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HIGH PERFORMANCE LIQUID CHROMATOGRAPH MASS SPECTROMETER

LCMS-8030
LCMS-8040

INSTRUCTION MANUAL

Read the instruction manual thoroughly before you use the product.
Keep this instruction manual for future reference.

SHIMADZU CORPORATION
KYOTO JAPAN

ANALYTICAL & MEASURING INSTRUMENTS DIVISION

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Introduction

Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing this product. This manual describes the installation, operation, usage cautions, accessories and options for this product. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Also, keep this manual for future reference.

■IMPORTANT

- If the user or usage location changes, ensure that this Instruction Manual is always kept together with the product.
- If this manual or a product warning label is lost or damaged, immediately contact your Shimadzu representative to request a replacement.
- To ensure safe operation, read all Safety Instructions before using the product.
- To ensure safe operation, contact your Shimadzu representative if product installation, adjustment, re-installation (after the product is moved) or repairment is required.

■NOTICE

- All rights are reserved, including those to reproduce this manual or parts thereof in any form without permission in writing from Shimadzu Corporation.
- Information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.
- Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.
- Note that Shimadzu will not be responsible for any damage resulting from operation of the product in accordance with this Instruction Manual.
- Note that Shimadzu will not be responsible for the results of operating the product.
- The contents of the hard disk of the personal computer (computer or PC) may be lost as the result of an unforeseen accident. Always create a backup to protect critical data from such accidents.
- Microsoft and Windows7, and Windows Vista are registered trademarks of Microsoft Corporation in the United States and/or other countries. Other company names and product names mentioned in this manual are trademarks or registered trademarks of their respective companies.
  The TM and ® symbols are omitted in this manual.
- Replacement parts for this product will be available for a period of seven (7) years after the product is discontinued. Thereafter, such parts may cease to be available.
  Note, however, that the availability of parts not manufactured by Shimadzu shall be determined by the relevant manufacturers.

Original version is approved in English.

Notes Regarding this Instruction Manual

■Indications Used in This Manual

Warnings, Cautions, and Notes are indicated using the following conventions:

Description	Meaning
WARNING	Indicates a potentially hazardous situation which, if not avoided, could result in serious injury or possibly death.
CAUTION	Indicates a potentially hazardous situation which, if not avoided, may result in minor to moderate injury or equipment damage.
NOTE	Emphasizes additional information that is provided to ensure the proper use of this product.

The following symbols are used in this manual:

Symbol	Meaning
Prohibitions	Indicates an action that must not be performed.
Instructions	Indicates an action that must be performed.
Hint	Indicates information provided to improve product performance.
Reference	Indicates the location of related reference information.
[ ]	Indicates buttons, menu items, settings, screens and windows, icon names, and other text displayed on-screen. Example: Click [OK].

Safety Instructions

To ensure safe product operation, read these important safety instructions carefully before use and follow all WARNING and CAUTION instructions given in this section.

Observe all of the WARNINGS and CAUTIONS described in this section. They are extremely important for safety.

■Product Applications

⚠ WARNING

Instructions

Use the product ONLY for the intended purpose.

This product is a high performance liquid chromatograph mass spectrometer. Using the product for any other purpose could cause accidents.

■Installation Site

⚠ WARNING

Prohibitions

Do NOT use naked flames.

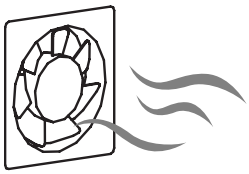
The use of naked flames is prohibited at the site where the high performance liquid chromatograph mass spectrometer is installed. You should also avoid installing other equipment that produces a naked flame in the same room. To ensure readiness in the event of an accident, install a fire extinguisher.

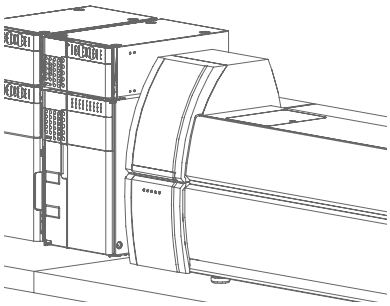
⚠ WARNING

Instructions

- Be sure to provide ventilation in the room.

  Some of the solvents that are used with a high performance liquid chromatograph mass spectrometer are inflammable or toxic. Also note that this instrument contains a large quantity of nitrogen gas. Its use in a room that is inadequately ventilated could cause oxygen deficiency.
  Install the instrument in a room that has a ventilation mechanism such as the type of draft chamber in general use (approx. 20 m^3/min), and feed the exhaust tube into the draft chamber.





- Install water supply equipment, such as a wash basin.

  If a solvent gets into someone's eyes or someone touches a toxic solvent, it has to be rinsed away immediately.
  Install water supply equipment, such as a wash basin, as close to the product as possible.

⚠ CAUTION

Prohibitions

Do NOT install the instrument close to any device that generates a strong magnetic field.

To ensure that the instrument can be operated normally, do not install it at a location where there is a strong magnetic field.
In addition, if there is a lot of noise in the power line add a noise filter.

⚠ CAUTION

Instructions

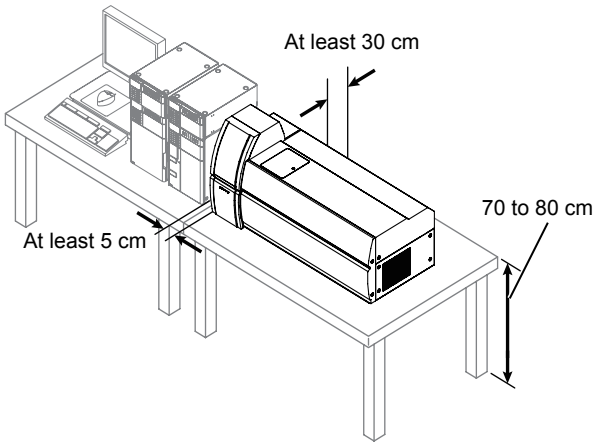
- Install the product on a desk or table that meets the following requirements.
  - Flat and stable

    Able to comfortably bear the weight of this product (approx. 130 kg) and the entire computer system

    Greater in depth than the product

    Failing to meet these requirements can cause accidents in which the table collapses or units fall off.
  - Allowing the instrument to be placed a sufficient distance from walls

    Make the distance between the rear face of the instrument and the wall at least 30 cm and the distance between the left and right faces and other units at least 5 cm. If these conditions are not met it will not be possible for the fans to provide adequate air cooling and there will be a risk that the instrument will overheat and its performance will drop.



  - Having an appropriate height

    Use a table with a height of about 70 to 80 cm. Using a table with a height outside this range will impair the operating convenience of the instrument, so care is required.
- Install the rotary pump on a stable floor.

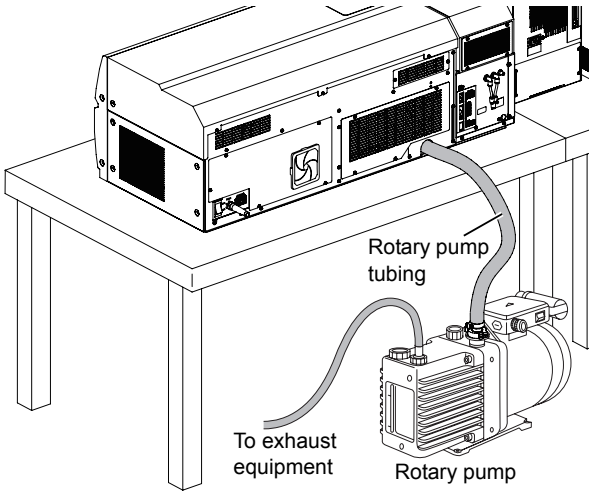
  Make the distance between the body of the instrument and the rotary pump a distance over which the tubing provided as an accessory can be connected. If the tubing is extended the intended performance of the machine cannot be guaranteed.

⚠ CAUTION

Instructions

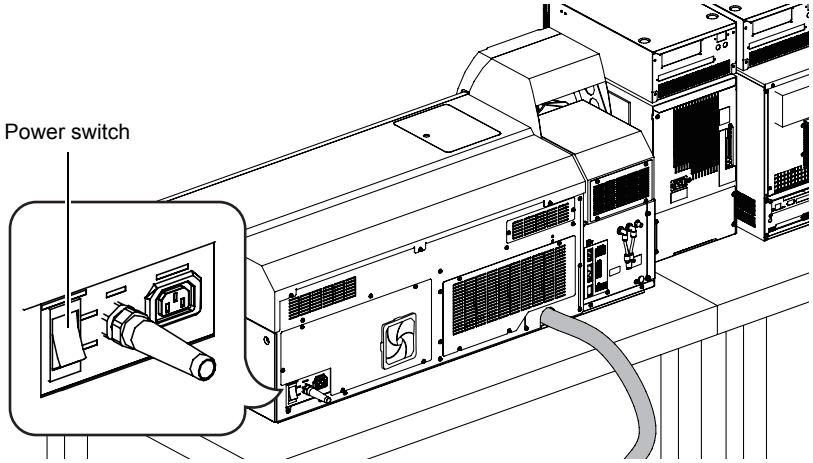
- Use a duct system for exhaust.

  Be sure to release the exhaust gas from the rotary pump, the solvent vapor that builds up in the waste container, and nitrogen gas into a duct system such as a draft chamber. Be sure to provide separate exhaust channels for the exhaust from the rotary pump and the nitrogen for ionization.
  Failure to do so will lead to contamination of the mass spectrometer.



- Install the instrument so that the power switch can be operated easily.

  If the power switch is difficult to operate, it will not be possible to switch the power off immediately in an emergency.



- Observe the installation conditions.
  - A room with a temperature within the range 18 to 28 °C and where the change in room temperature throughout the day is small
  - A location where the instrument is not directly exposed to the airflow from a heater/ air conditioner
  - A location not exposed to direct sunlight
  - A location where there is little vibration
  - A location where the humidity remains within the range 40 to 70 %
  - A location free from corrosive gas, contaminants and dust

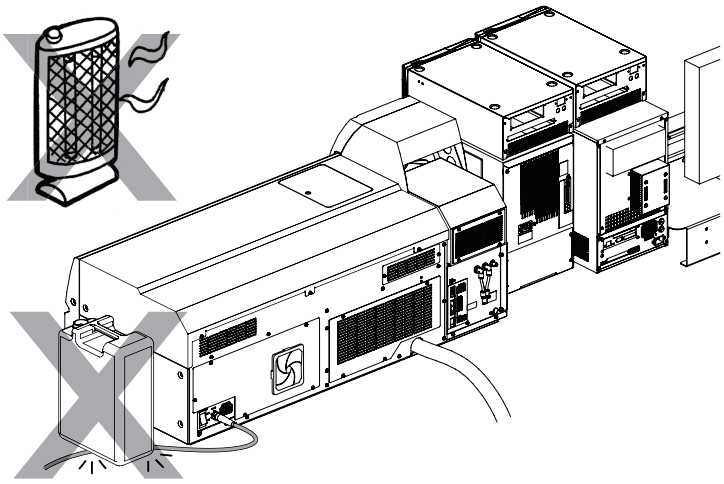
■Installation

To ensure safe operation, contact your Shimadzu representative if product installation, adjustment, or re-installation (after the product is moved) is required.

⚠ WARNING

Prohibitions

- Do NOT share the power supply to this product with any other equipment.
- The electric capacity of the instrument must not exceed the stipulated capacity of the earth leakage breaker.
- Do NOT rest anything heavy on the power cable.
  Do NOT run the power cable close to any heat-generating equipment.
  Such treatment could damage the cable, leading to fire, electric shock or instrument failure.
  If the cable becomes damaged, contact your Shimadzu representative immediately.



WARNING

Instructions

- Contact us or your Shimadzu service representative regarding installation, adjustment, or re-installation inquiries.

  Carrying out such work on your own may result in personal injury or damage to the product. Correct installation, adjustment, and re-installation are important to ensure stable operation of the instrument.

- Adopt measures to prevent the product falling in the event of an earthquake.

  The product may fall or drop due to vibration, and this may cause personal injury.

- Connect the instrument to a compatible power supply.

  This product has a power supply voltage of 230 V AC at 15 A and a power consumption of 3.45 kVA.
  Connect to a compatible power supply. A supply that is not compatible will cause fire or electric shocks.
  If the power supply voltage is unstable or the power supply capacity is insufficient, the intended performance of the instrument cannot be guaranteed.
  You must check the power supply capacity of the system as a whole and prepare an appropriate supply.

- The power supply that you connect to must be equipped with an earth leakage breaker.

- The instrument must be grounded (earthed).

  If you do not ground it, there will be a risk of instrument failure and electric shock in the event of current leaks. It is also essential to ground the instrument in order to stabilize it. (See "Power supply" in "8.1.1 Conditions for the Installation Site".)

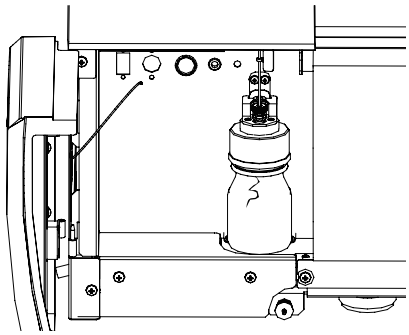
■Operation

⚠ CAUTION

Prohibitions

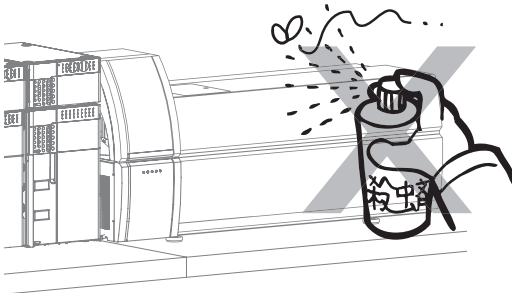
- Do NOT use the standard sample bottle if it is cracked.

  Doing so could ignite and cause a fire.
  Never use cracked standard sample bottles.
  When pressure is exerted on the bottle, it may break and cause injury.



- Do NOT use flammable sprays.

  Do NOT use flammable sprays (hair sprays, insecticide sprays, etc.) near the instrument.
  They could ignite and cause a fire.



- Do NOT use flammable solvents near the computer or printer.

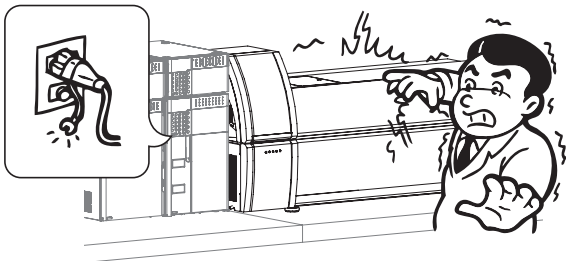
  Doing so could cause ignition and fire.

Instructions

- Provide electrostatic protection.

  Take thorough measures to prevent buildup of static electricity. Static electricity could result in fire or explosion.

Reference
"Static Electricity Precautions" P.xiii



- Wear protective goggles and protective gloves.

  Always wear protective gloves and protective goggles when handling solvents and samples. If solvent gets into the eyes, blindness could result. Should solvent get into the eyes, flush immediately with large amounts of water and get medical attention.
  Always wear protective gloves when handling any toxic or biologically infectious samples.

- Backup data periodically.

  The contents of the PC's hard disk may be lost as the result of an unforeseen accident. Always create a backup to protect critical data from such accidents.

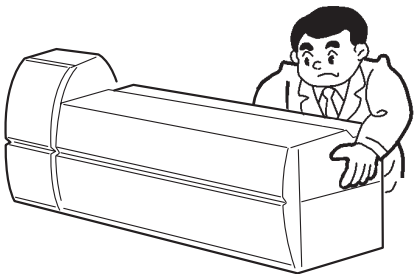
■Inspection and Maintenance

⚠ WARNING

Prohibitions

- Never remove the cover from the instrument.

  Doing so may cause personal injury or damage to the spectrometer.
  The cover does not need to be removed for routine maintenance or inspection. Repairs inside the product must be performed by Shimadzu service personnel. Contact your Shimadzu representative.



- Do NOT overhaul or modify the product without permission.

  This may cause injury or damage the instrument.

- Do NOT leave the instrument in wet condition nor use alcohol or thinner solvents for cleaning the instrument.

  Doing so could cause rust formation or discoloration.
  To clean the instrument, wipe it with a soft cloth moistened with a small amount of water or neutral detergent, and then wipe it with a soft dry cloth.

- Do NOT dispose of waste liquids illegally.

  Dispose of the waste liquid properly in accordance with the regulations and instructions issued by your administrative department.

Instructions

- Turn the instrument's power switch OFF before inspection, maintenance or part replacement.

  Otherwise, electric shock or short-circuit accidents could occur.

- Use the specified parts only.

  Replacement parts must be of the specifications given in "Component Parts" or "Maintenance Parts". Use of any other parts may result in malfunction in the instrument.

■Hazards Involved in Repair, Disassembly, or Modification

⚠ WARNING

Prohibitions

Do NOT disassemble or modify the product without permission.

Otherwise, you may receive an electric shock or a short circuit may occur. Personal injury or product damage can also result.

Instructions

Contact us or your Shimadzu service representative for repair inquiries.

Unauthorized repairs may cause a fire, electric shock, or injury.

■In the Event of an Emergency (Power Outage)

Take the following action in the event of an emergency (power outage), such as when a problem is found with the high performance liquid chromatograph mass spectrometer.

Perform a full inspection before using the product again, and if necessary, contact your Shimadzu representative.

Emergency stop procedure

1. Turn OFF the power switches at the mass spectrometer LCMS-8030/LCMS-8040 as well as the high performance liquid chromatograph units.
2. Turn OFF all the power switches at the peripheral equipment.
3. Close the main cock of the gas tubing.
4. Shut the power supply off.
    - If the power cable is fastened to the distribution board, turn OFF the switch at the distribution board.
    - If the power cable is connected with a plug, unplug the power cable.

NOTE

It is possible to make settings for automatic resetting when the power is restored.

Reference

"6.4 Power Outages" P.116

Static Electricity Precautions

A liquid chromatograph (LC) uses flammable organic solvent(s) as the mobile phase. LC systems are also often used where large amount of flammable substances are present. Thus, an accident can produce large scale damage. Operators must be constantly on guard against accidents involving fire or explosion.

The major cause of these accidents is static electricity. Devising preventative measures for static can be difficult, because the symptoms before an accident vary and can be hard to detect, since such accidents occur as a result of several simultaneous coincidences.

Recommended methods for preventing static electricity accidents are provided below. Take thorough safety measures based on this information.

