

Caution: *The Aux O/P connection must not be used, unless permitted by Waters.*

This connection is used for connecting to auxiliary equipment.

1.6.8 Pump Relay

This connects to a backing pump interlock box, which allows the instrument to remotely control the backing pump (Figure 1-7).

Note: *If the optional scroll pump is used, it may be supplied with a backing pump interlock box, or, alternatively, it may be supplied with a cable that directly connects the Quattro Premier XE to the scroll pump (Figure 1-8); this allows the Quattro Premier XE to control the scroll pump directly.*

The scroll pump's on/off switch must be set to "on" if it is connected to a backing pump interlock box.

The scroll pump's on/off switch must be set to "off" if it is directly connected to, and controlled by, the Quattro Premier XE.

Warning: *The backing pump is independently powered; hence, the pump interlock box can contain power even when the Quattro Premier XE is isolated from the mains power supply. To isolate the pump interlock box and backing pump, switch off the mains power to the pump interlock box.*

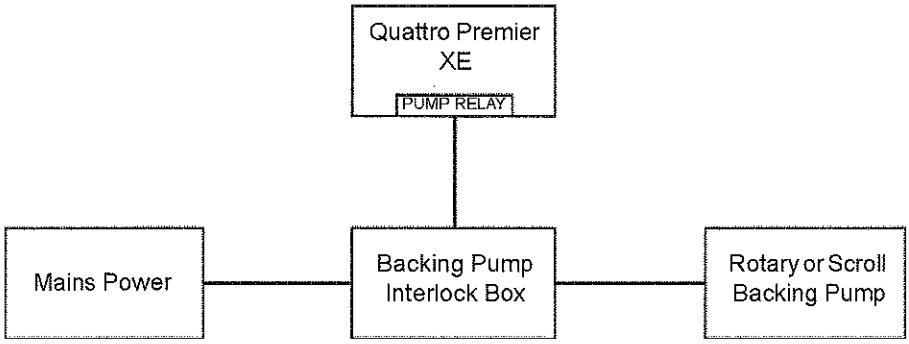

Figure 1-7 Rotary or Scroll Backing Pump Controlled Via a Backing Pump Interlock Box

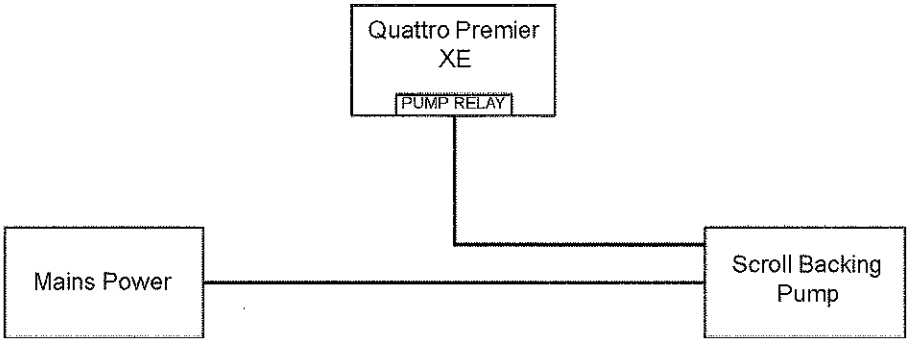

Figure 1-8 Scroll Backing Pump Controlled Directly by the Quattro Premier XE

1.6.9 GAS IN

Caution: *If the nitrogen supply pressure falls below 4 bar (58 psi), the instrument stops the nitrogen flow and admits air into the source. If flammable solvents are used, an ignition hazard exists under these conditions.*

The nitrogen gas supply is connected to this connection. The nitrogen must be dry and oil-free, with a purity of at least 95%. Regulate the supply at 6 to 7 bar (90 to 105 psi).

1.6.10 Collision Gas In

The collision gas supply is connected to this connection. The collision gas is argon; it must be dry and of high purity (99.9%). Regulate the supply at 0.5 bar (7 psi).