■Typical Cause of Static Electricity Accidents

Static electricity accidents are generally caused by this sequence of events:

Generation of static electricity

↓

Accumulation of static electricity

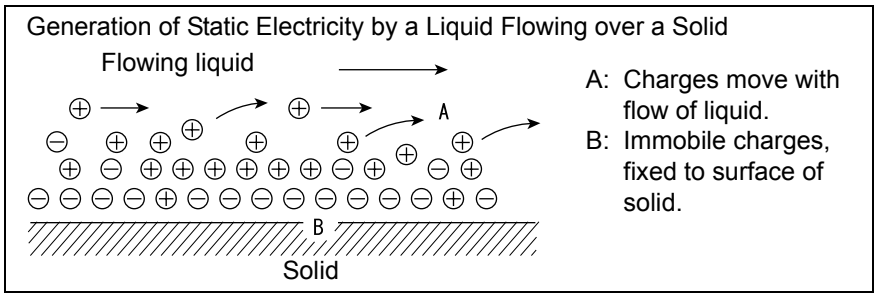
↓

Release of energy through

↓

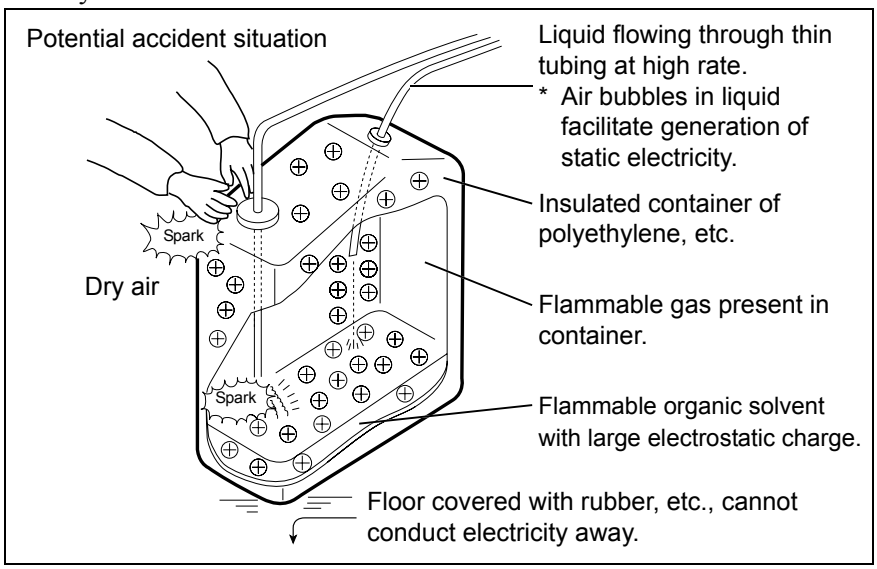
Ignition of flammable substances

When liquid is passed through thin tubing at high flow rates, as in a liquid chromatograph, the electrostatic charges of the flowing matter generate static electricity as shown below.



If electrostatically charged liquid is allowed to accumulate in an electrically insulated container, the charge will gradually increase, and can eventually reach several thousand volts.

If this happens and an electrical conductor is brought within a certain distance of the container, electrical discharge will occur, releasing thermal energy which will ignite any flammable gas of sufficient density in the vicinity.



■Preventing Static Electricity Accidents

The best way to prevent static electricity accidents is simply to prevent the occurrence and accumulation of electrostatic charges.

⚠ CAUTION

Instructions

It is important to take multiple preventive measures simultaneously.

If large amounts of flammable solvents are collected in a large container, implement preventive measures 1 - 5 below.

Preventive Measure 1

Use a conductive metal container for the waste liquid, and ground the container.
This will ensure that the electrical charges of the container and liquid pass to the ground.

<Optional accessories for this measure>

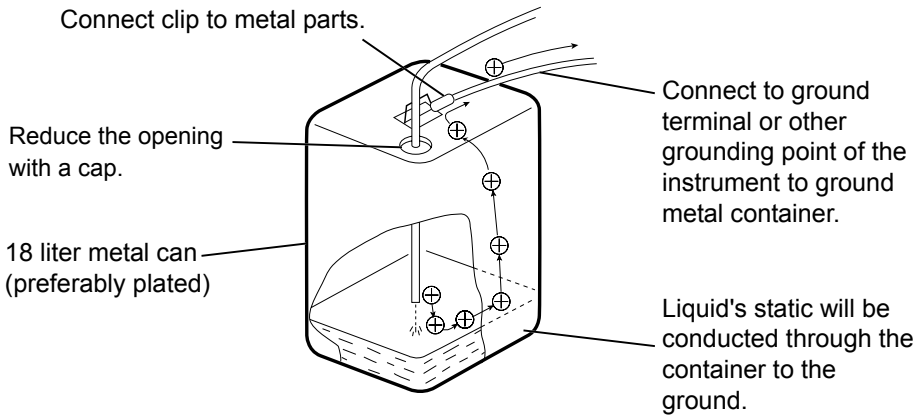
(1) Grounding wire with clip Part No.: S228-21353-91
(2) 18 liter metal container Part No.: S038-00044
(3) 4 liter metal container Part No.: S038-00043-01

⚠ CAUTION

Instructions

- Be sure to ground the metal waste container properly.
  If the grounding wire is not properly attached or connected to the ground, static electricity can build up in the container.
- Be sure to use a tester to verify that electricity is conducted to the ground.
  Some metal containers have surfaces that are laminated or oxidized, and therefore do not conduct electricity.
- If the liquid to be drained into the waste container is virtually non-conductive (10^{-10} S/m or less), it will be necessary to add properly conductive, and therefore safe, liquid to the tank.
  This conductive liquid may be added to the waste container beforehand.

Preventive Measures for Static Electricity



Preventive Measure 2

Restrict the openings at the waste container with caps or other protective covering to prevent sparks generated outside the container from getting inside.

<Optional accessories for this measure>
Caps for 18 liter or 4 liter containers
(with three 3 mm diameter openings) Part No.: S228-21354-91

Preventive Measure 3

Keep electrostatically charged objects, including the human body, away from the waste container. To prevent electrostatic charging of the human body, take the following precautions:

- Wear anti-static clothing and shoes.
- Ground the human body with anti-static wrist straps. (For safety, the wrist strap should be connected to the ground using an intervening resistor of about 1 MΩ.)
- Spread anti-static matting or the like on the floor, to make the floor conductive.

⚠ CAUTION

Instructions

Provide antistatic measures.

Persons who have not taken anti-static precautions should touch some grounded metal object before coming near the waste container, in order to drain static charges.

Preventive Measure 4

Use tubing with an inner diameter of at least 2 mm for drain lines with high flow rates.

⚠ CAUTION

Instructions

Periodically check the tubing connections for air bubbles.

Air bubbles in liquid can multiply the electrostatic charge by a factor of 20, 30 or more.

Preventive Measure 5

If it is not possible to use a conductive waste container, take the following precautions:

Ensure that the end of the inflow tubing is always submerged inside the container. Also, place some type of grounded metal object, such as a ground wire connected to the instrument, into the liquid.

⚠ CAUTION

Instructions

- The above precaution will be ineffective for low conductivity (less than 10^{-10} S/m) liquids.
- Use as small a container as possible to minimize damage in the event of fire.
- Keep the room at a proper humidity.
  Ambient humidity exceeding 65 % will prevent static electricity.

- Reference

  Anti-static equipment (anti-static clothing, shoes and matting) and charge measurement equipment (electrometer) are sold by specialty manufacturers.

Precautions for Mobile Phase Selection and Use

⚠ CAUTION

Prohibitions

If PEEK resin parts are used in the plumbing, do NOT use the following mobile phases.

These mobile phases weaken the PEEK resin, which could result in cracked plumbing and mobile phase leaks.

Concentrated sulfuric acid, concentrated nitric acid, dichloroacetic acid, acetone, tetrahydrofuran (THF), dichloromethane, chloroform, dimethyl sulfoxide (DMSO).

Note: Briefly using a weak solution of less than 0.5 % acetone in water (e.g. in order to check gradient performance) will present no problems.

Instructions

- When performing APCI analysis in which a halogenated mobile phase additive is used, note the following:

  In the APCI method, the analyte is heated to high temperatures. If the mobile phase contains a halogenated compound such as chloroform, a corrosive gas will be produced. Even a small percentage concentration of halogens in the mobile phase can cause corrosion.

  Use SUS tubes to connect the high performance liquid chromatograph to the instrument. PEEK resin tubes do not have sufficient strength and should they rupture, solvent may blow out.

  Black particles may build up on the APCI probe or inside the probe holder.
  Because of exposure to corrosive gases, you may need to replace parts at a shorter interval than specified.

- Plastic connections are used regardless of the tubing material.

  Do NOT use a mobile phase that contains hexafluoroisopropanol (HFIP) because it may weaken or break the plastic joints resulting in splashing of the solvent.

NOTE

- Select an HPLC compliant or HPLC compatible mobile phase and remove any fine particles and contaminants from the filter (part No.: S228-45707-91) before use.
- Whenever possible, avoid using mobile phases that contain halogen ions, such as KCI, NaCl and NH_4CI, or that generate halogen ions in certain reactions. Halogen ions can corrode the stainless steel material (SUS316L) used in plumbing. If such mobile phases must be used, clean all flow lines thoroughly with distilled water immediately after analysis.
- A less volatile buffer solution (such as phosphate buffer solution) will cause precipitation at the interface area, which will decrease sensitivity. Avoid less volatile buffer solutions.
- Always degas the mobile phase, as air bubbles may tend to form during solvent mixing or during temperature or pressure changes. Air bubbles may cause pump malfunctions and detector signal noise.
- For information on the characteristics of the mobile phase to be used, such as its boiling point or viscosity, refer to the "Mobile Phase Characteristics" section in the relevant instruction manual of the high performance chromatograph system you are using.

■Warning Labels

For safe operation, warning labels are affixed where special attention is required.

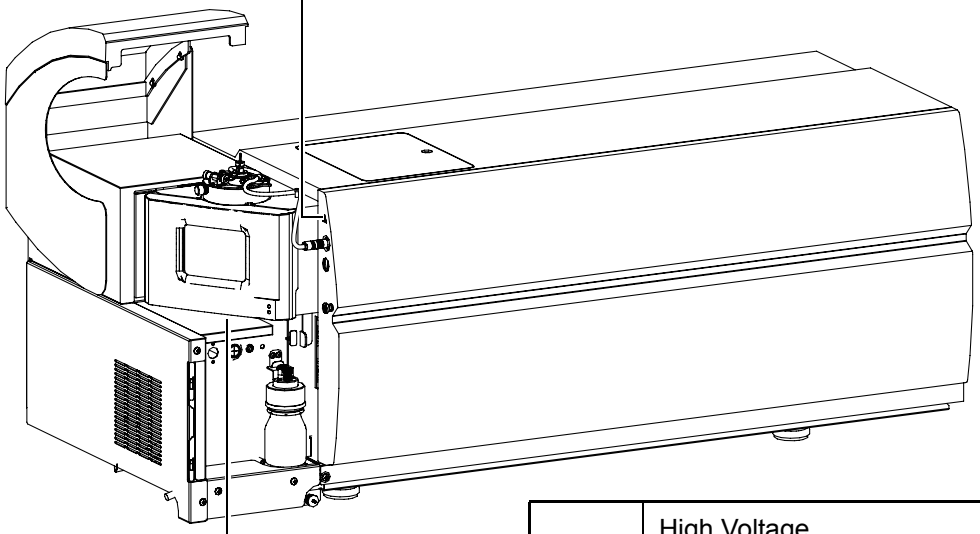
Should any of these labels peel off or be damaged, obtain replacements from your Shimadzu representative.

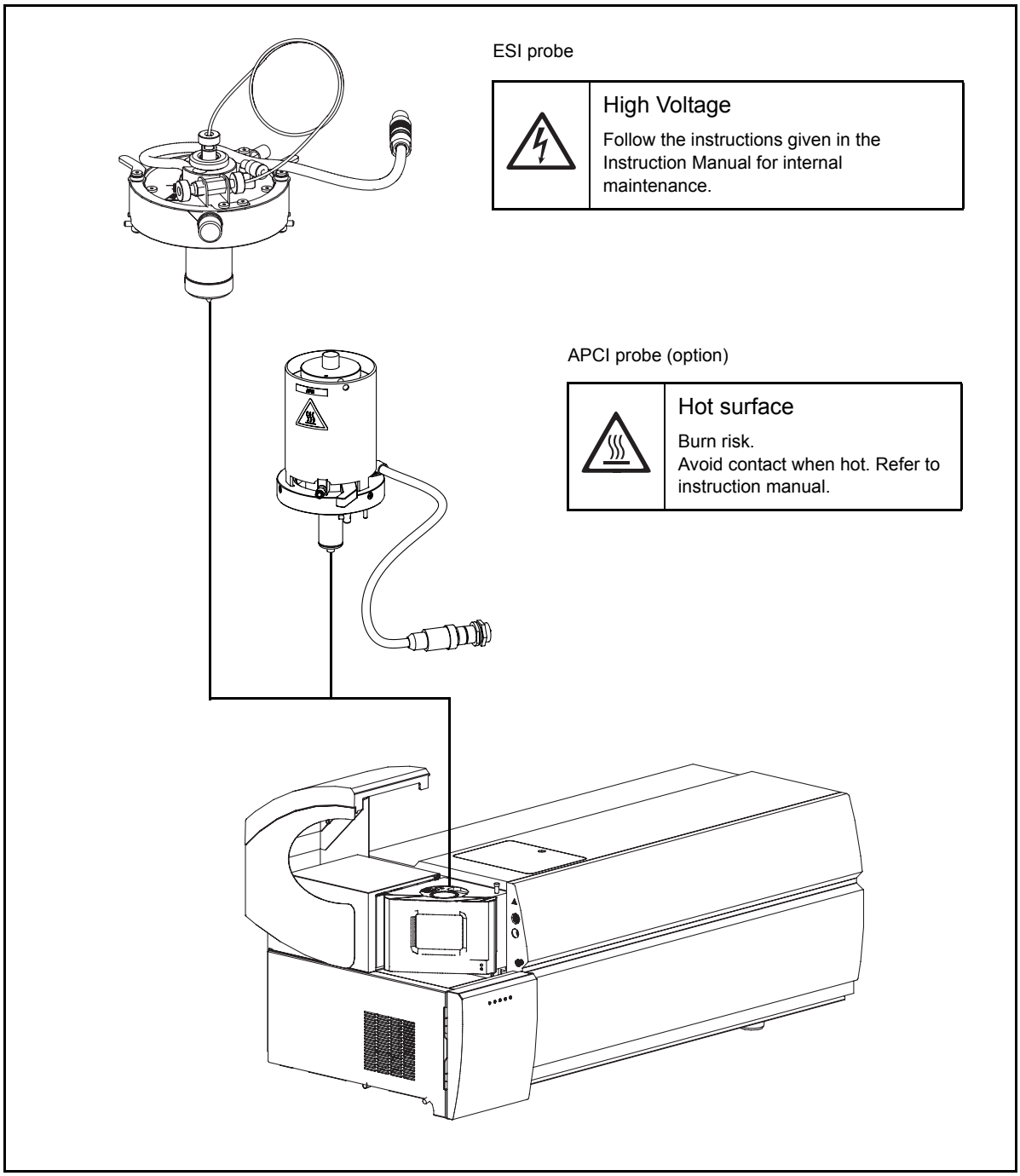
When handling or operating the instrument, thoroughly read the Instruction Manual and follow the instructions given.

Indicates that lethal voltage is present.

Indicates that some parts will reach high temperatures.

Refer to the Instruction Manual when handling or operating any section marked with this symbol.




ESI probe
High Voltage
Follow the instructions given in the Instruction Manual for internal maintenance.
APCI probe (option)
Hot surface
Burn risk.
Avoid contact when hot. Refer to instruction manual.

Warranty

Shimadzu provides the following warranty for this product.

1. Period:

Please contact your Shimadzu representative for information about the period of this warranty.

2. Description:

If a product/part failure occurs for reasons attributable to Shimadzu during the warranty period, Shimadzu will repair or replace the product/part free of charge (including the USB dongle). However, in the case of products which are usually available on the market only for a short time, such as personal computers and their peripherals/parts, Shimadzu may not be able to provide identical replacement products.

3. Limitation of Liability:

1. In no event will Shimadzu be liable for any lost revenue, profit or data, or for special, indirect, consequential, incidental or punitive damages, however caused regardless of the theory of liability, arising out of or related to the use of or inability to use the product, even if Shimadzu has been advised of the possibility of such damage.
2. In no event will Shimadzu's liability to you, whether in contract, tort (including negligence), or otherwise, exceed the amount you paid for the product.

4. Exceptions:

Failures caused by the following are excluded from the warranty, even if they occur during the warranty period.

1. Improper product handling
2. Repairs or modifications performed by parties other than Shimadzu or Shimadzu designated companies
3. Product use in combination with hardware or software other than that designated by Shimadzu
4. Computer viruses leading to device failures and damage to data and software, including the product's basic software
5. Power failures, including power outages and sudden voltage drops, leading to device failures and damage to data and software, including the product's basic software
6. Turning OFF the product without following the proper shutdown procedure leading to device failures and damage to data and software, including the product's basic software
7. Reasons unrelated to the product itself
8. Product use in harsh environments, such as those subject to high temperatures or humidity levels, corrosive gases, or strong vibrations
9. Fires, earthquakes, or any other act of nature, contamination by radioactive or hazardous substances, or any other force majeure event, including wars, riots, and crimes
10. Product movement or transportation after installation
11. Consumable items
    Note: Recording media such as floppy disks and CD-ROMs are considered consumable items.

* If there is a document such as a warranty provided with the product, or there is a separate contract agreed upon that includes warranty conditions, the provisions of those documents shall apply.
* A separate warranty period shall be determined for custom specification parts and system parts.
* Note that a license cannot be reissued in the event that the license key disk or USB dongle supplied with the product is lost.

After-Sales Service and Availability of Replacement Parts

After-Sales Service

If any problem occurs with this product, perform an inspection and take appropriate corrective action as described in the section "6 Troubleshooting".

If the problem persists, or the symptoms are not covered in the troubleshooting section, contact your Shimadzu representative.

Replacement Parts Availability

Replacement parts for this product will be available for a period of seven (7) years after the discontinuation of the product. Thereafter, such parts may cease to be available. Note, however, that the availability of parts not manufactured by Shimadzu shall be determined by the relevant manufacturers.

If Shimadzu receives notice of the discontinuation of units or parts, the necessary quantity for the above period is immediately calculated and secured. However, such units or parts may cease to be available within seven years after the discontinuation of the product, depending on individual manufacturer conditions and on changes in the quantity required.

Maintenance, Inspection, and Servicing

To prolong instrument performance and to obtain the correct measurement data, you need to carry out daily and periodic inspections as well as periodic calibrations.

- For information on daily maintenance and inspection and replacement parts, see Chapter "7 Maintenance" and Chapter "10 Maintenance Parts".
- For periodic inspection or calibration, contact your Shimadzu representative or Shimadzu service representative.
- The replacement frequencies for periodic replacement parts are shown as guidelines.
  Depending on the operating conditions and frequency of use, you may need to replace the parts at a shorter interval than specified.

Electromagnetic Compatibility

Take the following measures before installing and/or using the instrument in industrial locations:

- Install the instrument away from devices that generate strong electromagnetic noise.
- Supply power from an independent power source.
- Take measures to prevent buildup of static electricity.

Regulatory Information

For Europe:
The product complies with the requirements of the Low Voltage Directive 2006/95/EC and EMC Directive 2004/108/EC.

Product Name:	High Performance Liquid Chromatograph Mass Spectrometer
Model Name:	LCMS-8030, LCMS-8040, APCI-8030 Set, DUIS-8030 Set, APCI/DUIS-8030 Common Parts
Manufacturer:	SHIMADZU CORPORATION ANALYTICAL & MEASURING INSTRUMENTS DIVISION
Address:	1, NISHINOKYO-KUWABARACHO, NAKAGYO-KU, KYOTO, 604-8511, JAPAN
Authorized Representative in EU:	SHIMADZU EUROPA GmbH
Address:	Albert-Hahn-Strasse 6-10, 47269 Duisburg, F.R. Germany

Action for Environment (WEEE)

To all users of Shimadzu equipment in the European Union:

WEEE Mark

Equipment marked with this symbol indicates that it was sold on or after 13th August 2005, which means it should not be disposed of with general household waste. Note that our equipment is for industrial/professional use only.

Contact Shimadzu service representative when the equipment has reached the end of its life. They will advise you regarding the equipment take-back.

With your co-operation we are aiming to reduce contamination from waste electronic and electrical equipment and preserve natural resource through re-use and recycling.

Do not hesitate to ask Shimadzu service representative, if you require further information.

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1 Outline and Configuration

1.1 Outline

The Shimadzu LCMS-8030/LCMS-8040 is a quadrupole type tandem mass spectrometer. Shimadzu offers this LC/MS/MS unit as a high speed and high separation solution, which is compatible with Shimadzu's ultra fast LC series, by enhancing the LCMS-2020's high-speed performance and through the development of a high-speed collision cell.

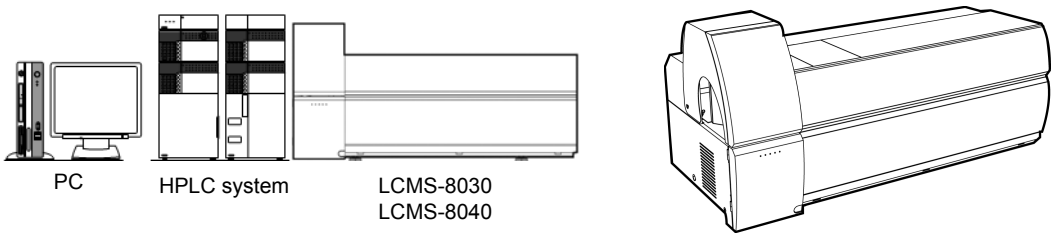


Fig. 1-1

The sample introduced from the liquid chromatograph is ionized by the atmospheric pressure ionization probe (e.g. ESI or APCI probe).

1.2 Features

- **High sensitivity**
  High ion transmission has been achieved by developing a new design for the DL (desolvation line), Qarray, skimmer, multipoles, and entrance lens that make up the ion-optical system. This gives the system even greater sensitivity.
- **High throughput**
  Ultra high speed MRM measurement has been achieved through the development of a high speed collision cell. High speed MRM measurement at 250 ch/sec can be conducted without cross talk or any reduction in signal intensity. In addition, ultra high speed MRM measurement can be conducted at more than 500 ch/sec.
  The scan speed is the same as the Shimadzu LCMS-2020 at 15,000 u/sec.
  The instrument features a high speed polarity switching time of 15 msec and you will never miss sharp peaks when used in combination with Shimadzu's ultra fast LC series.
- **Ruggedness and stability**
  After being sprayed and ionized by the atmospheric pressure ionization probe, the sample passes through the sample introduction unit (DL) oriented at 90°, which efficiently introduces it into the vacuum. Since excess solvent is expelled through the drainage port, the effects of contamination are minimized and stable analysis is possible.
- **Designed for ease of use**
  The LabSolutions software package enables easy control of the liquid chromatograph (LC) and mass spectrometer (MS) units, analysis, data processing, and report creation.

1.3 Mechanism of Analysis

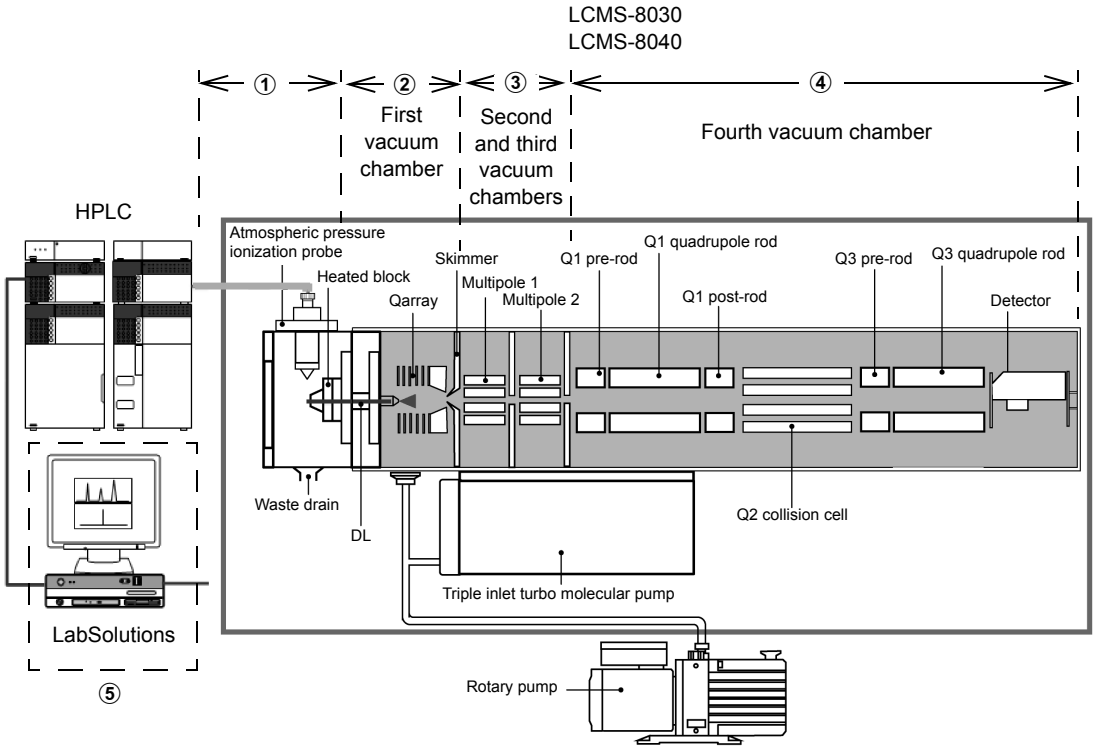
① The sample introduced from the liquid chromatograph is sprayed and ionized under atmospheric pressure by the atmospheric pressure ionization probe (e.g. ESI or APCI probe).

② The ionized sample is introduced through the sample introduction unit (DL), which is oriented at 90° to the spray, into the first stage primary vacuum chamber, where it is efficiently focused at the tip of the skimmer by the Qarray where multi-stage high frequency ion guides are arranged.

③ The rear section of the skimmer passes through the high frequency ion guides (multipoles) arranged in the second and third vacuum chambers.

④ Subsequently, the ions are separated according to their mass-to-charge ratio (m/z) by the quadrupole mass filter with pre-rod and the collision cell and are detected by the detector.

⑤ The detected ion signals are first amplified by the amplifier and then processed by the LabSolutions data processing software.



Configuration of the LCMS-8030/LCMS-8040 Unit

Fig. 1-2

1.4 Component Parts

This product is composed of the following parts. When unpacking the product, check the details and quantity of each item.

Packed parts

Part Name	Part No.	Q'ty	Remarks
LCMS-8030/LCMS-8040 body • LCMS-8030/LCMS-8040 • Packed parts (1) • Packed parts (2) • Packed parts (3)	-	1	230 V AC, 50/60 Hz
Rotary pump E2M28	S225-09309-02	1	230 V AC, 50/60 Hz

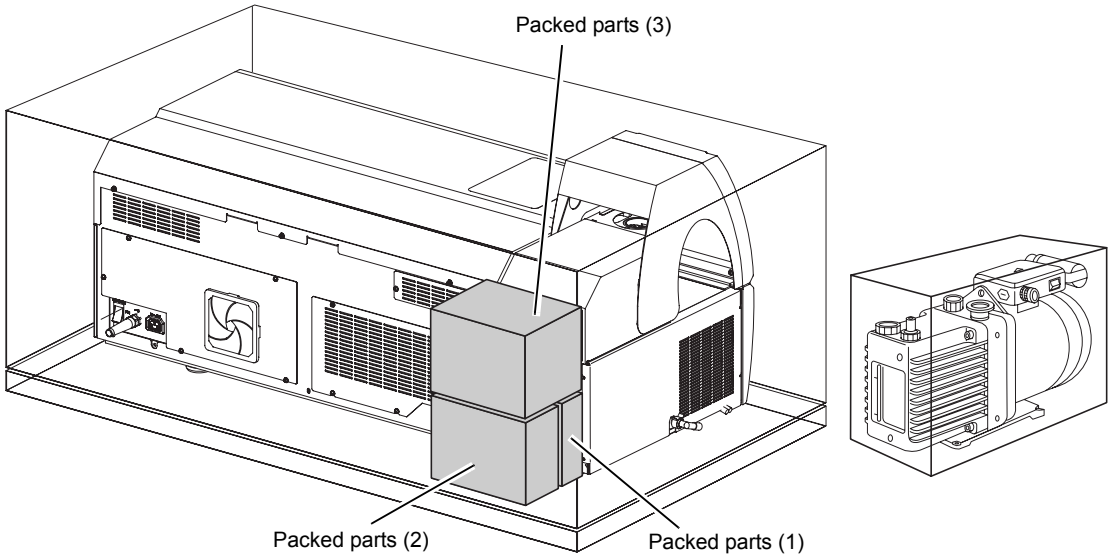


Fig. 1-3

1.4.1 Packed Parts (1)

Part Name	Part No.	Q'ty	Remarks
Accessory kit	-	1	Tools

Accessory kit details

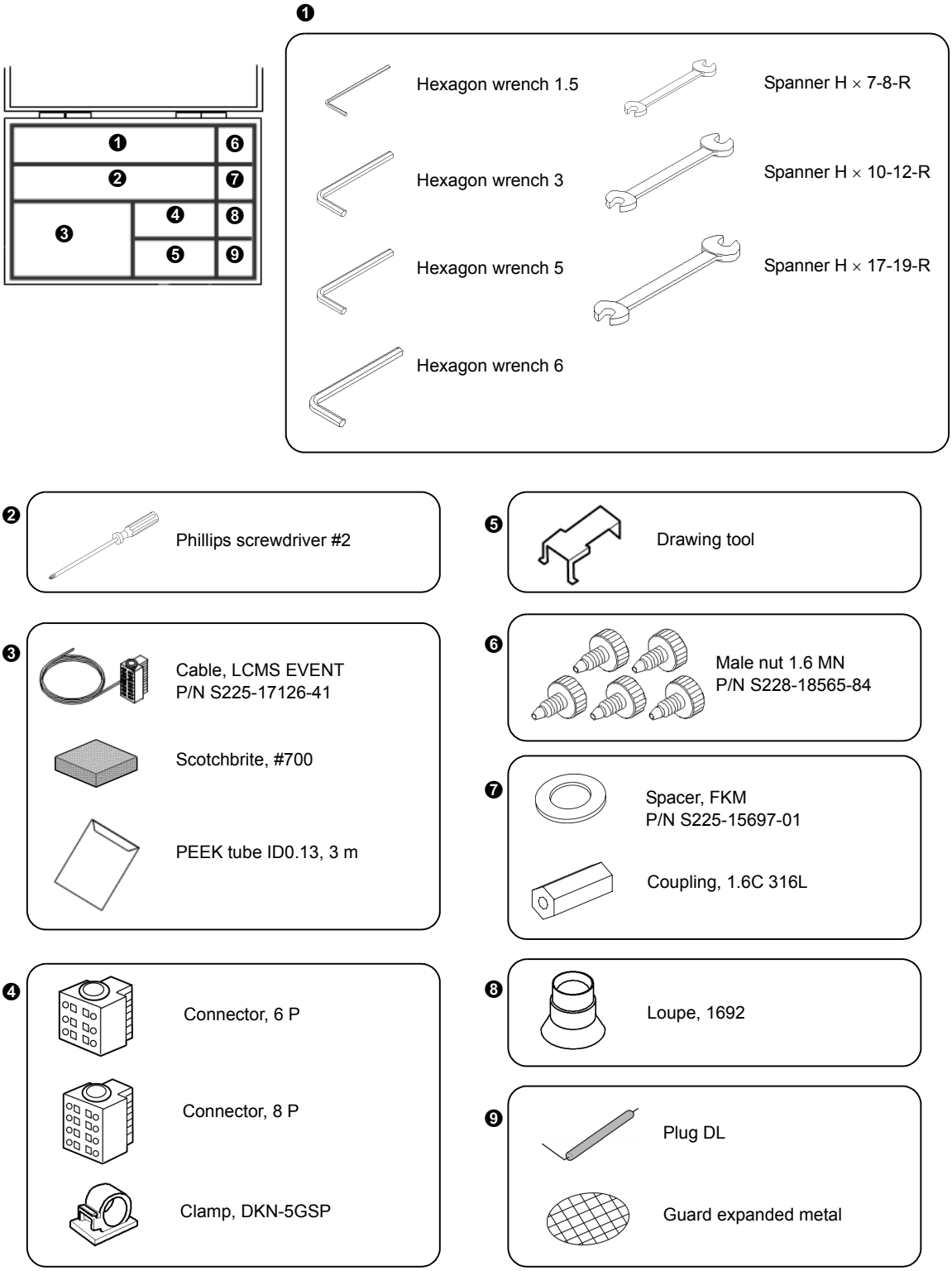


Fig. 1-4

1.4.2 Packed Parts (2)

No.	Part Name	Part No.	Q'ty	Remarks
1	Standard sample bottle ASSY	-	1	Includes capillary tubing
2	ESI probe ASSY	S225-14949-41	1	
3	Stand	-	1	ESI probe, stand

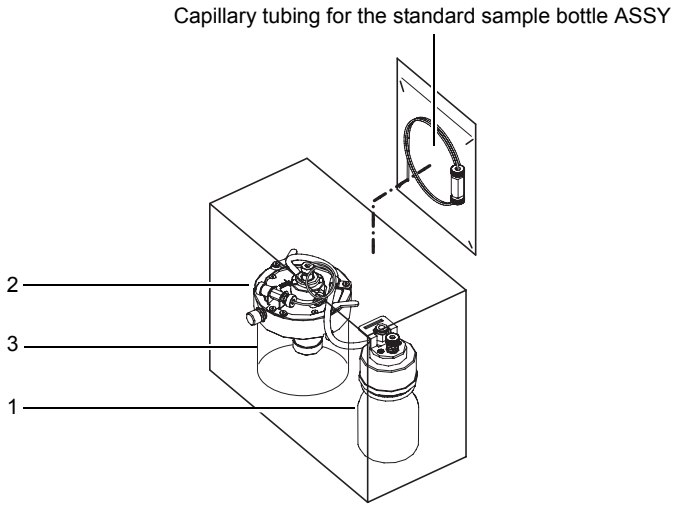
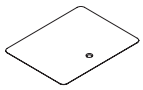
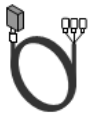
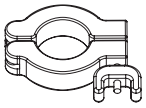
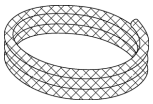


Fig. 1-5

1.4.3 Packed Parts (3)

Fig.	Part Name	Part No.	Q'ty	Remarks
	Clear file	-	1	Includes the inspection results sheet, auto tuning data, and packing list.
	Instruction manual	-	1	Includes the instruction manual for the triple inlet turbo molecular pump
	OP cover	-	1	
	Rotary pump cable	S225-17224-41	(1)	Only supplied when there is no rotary pump
	Clamp, KF25	S035-06004-02	(1)	Only supplied when there is no rotary pump
	RP exhaust hose set	-	1	Includes hose clamp
	Vinyl tube R3603 1/2 × 3/4	S016-31414	1 m	
	SI rubber tube 7 × 10 NL	S016-31350-19		1300 mm
	Rubber plug ASSY	S225-06482-92	1	
	Joint, L1252	S035-61561-11	1	
	Clamp, TS185-08-00-T	-	1	
	Cable tie GT-1401	-	6	
	Tetoron sleeving 12 × 18	S018-31510	5 m	

1.5 Optional Parts

The optional parts for this unit are shown in the table below.

For optional parts that are not listed in the table below and details on optional parts, consult your Shimadzu representative.

Optional Part Name	Part No.	Features
APCI set	S225-14271-41	Atmospheric pressure chemical ionization probe and corona needle
DUIS set	S225-12229-41	Set comprising a corona needle capable of simultaneous analysis in both ESI and APCI modes and a high voltage power supply
APCI/DUIS socket ASSY	S225-14232-41	Corona needle socket and HV cable
Rotary pump oil return kit	S225-05990-92	Kit that traps the exhaust gas from the rotary pump and returns oil to the rotary pump
Startup kit	S225-13915-42	A kit of recommended accessories such as consumables

1.5.1 APCI Set: S225-14271-41

No.	Part Name	Part No.	Q'ty	Remarks
1	APCI probe	-	1	
2	Probe stand ASSY	-	1	
3	Needle unit ASSY	S225-14290-41	1	
4	Cable APCI	-	1	Wiring inside the unit, for the APCI heater
5	APCI pipe ASSY	S225-15845-91	1	
6	Corona needle plug	-	1	High voltage socket blank
7	Needle scale	-	1	Needle alignment tool
8	Loupe, 1962	-	1	
9	Hexagon wrench 1.5	-	1	
10	Spanner, double open-end, 7 × 8	-	1	
11	Spanner, double open-end, 10 × 14	-	1	
12	Screwdriver, DS-13	-	1	

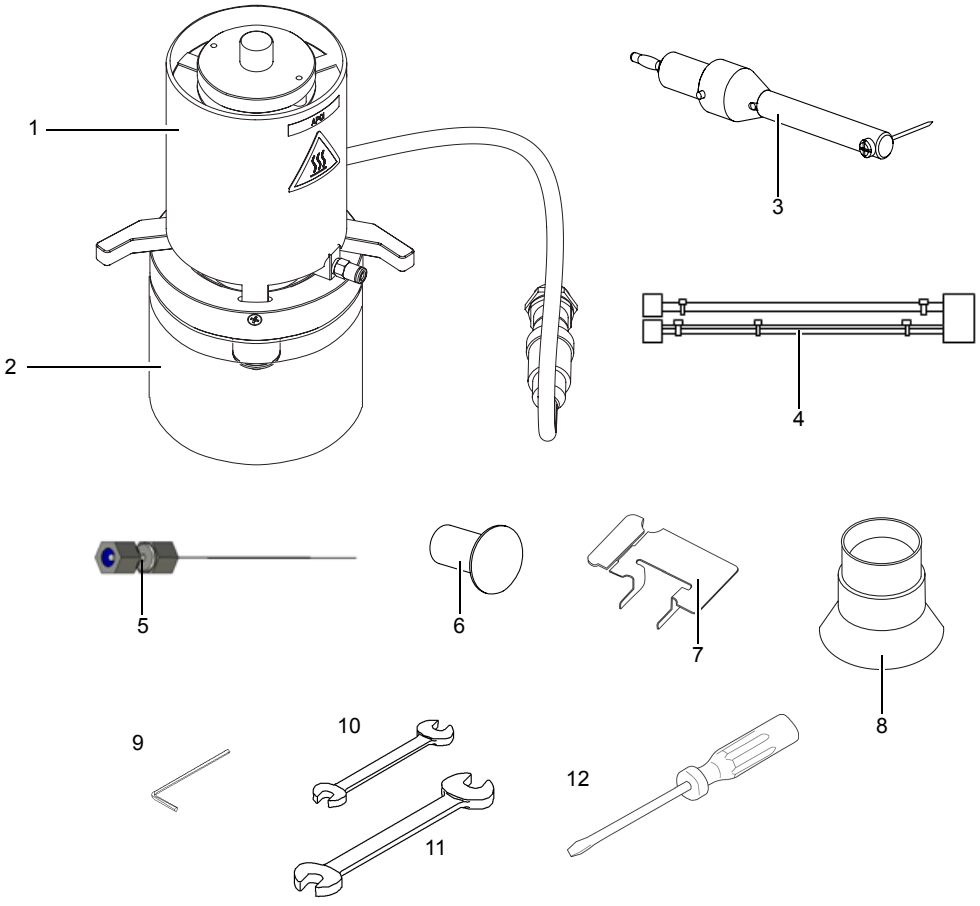


Fig. 1-6

1.5.2 DUIS Set: S225-12229-41

No.	Part Name	Part No.	Q'ty	Remarks
1	DUIS needle unit ASSY	S225-14290-41	1	
2	TQ-HV DUAL ASSY	S225-17101-41	1	High voltage power supply for DUIS