1.6.11 Exhaust

Warning: *LC solvents and analytes may be carried in the nitrogen exhaust, which must be vented via the nitrogen exhaust waste bottle and laboratory exhaust system, which must provide a minimum vacuum of 2 millibar below atmospheric pressure (negative pressure).*

Warning: *To avoid the build-up of hazardous gases, do not place the nitrogen exhaust waste bottle in an enclosed cabinet.*

This is the nitrogen gas exhaust connection, which is connected to a nitrogen exhaust waste bottle (see Figure 1-9), which, in turn, is connected to the laboratory exhaust system. The nitrogen exhaust waste bottle must be located in an area where it is visible, so that you can monitor and empty it, and then perform a leak test on it, at regular intervals, as described in Section 7.4.

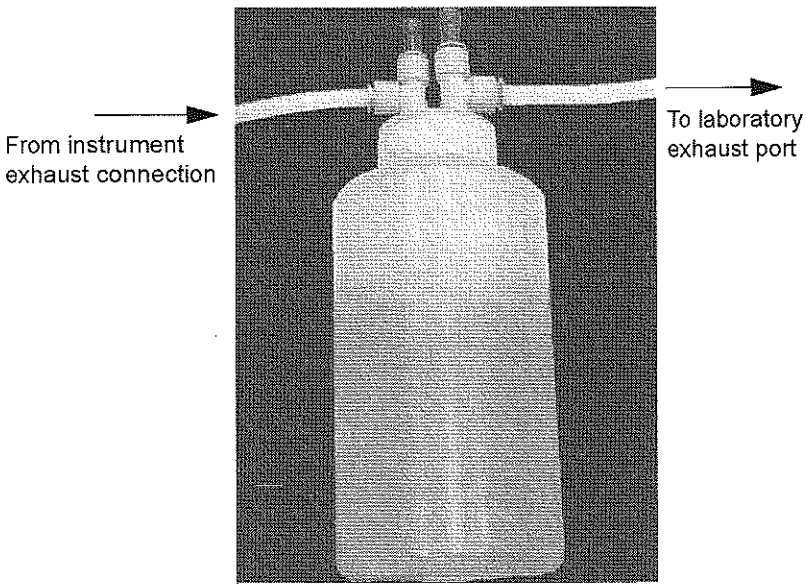

Figure 1-9 Nitrogen Exhaust Waste Bottle

1.6.12 Waste

Warning: *The waste liquid from the source enclosure and the divert/injection valve comprises LC solvents and analytes. Always wear nitrile gloves while handling the drain bottle, and ensure that the waste liquid is correctly disposed of according to local environmental regulations.*

Waste liquid from the top of the instrument, the source enclosure, and the divert/injection valve is drained from the instrument via this connection. The liquid passes into a drain bottle. This must be located in an area where it is visible, so that you can monitor and empty it at regular intervals.

1.6.13 Mains Power Connection

This is the mains power connection for the instrument.

1.6.14 Mains Power Fuses

Warning: *Parts of the instrument may be electrically live even when a mains fuse has failed. To avoid electrical shock, isolate the instrument from the mains supply before replacing the mains fuses.*

Two mains power fuses are located adjacent to the mains power connection. The fuses are rated at T10 AH 250 V.

If a one fuse fails, replace both fuses.

1.6.15 Vacuum Connections

Two vacuum connections are provided for connection to the backing pump.

1.7 Top Panel

Caution: *To avoid accidental spillage damaging the instrument, the instrument's top panel must not be used for storing large volume solvent reservoirs.*

The instrument's top panel may be used for storing small items, for example, small solvent bottles.

1.8 Mass Flow Controllers

The cone gas, desolvation gas, and collision gas flow rates are regulated by electronic mass flow controllers, which are controlled from the MassLynx Tune window. Table 1-3 shows the flow rate ranges for these gasses.

If the nitrogen supply fails, solvent is prevented from accumulating in the source enclosure as described in Section 1.6.3.

Table 1-3 Gas Flow Rate Ranges

Gas	Flow Rate Range
Cone (nitrogen)	0 to 300 L/h
Desolvation (nitrogen)	0 to 1200 L/h
Collision (argon)	0 to 1 mL/min