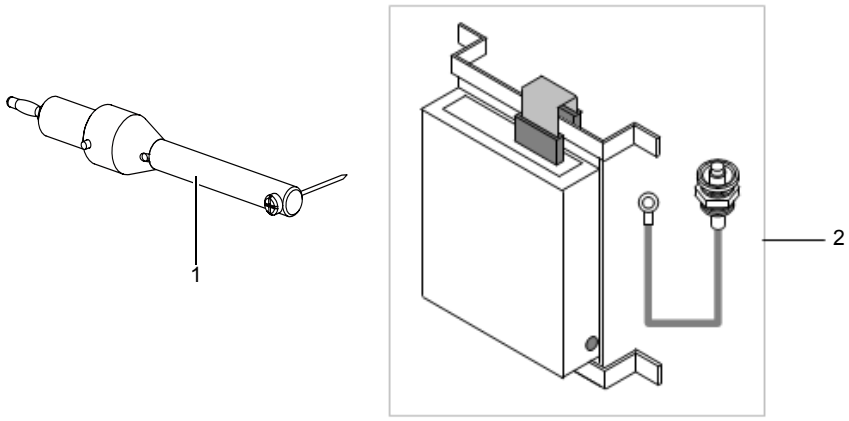


Fig. 1-7

1.5.3 APCI/DUIS Socket ASSY

No.	Part Name	Part No.	Q'ty	Remarks
1	APCI/DUIS socket ASSY	S225-14232-41	1	

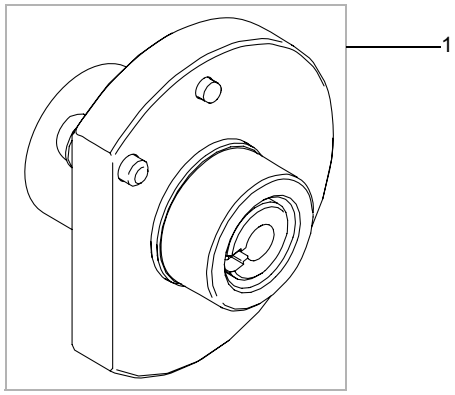


Fig. 1-8

1.5.4 RP Oil Return Kit: S225-05990-92

No.	Part Name	Part No.	Q'ty	Remarks
1	Oil return kit, E2M28	-	1	
2	Oil mist filter EMF20	S042-00124-33	1	
3	Flange, KF25-#15 straight	-	1	
4	Center ring, KF25ANCR	S035-06004-13	1	
5	Clamp, KF25C	S035-06004-02	1	
6	Hexagon wrench 8	-	1	

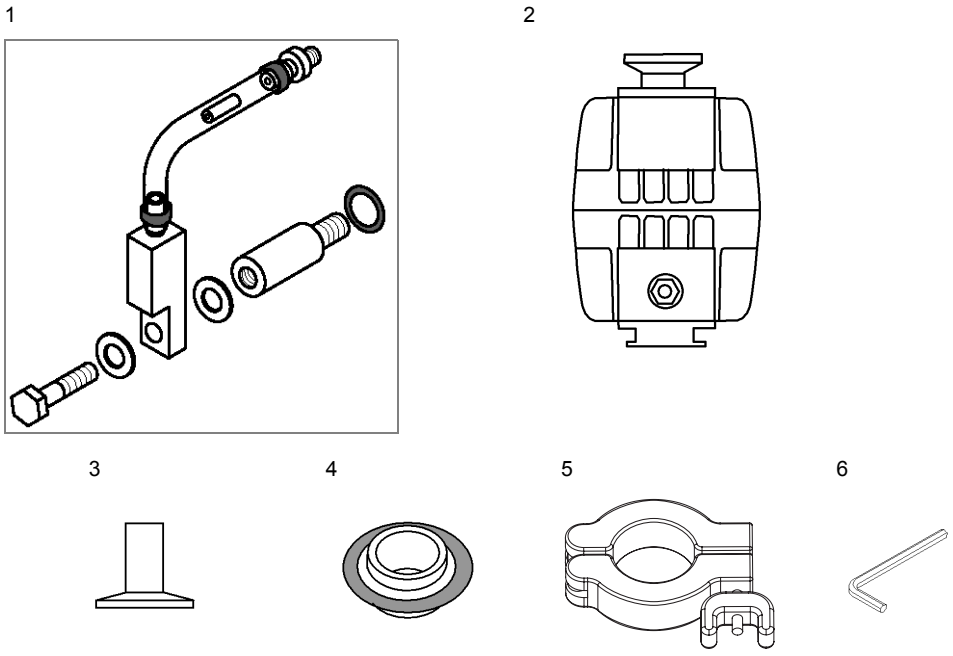


Fig. 1-9

1.5.5 Startup Kit: S225-13915-42

No.	Part Name	Part No.	Q'ty	Remarks
1	Ferrule 1.6FP, total of 3	S228-33513-91	1	PEEK ferrule, total of 3
2	DL ASSY	S225-15718-91	1	
3	Pump oil, H11025013	S017-30163-02	1	Rotary pump oil, 4 L
4	Male nut 1.6 MN PEEK (total of 5)	S228-18565-84	1	
5	Ferrule 1.6F-T (total of 5)	S228-16007-84	1	PTFE ferrule (total of 5)
6	PEEK tube, ID0.13S	-	1	ID0.13 mm PEEK tube, 3 m
7	PTFE tube 1.6 × 0.5	S228-18495-04	1 m	
8	Reflex fitting set	S228-32651-41	1	Nut, ferrule, total of 5
9	ESI pipe ASSY	S225-14948-91	1	
10	SI filter	S228-48607-91	1	Line filter for standard sample bottle
11	0.1SUS pipe	S228-49120-00	1	ID0.1 mm SUS pipe, 2 m
12	PEEK tube cutter	S228-32930-01	1	
13	Filter	S042-60935-14	1	
14	Gloves, 559-2150 (1 pair)	S086-72599-01		
15	Resistance tube, GLP cleaner	S228-32722-94	1	

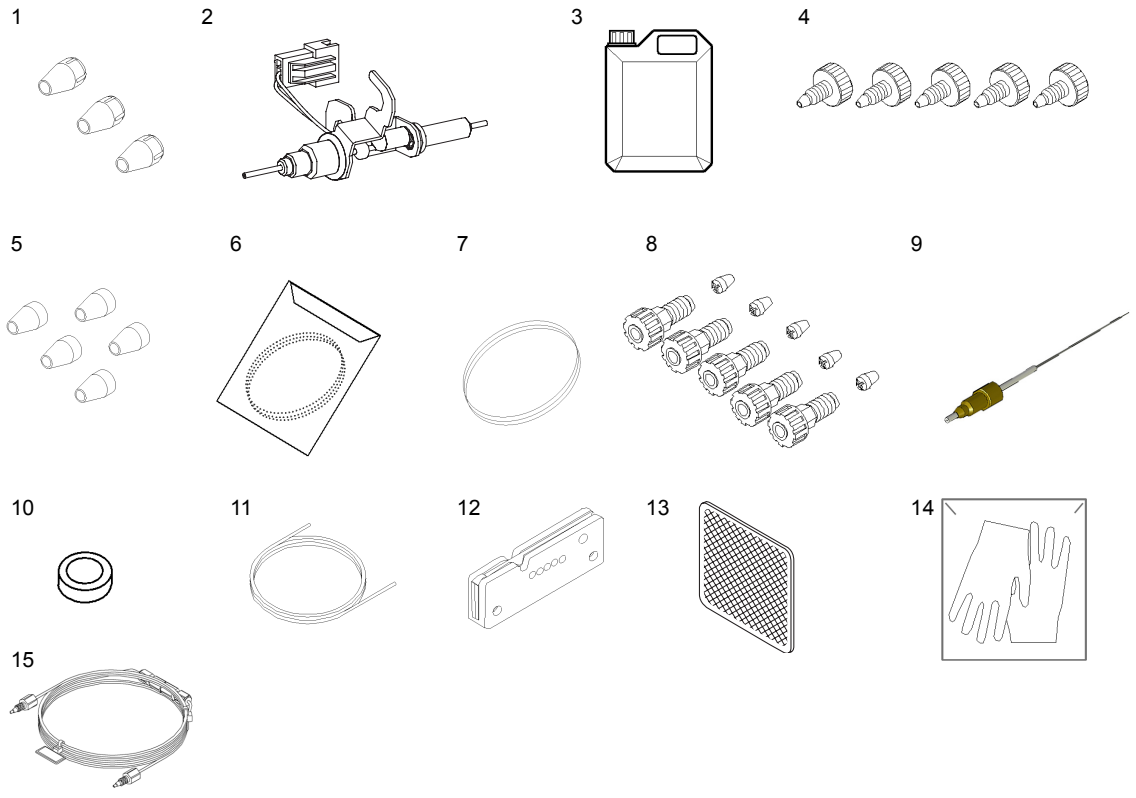


Fig. 1-10

1.5.6 FCV-20AH Mounting Kit

No.	Part Name	Part No.	Q'ty	Remarks
1	CABLE, TQ-FCV	S225-17127-41	1	

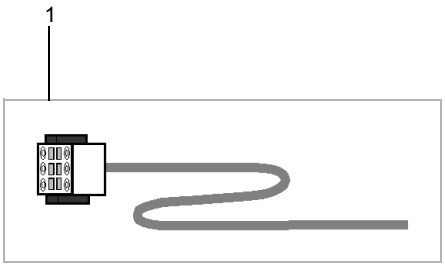
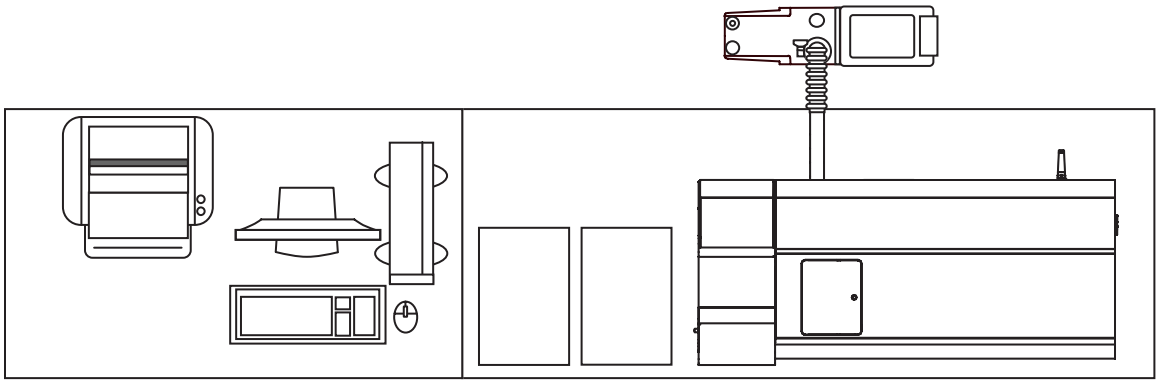


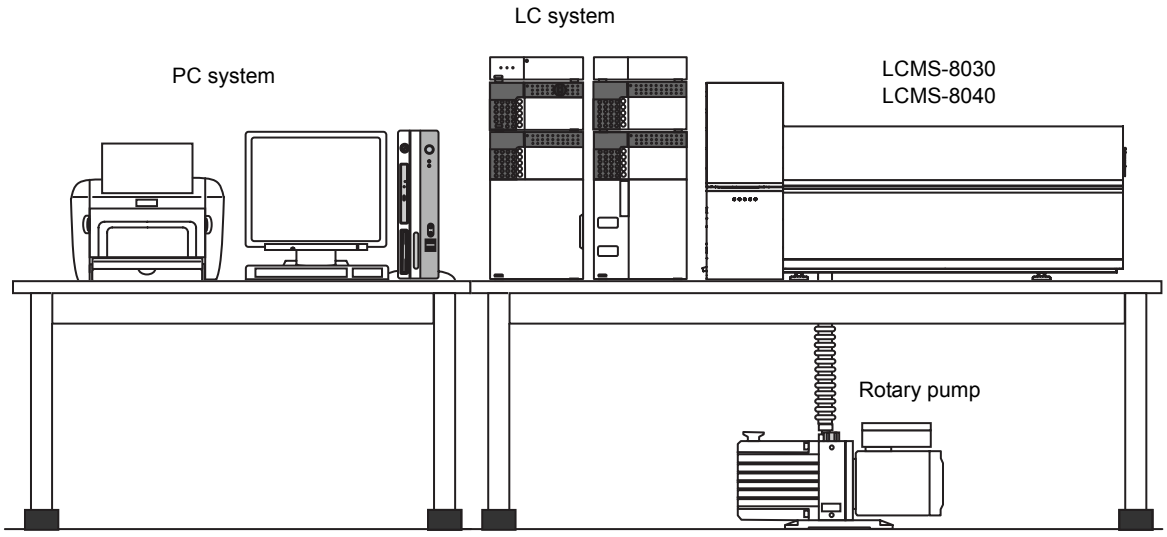
Fig. 1-11

2 Part Nomenclature and Functions

2.1 Arrangement of Component Units



[Plan View]



[Front Elevation]

Fig. 2-1

2.2 Names of Parts

[Front Elevation]

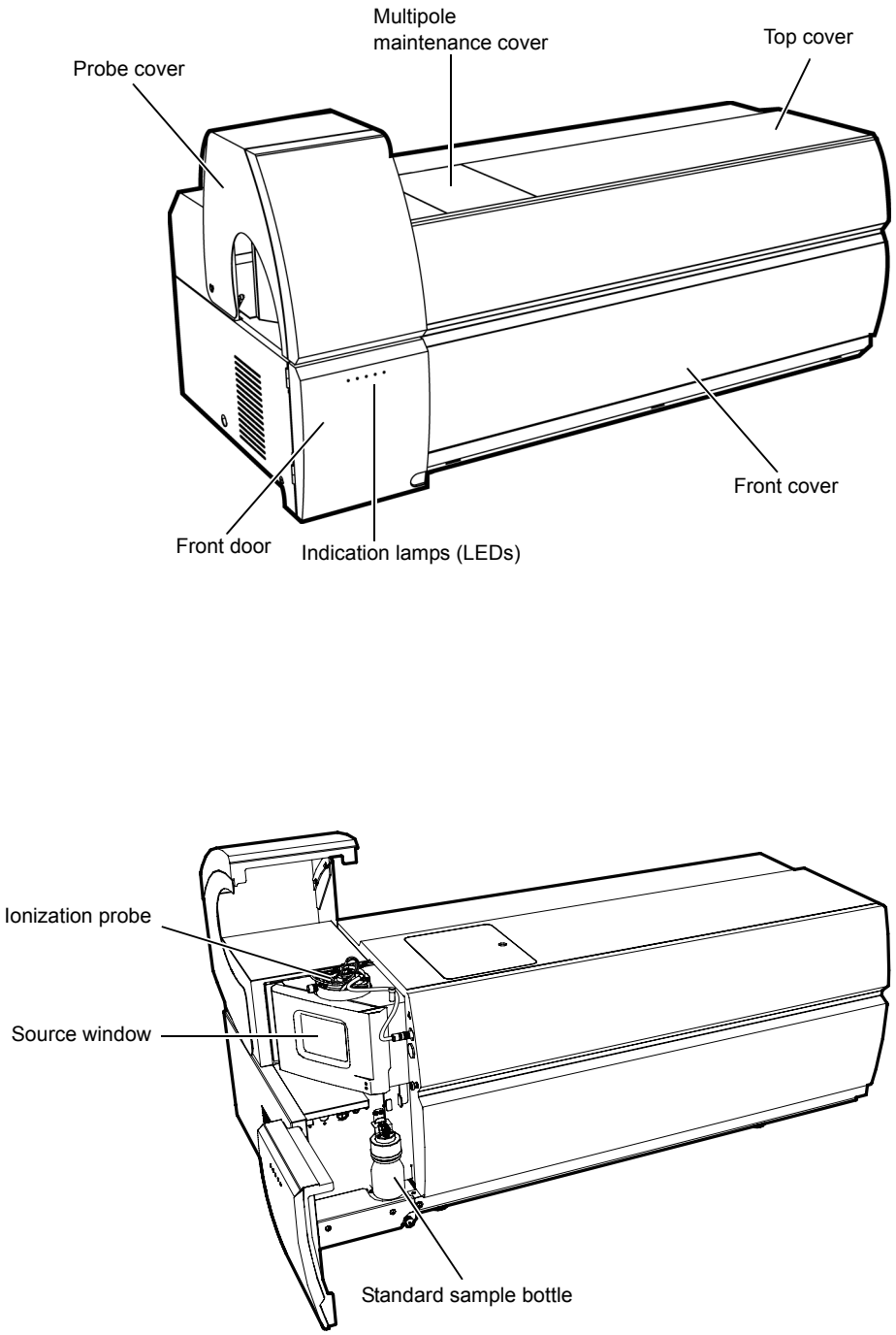


Fig. 2-2

[Rear view]

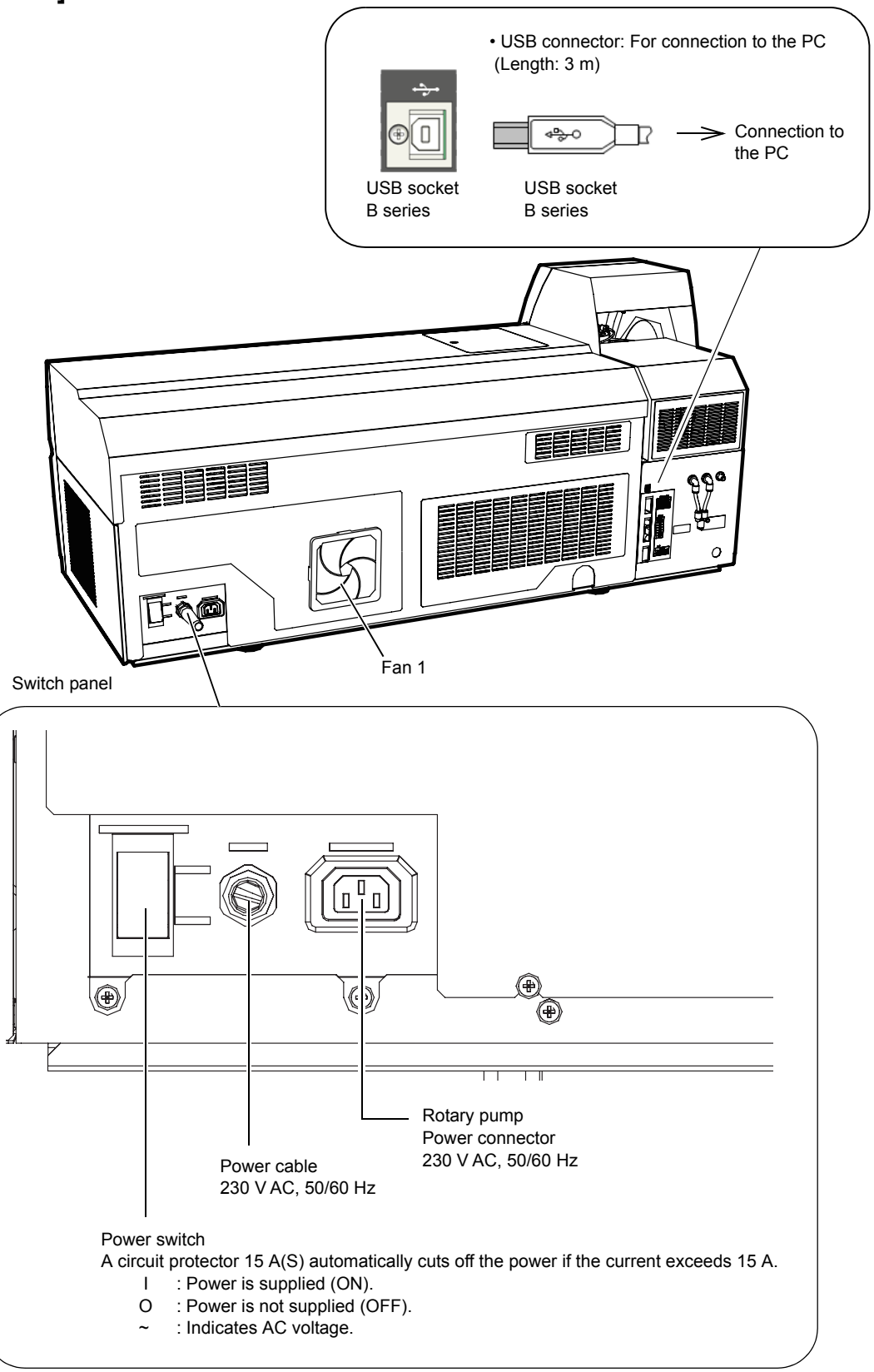


Fig. 2-3

[Rear view]

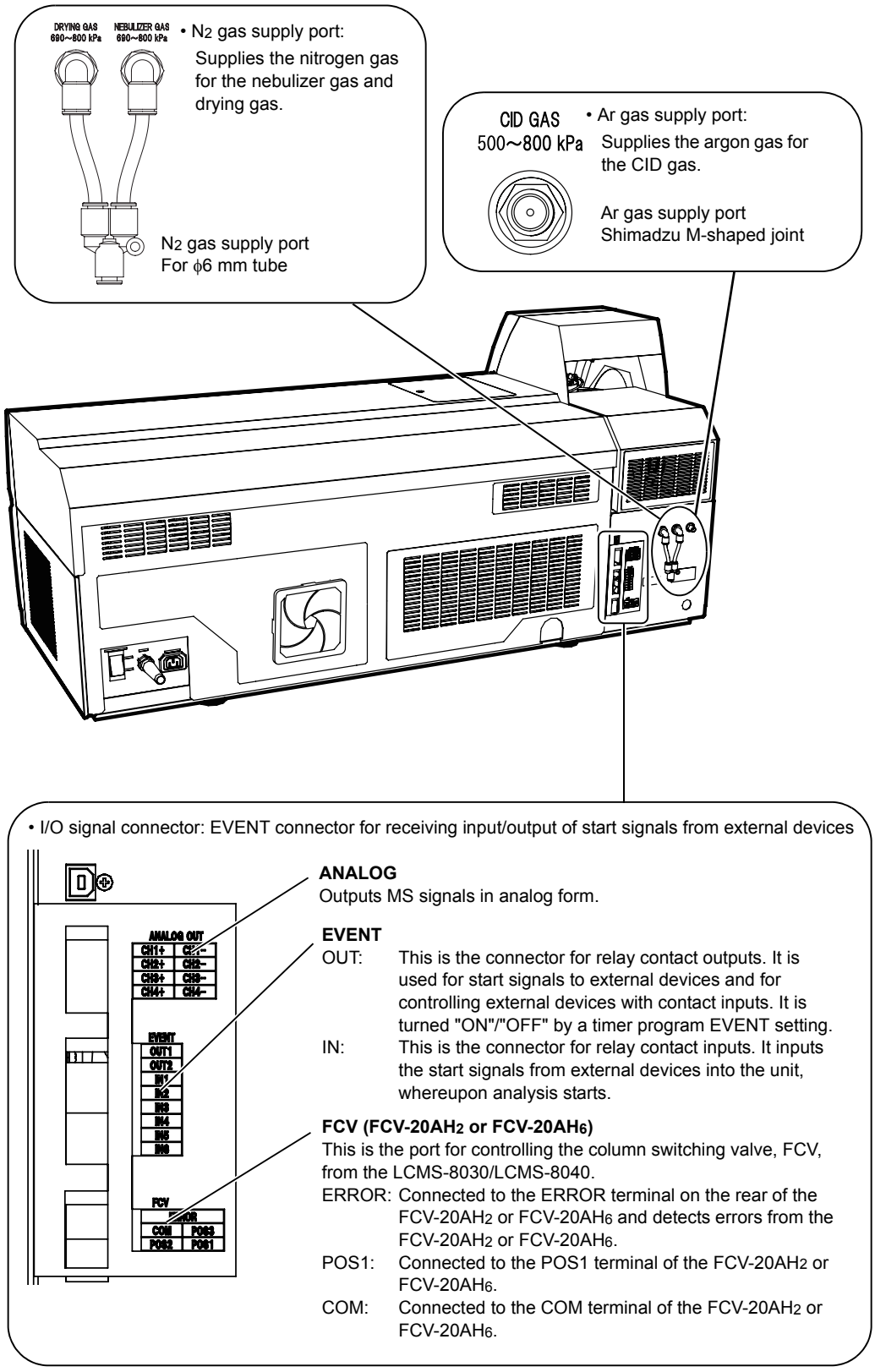


Fig. 2-4

2.3 Unit Configuration

Fig. 2-5 shows the configuration of the parts in the unit from the loading of the sample to detection. For details on the function of each part, refer to the relevant sections in this manual.

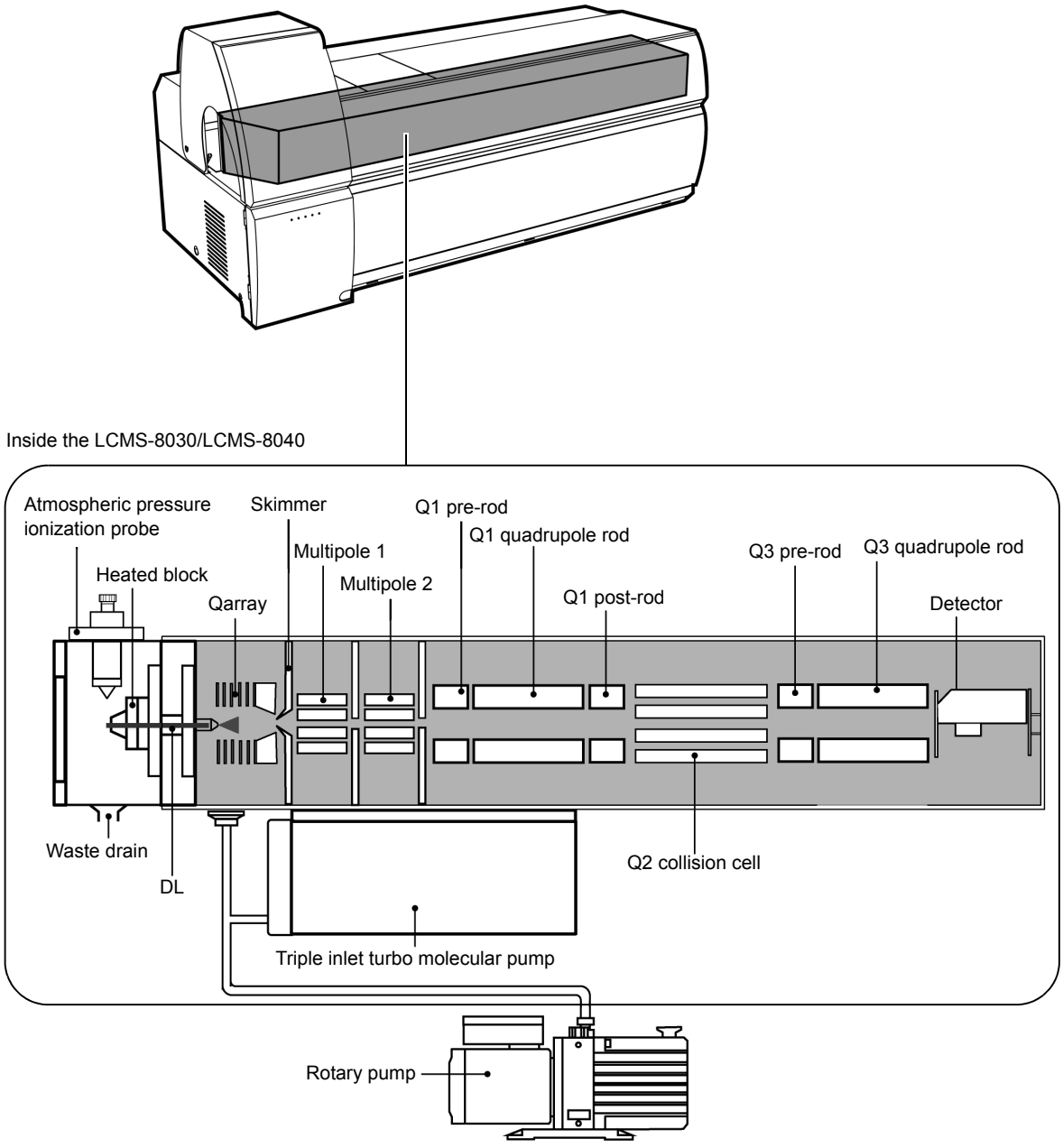


Fig. 2-5

2.4 Atmospheric Pressure Ionization Unit

This is the section that ionizes, under atmospheric pressure, the sample sent from the liquid chromatograph.

The LCMS-8030/LCMS-8040 features electrospray ionization (ESI) as standard, but by using the optional ionization probe and corona needle it is also possible to use the atmospheric pressure chemical ionization (APCI) method and dual ion source (DUIS) ionization.

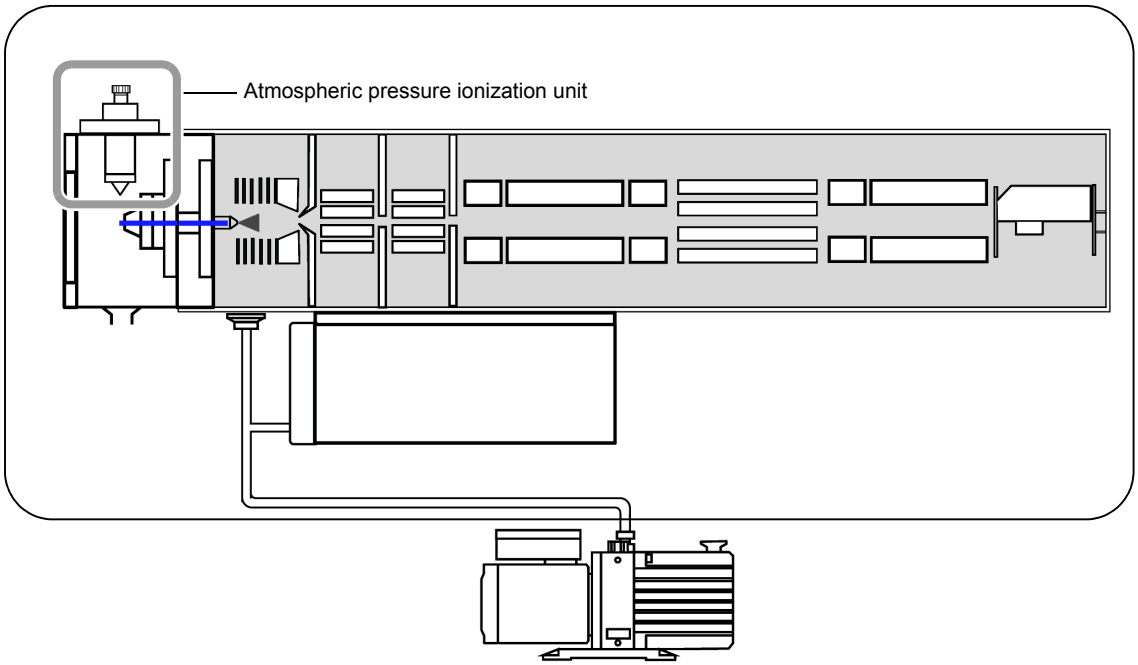


Fig. 2-6

2.4.1 Using the ESI Probe

The ESI probe can be used for effective ionization of samples containing compounds with ionicity and high polarization.

■ Principle of ionization

1. The sample solution is drawn into a capillary tube with a high voltage of around 3 to 5 kV applied to it.
2. Nebulizer gas is blown out around the outside of the capillary tube, spraying the solution and generating fine droplets that are electrostatically charged with the same sign as the applied voltage.
3. During the course of movement the charged droplets are subject to vaporization of the solvent, and they disintegrate when the repulsive force among the charges exceeds the surface tension of the liquid.
4. Through repetition of vaporization and disintegration, very fine droplets are achieved, and ultimately it is thought that sample ions are released in the vapor phase. This state is called ion vaporization.

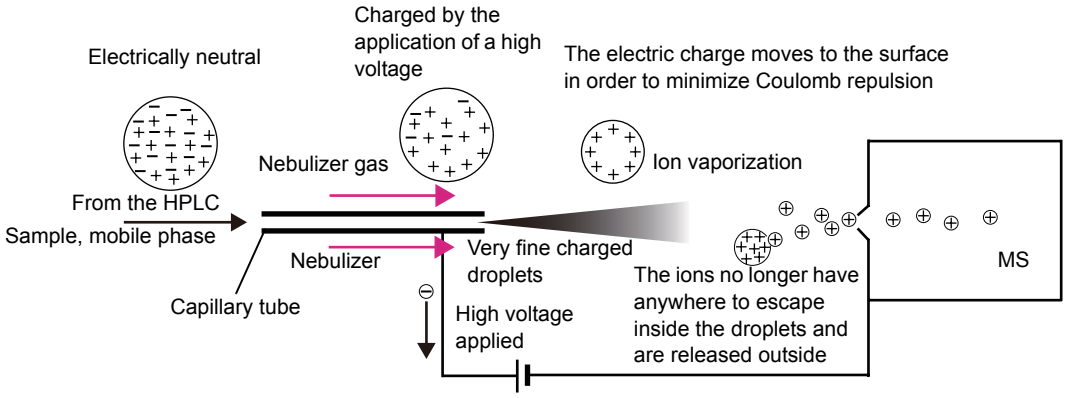


Fig. 2-7

■ ESI probe construction

Fig. 2-8 shows the component parts of the ESI probe.

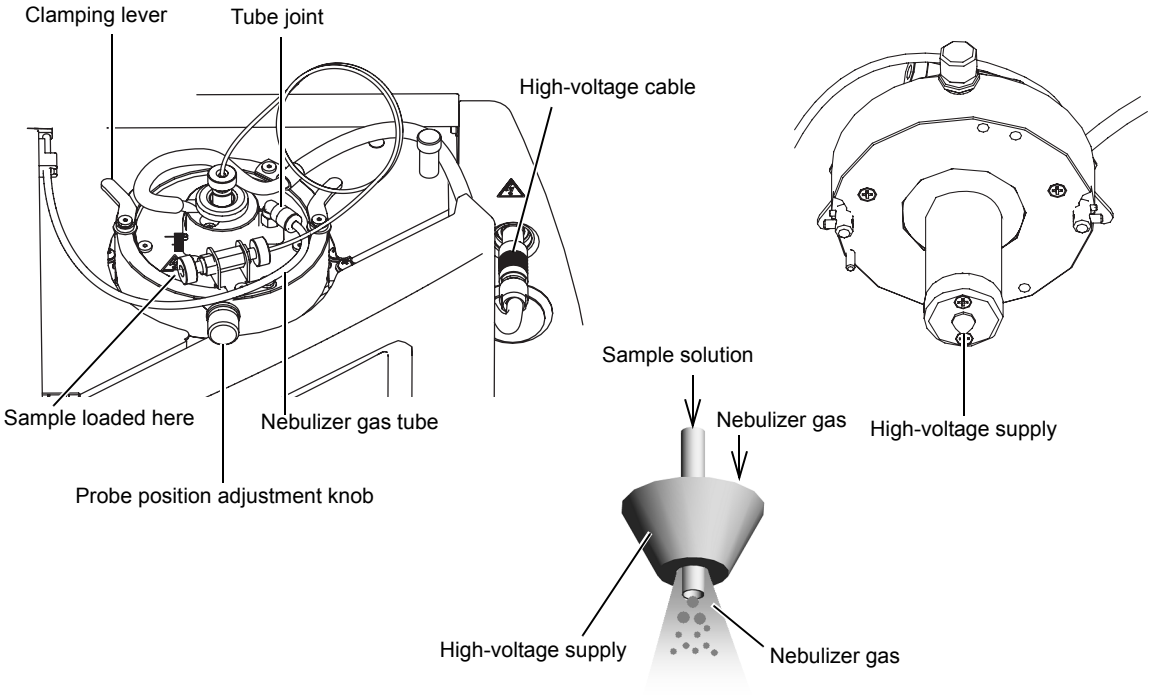


Fig. 2-8

2.4.2 Using the APCI Probe

The APCI probe can be used effectively to ionize compounds with low and medium polarity.

■ Principle of ionization

1. The solvent gas heated (from 300 to 500 °C) inside the APCI probe is ionized on the occurrence of corona discharge due to the application of a high voltage (± 3 to 5 kV) to the needle.
2. The sample molecules are ionized as a result of ion-molecular reactions (Cl reactions) with the solvent ions. Nebulizer gas is used to spray the liquid in the same way as with ESI.

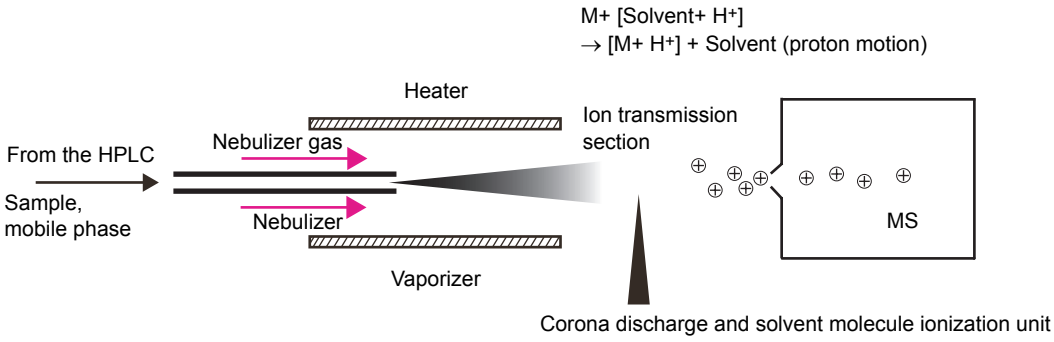


Fig. 2-9

■ APCI probe

Fig. 2-10 shows the component parts of the APCI probe.

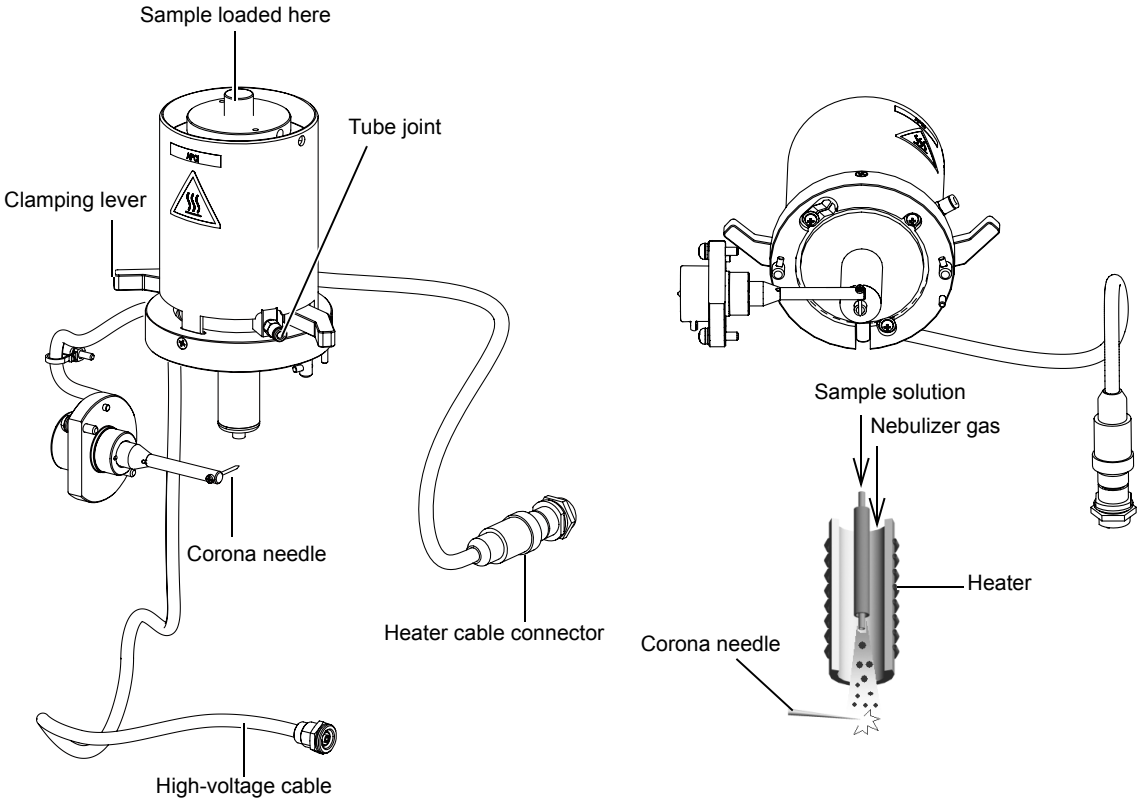


Fig. 2-10

2.4.3 Using DUIS (Dual Ion Source)

This is an ionization method in which data can be obtained in both ESI and APCI modes.

High voltages are applied simultaneously to the nebulizer for ESI and the corona needle for APCI, and heated dry gas is used to assist ionization in the APCI mode. The ESI probe provided as the standard accessory is used as the nebulizer for ESI.

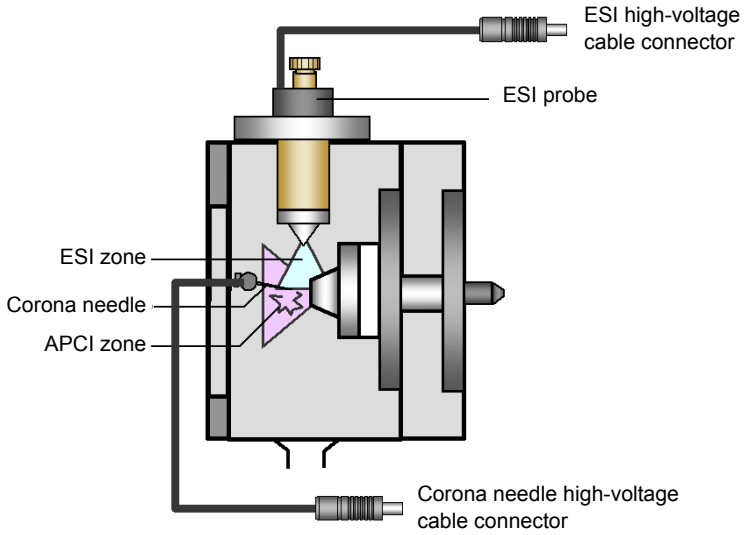


Fig. 2-11

■ ESI probe and corona needle

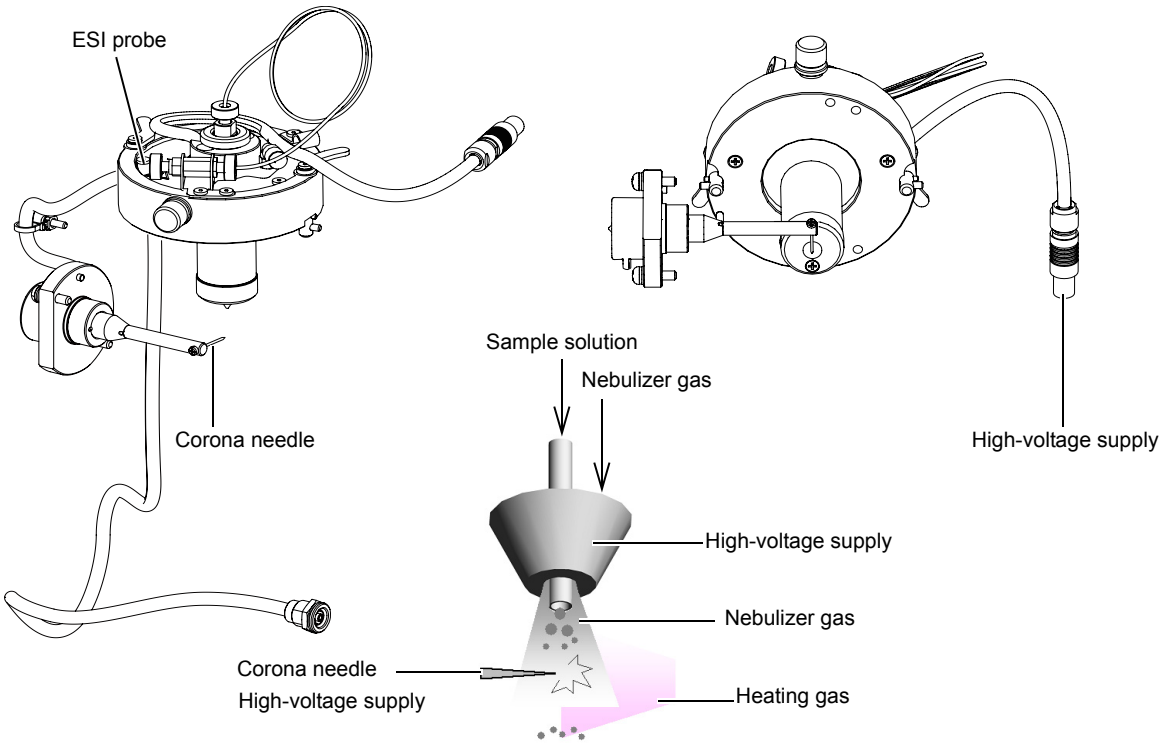


Fig. 2-12

2.5 Interface Section

The interface section introduces the ions generated by the ionization probe into a vacuum.

The status of the spray generated under atmospheric pressure can be observed through the source window at the front of the unit.

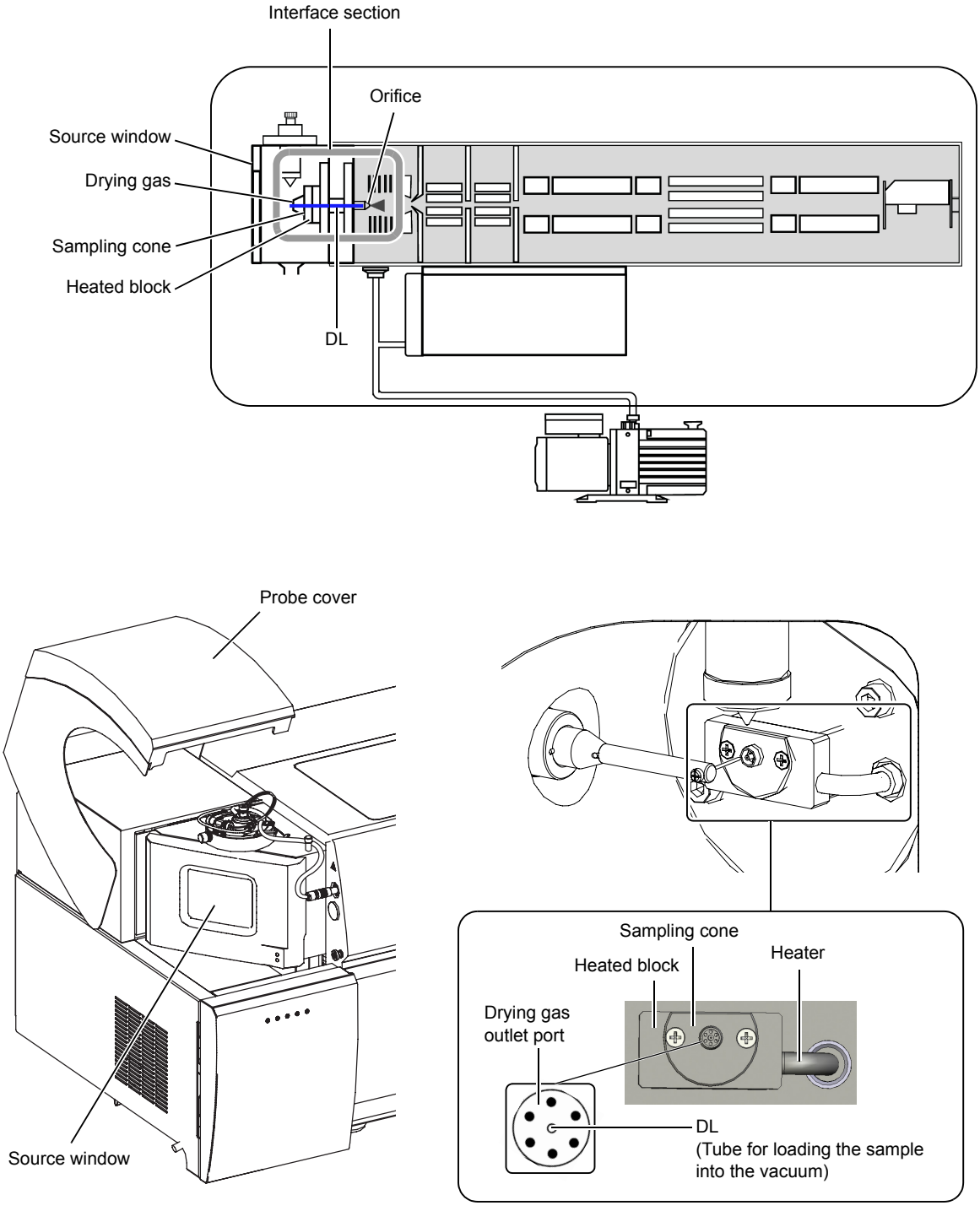


Fig. 2-13

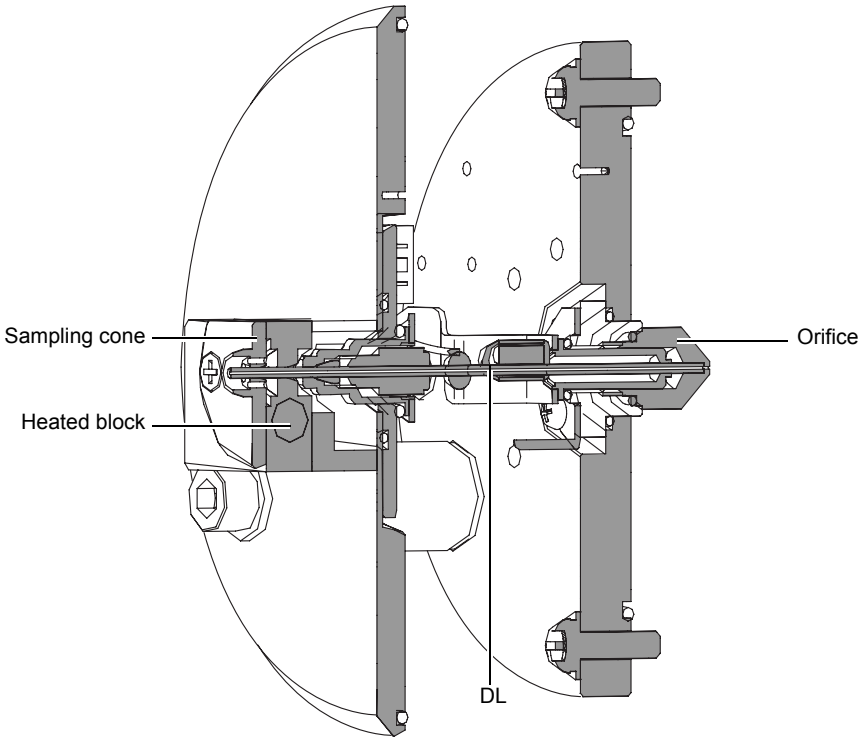


Fig. 2-14

2.5.1 DL (Desolvation Line)

The charged droplets that have been spray ionized under atmospheric pressure are heated by the DL. This heating serves to remove the solvent and introduce ions into the vacuum.

The DL can be changed without stopping the vacuum.

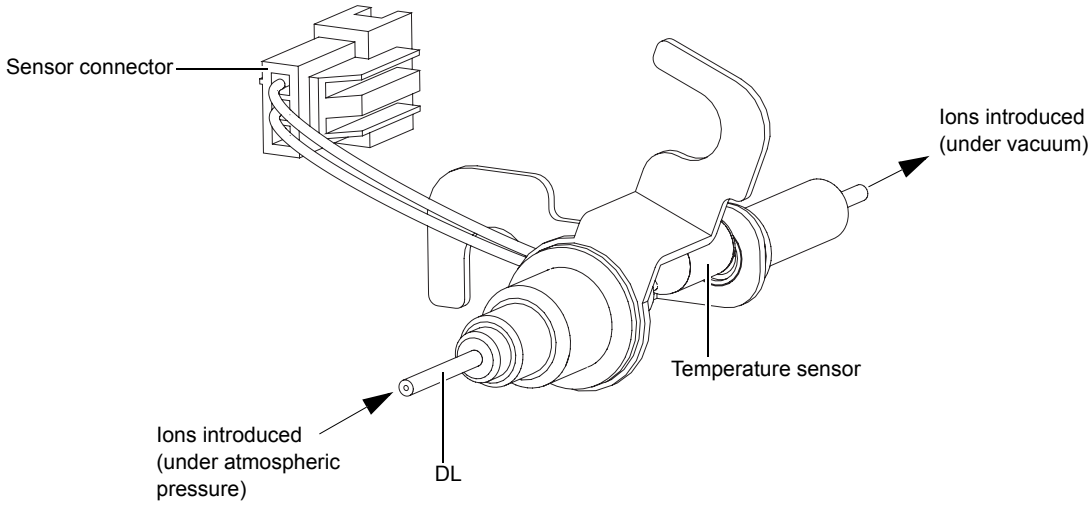


Fig. 2-15

2.5.2 Orifice

The orifice is located at the tip of the DL. The orifice maintains the vacuum and the DL can be changed without stopping the vacuum.

NOTE

Stop the vacuum before removing the orifice.

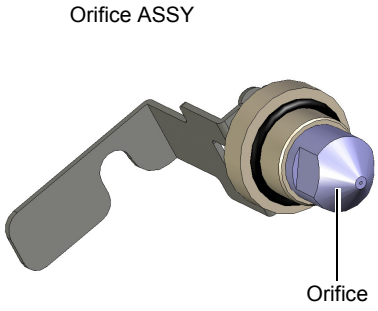


Fig. 2-16

2.6 Lens System

The ions generated under atmospheric pressure are efficiently focused, and then introduced into the quadrupole rods by the lens system.

The lens system comprises the Qarray, skimmer, multipole and entrance lens.

Each part can be removed by opening the instrument's top cover and the lens system door.

* Octapoles are used in the LCMS-8030 and quadrupoles are used in the LCMS-8040. Octapoles and quadrupoles are collectively referred to as "multipoles".

NOTE

Stop the vacuum before handling the parts of the lens system.

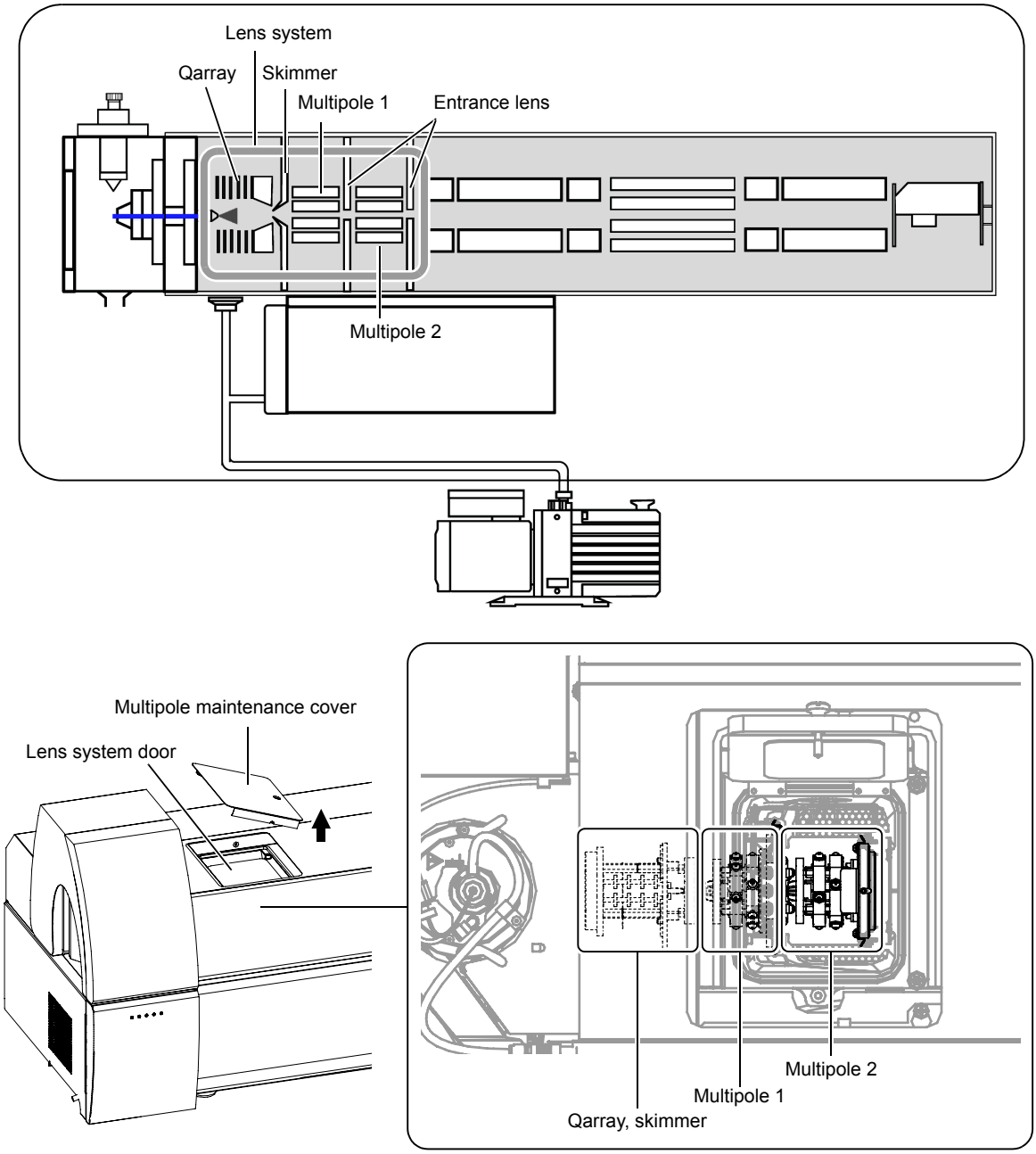
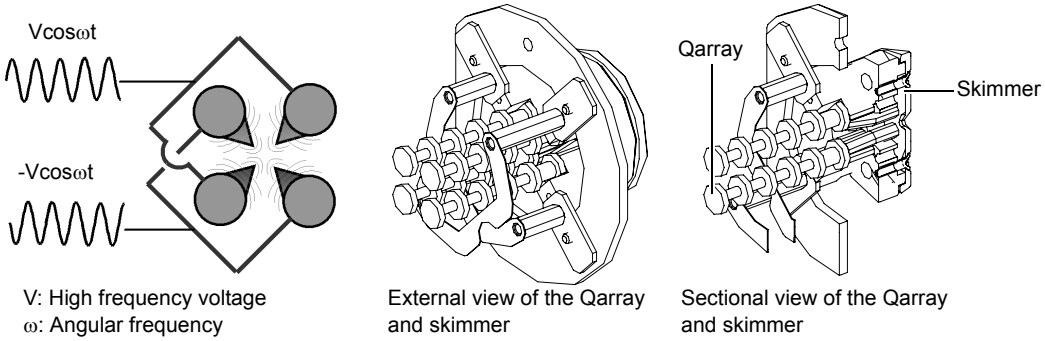


Fig. 2-17

2.6.1 Qarray, Skimmer

The Qarray and skimmer located inside the first stage vacuum chamber focus the scattering of the ions emitted from the DL. The Qarray arranges the quadrupole electric field as a number of stages which progressively focus the ions in their direction of progress, and this constriction makes the ions converge efficiently on the hole in the tip of the skimmer. The same high-frequency voltage is supplied to opposing electrodes, while adjacent electrodes are supplied with high frequency voltages with a phase difference of 180 degrees. The high frequency voltage acts as a force to confine the ions and because, in contrast to a quadrupole mass filter for mass separation, DC voltage is not used, it functions as an ion guide.

The skimmer is a partition that separates the first vacuum chamber and the second vacuum chamber.



V: High frequency voltage
ω: Angular frequency

External view of the Qarray and skimmer

Sectional view of the Qarray and skimmer

Fig. 2-18

2.6.2 Multipole and Entrance Lens

These are lens components that lead the ions that emerge from the skimmer into the quadrupole rods.

Multipole 1 and multipole 2 are located in the second and third vacuum chambers respectively.

The multipole is a high-frequency ion guide that is located at the rear of the skimmer. A radio-frequency voltage is applied to the electrodes to confine and focus the ions. Adjacent electrodes are supplied with high-frequency voltages with a phase difference of 180 degrees. Like the Qarray, it functions as an ion guide that does not use DC voltage.

The entrance lens comprises the second and third partitions.

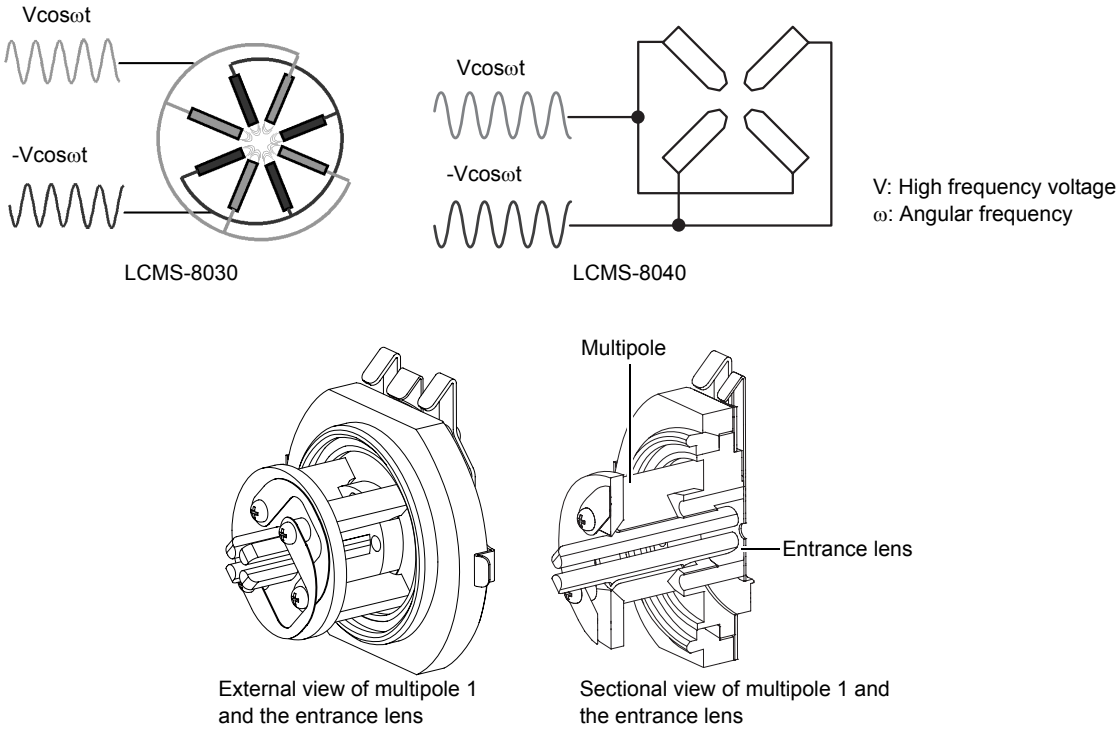


Fig. 2-19

CAUTION

Prohibitions

Do NOT disassemble the assembly components of the Qarray, multipoles and so on.

This may cause injury or damage the instrument.

2.7 Analysis Unit

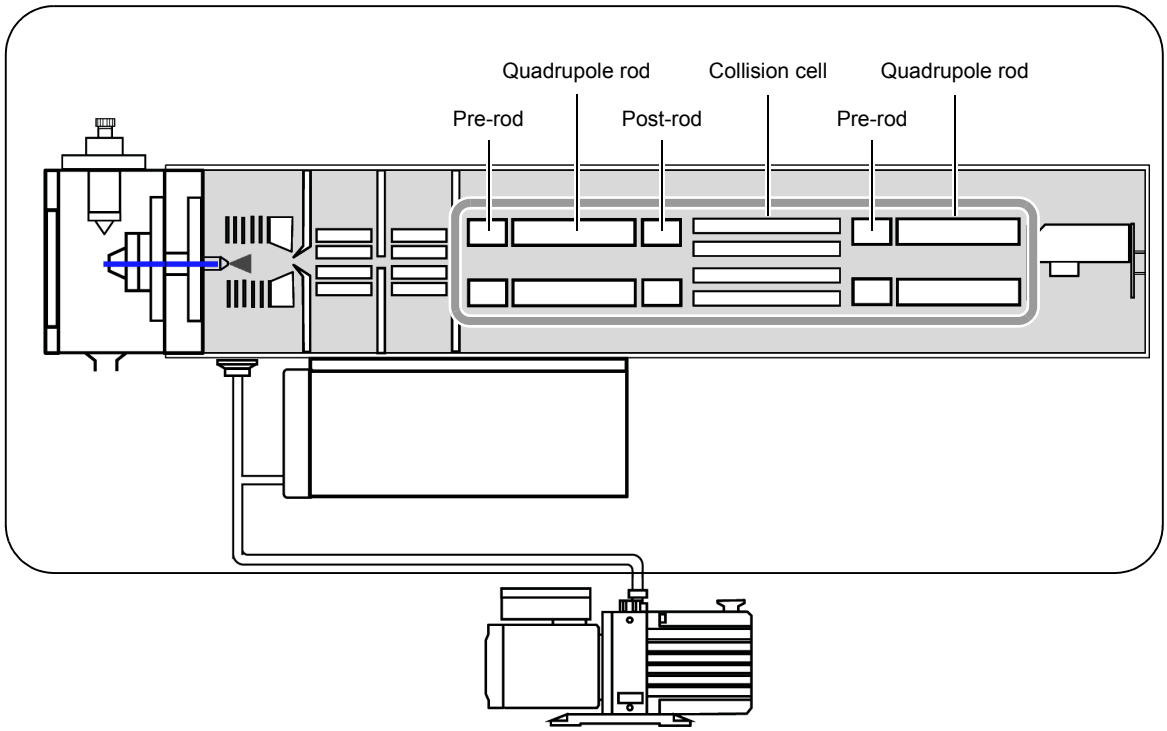


Fig. 2-20

The analysis unit is composed of four precision machined hyperbolic electrodes and pre-rods, and the four electrodes are arranged an equal distance from, and parallel to, the center axis.

The ions generated in the ionization unit are accelerated in the Z-axis direction by a relatively weak voltage of several volts and introduced into the quadrupole zone through a small hole. Within the quadrupole, voltages of the same polarity are applied to opposing electrodes, while voltages with positive and negative reversed are applied to adjacent electrodes. When both DC voltage U and high-frequency AC voltage $V\cos\omega t$ (ω: high angular frequency, t: time) are applied to each of the electrodes, an electric field that changes phase at high speed is generated within the quadrupole.

This electric field causes the ions that pass through it to oscillate in the X and Y axis directions. If specific conditions (U, V, ω) are imposed at this time, ions within a particular range of mass-to-charge ratios (m/z) go into the "stable oscillation" state and can pass through the quadrupole and reach the detector. Ions with m/z ratios outside this range oscillate unstably and collide with the electrodes or fly out of the system, and so are not detected.

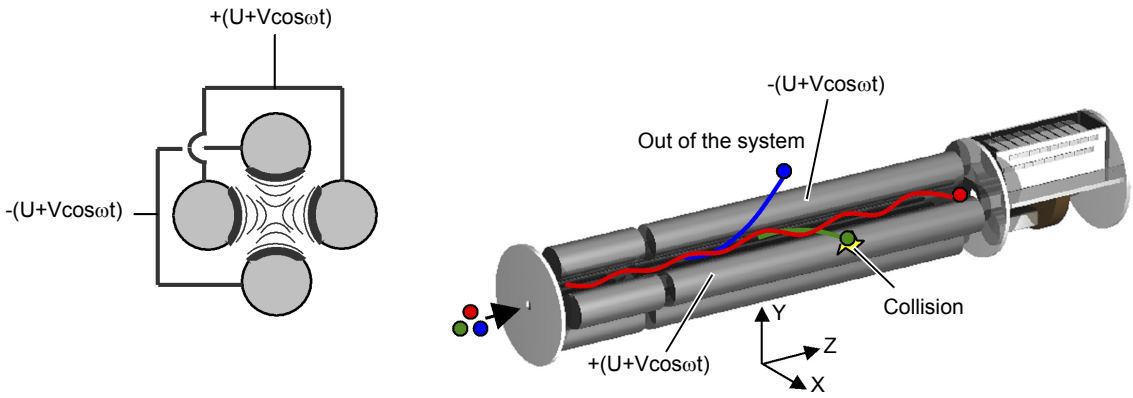
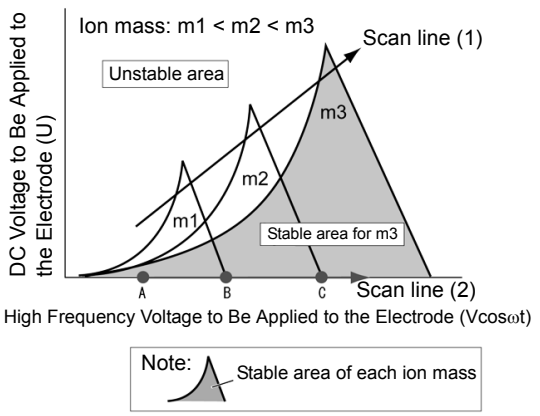


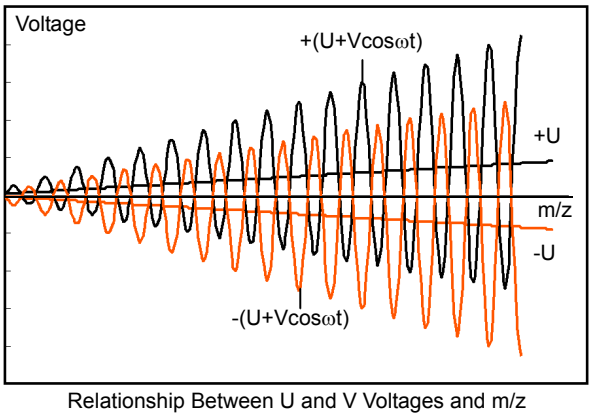
Fig. 2-21 Side View of a Quadrupole Type Mass Spectrometer

It is known that the vibration of ions inside the quadrupole follows an equation called Mathieu's equation. The ions move so that they satisfy equation (1) below regardless of their initial speed or initial position.

$$\frac{m}{z} = K\frac{V}{r^2\omega^2} \quad \ldots . (1)$$ (K: constant, r: distance between electrodes)

The conditions under which the ions vibrate stably are expressed by the areas bounded by the lines of m1, m2 and m3 in Fig. 2-22 when the masses of the ions, m, and their angular frequencies, ω, have been determined. There are different stable areas for the ions with masses m1, m2, and m3. If we vary the voltage while maintaining a constant ratio between the direct current voltage and the high frequency alternating current voltage so that it passes through each of the stable areas for m1, m2 and m3, this will mean that ions in the area above the scan line (1) will pass through. This means that we can pass the ions m1, m2, and m3 through in order. In this way, we can obtain a mass spectrum for ions with low masses through to ions with high masses.





Relationship Between U and V Voltages and m/z

Fig. 2-22

CAUTION

The quadrupole rods are assembled with precision and should not be touched.

Prohibitions

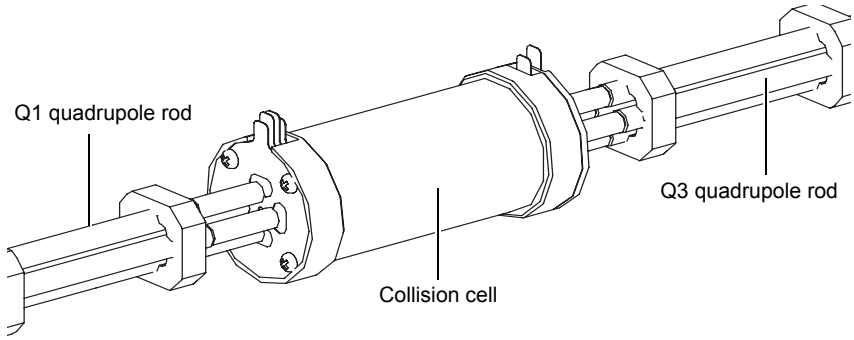


Fig. 2-23

The collision cell is a high frequency ion guide that is located between the Q1 and Q3 quadrupole rods. In the same manner as the high frequency ion guide in the lens system, ions are confined through the application of a high frequency voltage with a phase difference of 180° to the adjacent electrodes.

The pseudo-potential can be expressed by the following equation through the high frequency voltage in the high frequency ion guide.

$$V^*(R_0) = \frac{qn^2}{4m\Omega^2}\left(\frac{V_0}{r_0}\right)^2\left(\frac{R_0}{r_0}\right)^{2(n-1)}$$

r_0 : radius of the incircle of the high frequency ion guide, V_0 : high frequency voltage, n: number of electrodes in the ion guide.

The r_0 value for the Shimadzu collision cell becomes larger closer to the detector. Such a construction sets up an inclination that accelerates ions. This enables the high speed transfer of ions and makes high speed analysis possible.

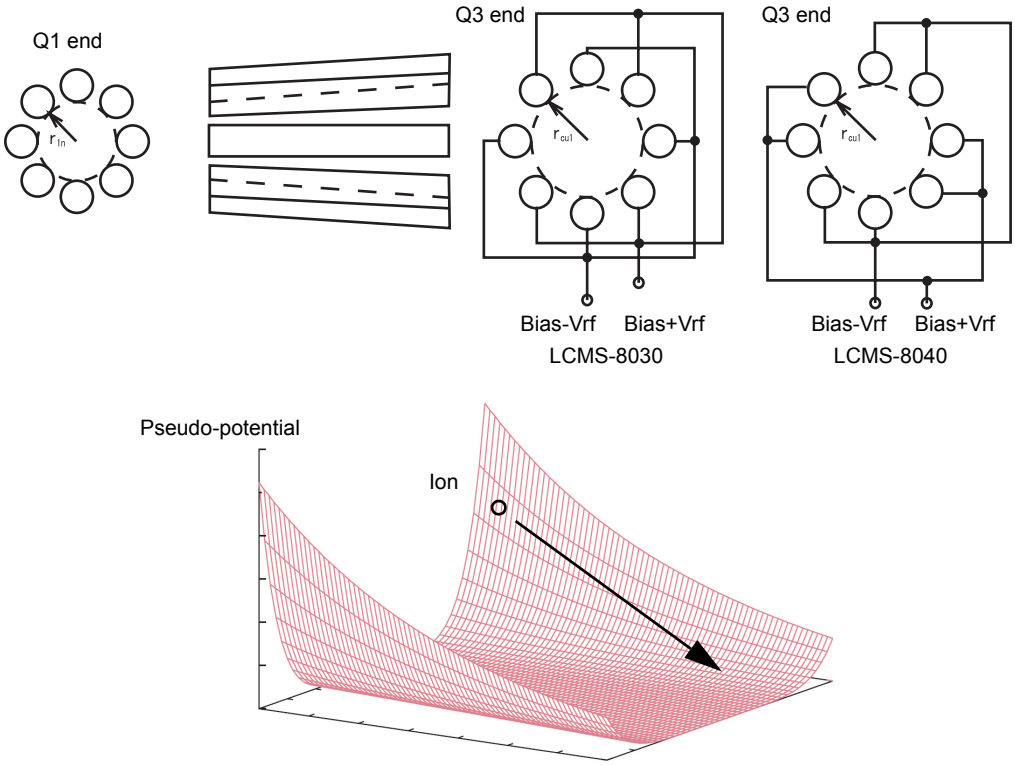


Fig. 2-24

2.8 Detection Unit

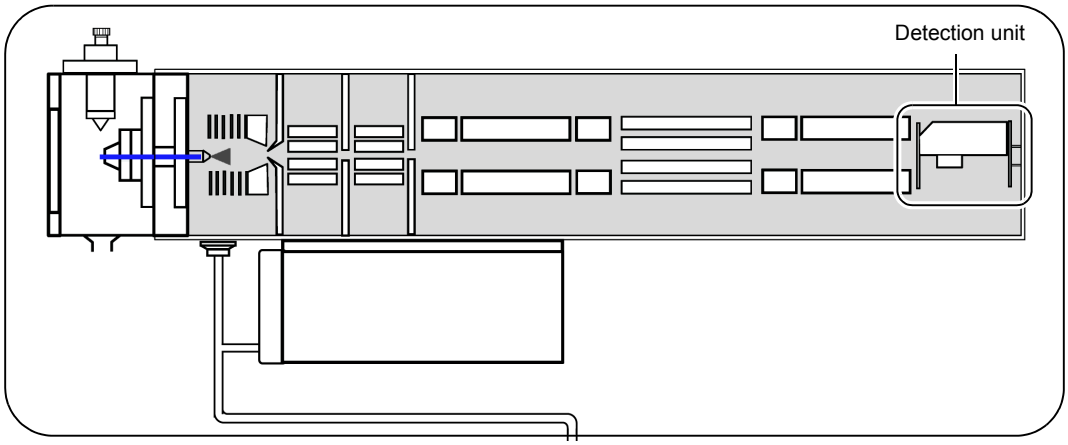


Fig. 2-25

2.8.1 Detector

The detector comprises the conversion dynode and the electron multiplier (secondary electron multiplier), and it detects positive and negative ions that have passed through the quadrupole rods.

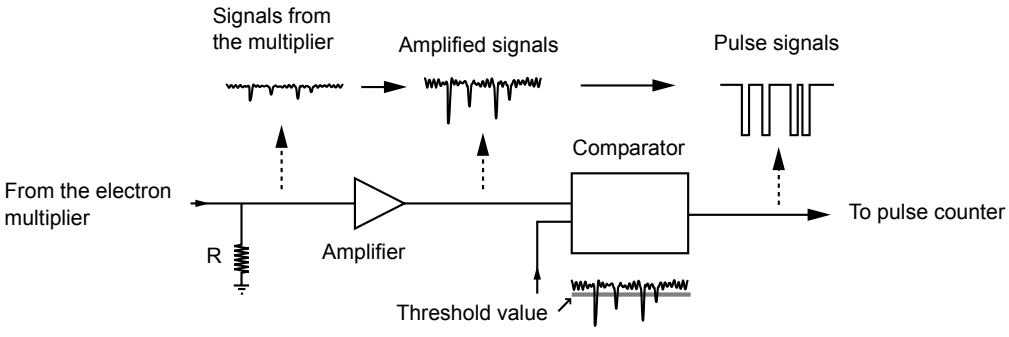
The ions that pass through the quadrupole rods are accelerated by the conversion dynode, to which a voltage of 6 kV is applied, and they collide with the conversion dynode electrode. The collision of these ions releases ions and secondary electrons, which are further accelerated toward the electron multiplier.

The electron multiplier comprises electrodes arranged in a number of stages: the secondary electrons are progressively amplified here and the amplified current is detected at the final stage.

The voltage that is applied to the electrode at each stage is set as the detector voltage, and this voltage value contributes to the amplification factor.

The secondary electrons are detected by the electron multiplier, amplified, and then sent to the pulse count detection system.

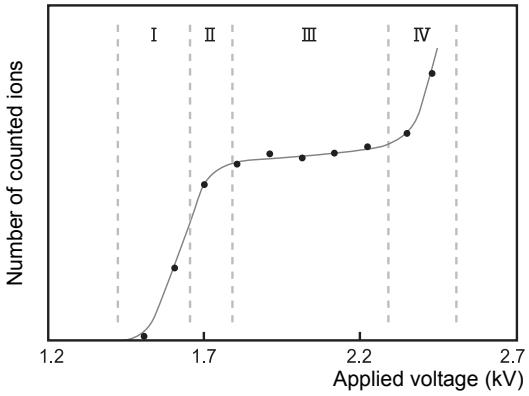
The pulse count detection system converts signals that exceed a threshold value into pulses and counts these pulses. Setting the threshold value above the electrical noise level eliminates electrical noise and allows counting of ion signals only.



Pulse Count Detection System

Fig. 2-26

The relationship between the voltage applied to the electron multiplier and the number of counted ions is shown in the Fig. 2-27. Ion signals can be counted accurately if the detector is operated in the plateau region of the graph.



Ion Signal Count Plateau Curve

Fig. 2-27

Hint

The LCMS-2020 employs an analog detector and increasing the detector voltage by 0.1 kV causes the signal intensity to approximately double (S/N does not change). In contrast, the LCMS-8030/LCMS-8040 measures the number of ions in the plateau region of the graph, which means the signal intensity stays about the same even if the detector voltage is changed.

If changing the detector voltage by 0.05 kV changes the signal intensity by more than 30 %, the detector may have deteriorated. Try performing auto tuning first to fix the variation.

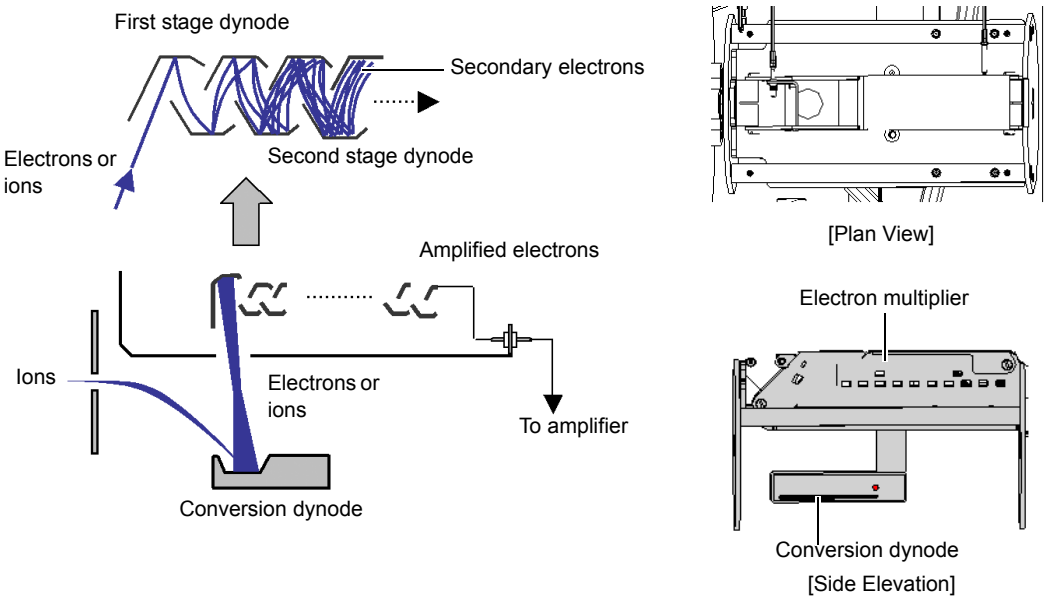


Fig. 2-28

2.9 Vacuum System

The vacuum housing comprises the atmospheric pressure chamber and the first, second, third, and fourth vacuum chambers. The rotary pump evacuates the first vacuum chamber and the rear part of the triple inlet turbo molecular pump, while a single triple inlet turbo molecular pump evacuates the second, third, and fourth vacuum chambers.

Both of the vacuum pumps are started and stopped by the LabSolutions software.

The pressure is measured by the Pirani gauge fitted to the first vacuum chamber and the ion gauge fitted to the fourth vacuum chamber.

The approximate pressures during measurement are listed below. The analysis detection section is maintained at a high vacuum.

First vacuum chamber (Qarray section):	100 to 200 Pa (when the DL temperature is 250 °C)
Second vacuum chamber (multipole 1 section):	Approx. 5 Pa (no vacuum gauge connected)
Third vacuum chamber (multipole 2 section):	Approx. 0.1 Pa (no vacuum gauge connected)
Fourth vacuum chamber (analysis detection unit):	3×10^{-3} Pa (when CID gas is introduced)

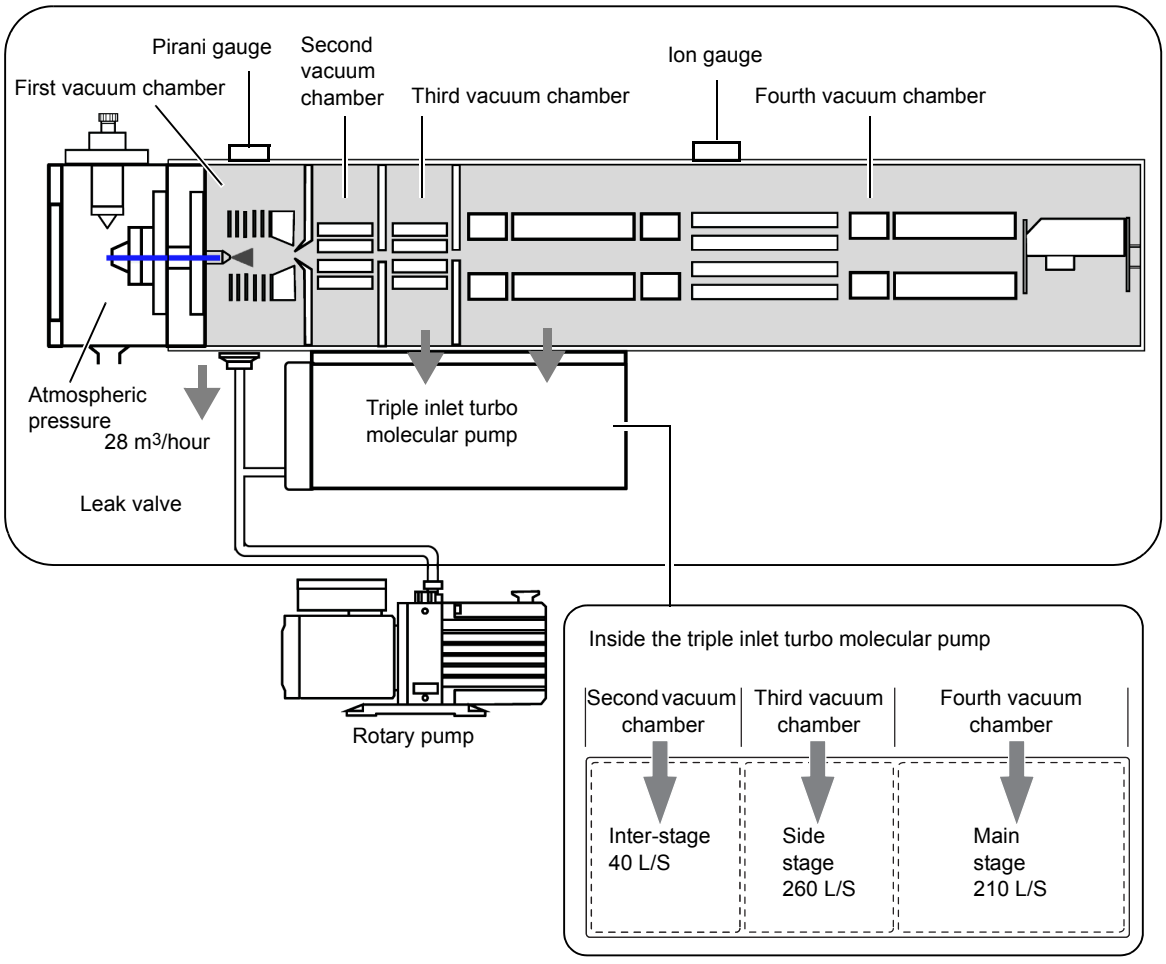


Fig. 2-29

2.10 Standard Sample Introduction Unit

The standard sample is delivered to the ESI probe for sensitivity adjustment, resolution adjustment and mass calibration (auto tuning) of the instrument.

To deliver the standard sample, the standard sample bottle is pressurized with nitrogen gas.

In order to pressurize the standard sample bottle to a constant pressure, tubing is connected by branching from the drying gas flow line.

Sample delivery is performed automatically when using auto tuning, but is started and stopped with the LabSolutions software when using manual tuning.

Since pressurization with nitrogen gas is carried out with the standard sample bottle sealed up, if the sample is delivered over a long period of time you may see a decrease in the flow rate caused by a drop in pressure. In this case, deliver the standard sample again.

You can keep delivering the sample for about 30 minutes with no decrease in the flow rate.

NOTE

The sample will not flow out for approximately one minute while the sample tubing becomes filled with the sample.

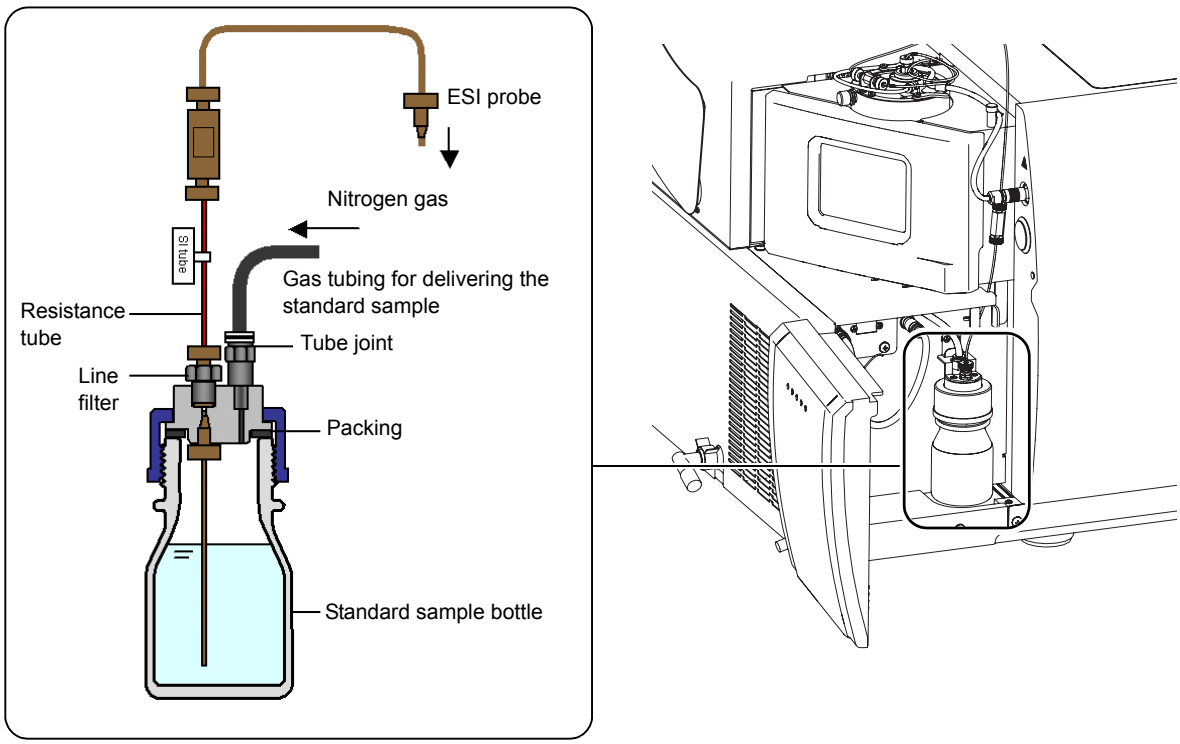


Fig. 2-30

■ Operation of the standard sample introduction unit

When the standard sample is ON:

1 Pressurize the inside of the standard sample bottle to 100 kPa.

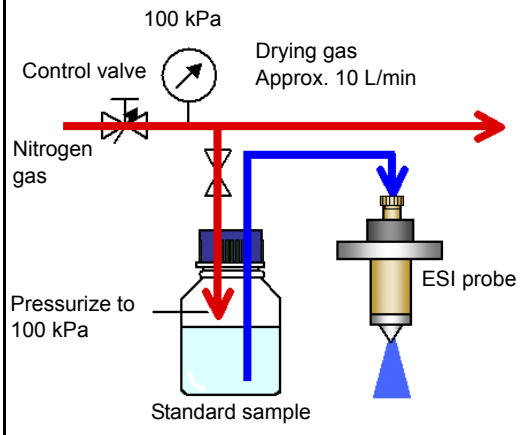


Fig. 2-31

2 After 10 seconds, close the valve to the standard sample and control the drying gas to the set flow rate.

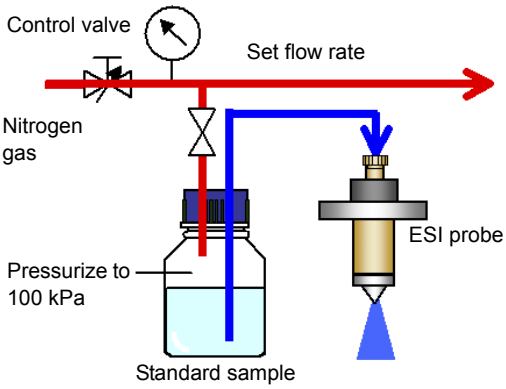


Fig. 2-32

When the standard sample is OFF:

1 Turn the drying gas OFF and open the valve to the standard sample to open the inside of the standard sample bottle to atmospheric pressure.

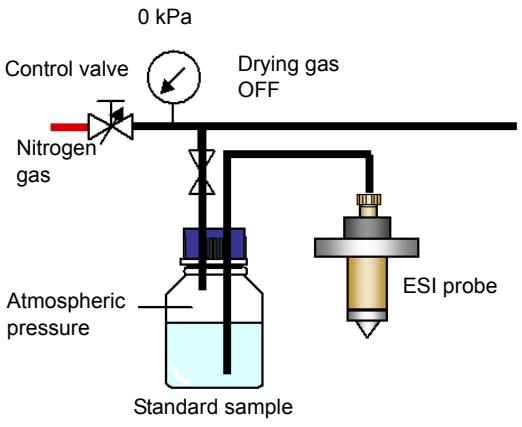


Fig. 2-33

2 Close the valve to the standard sample and control the drying gas to the set flow rate.

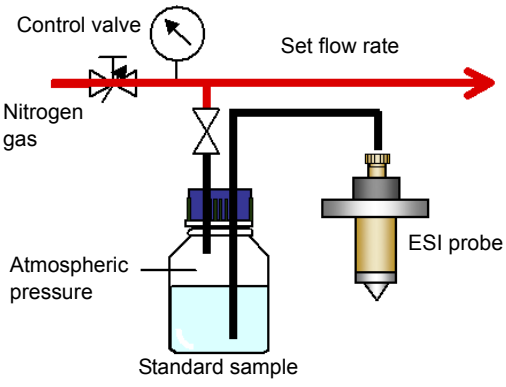


Fig. 2-34

2.11 Gas Control System

In the LCMS-8030/LCMS-8040, the nitrogen gas supply is branched so that it can be used as three types of gas: nebulizer gas, drying gas, and standard sample delivery gas. The gas is controlled and turned ON and OFF with the LabSolutions software.

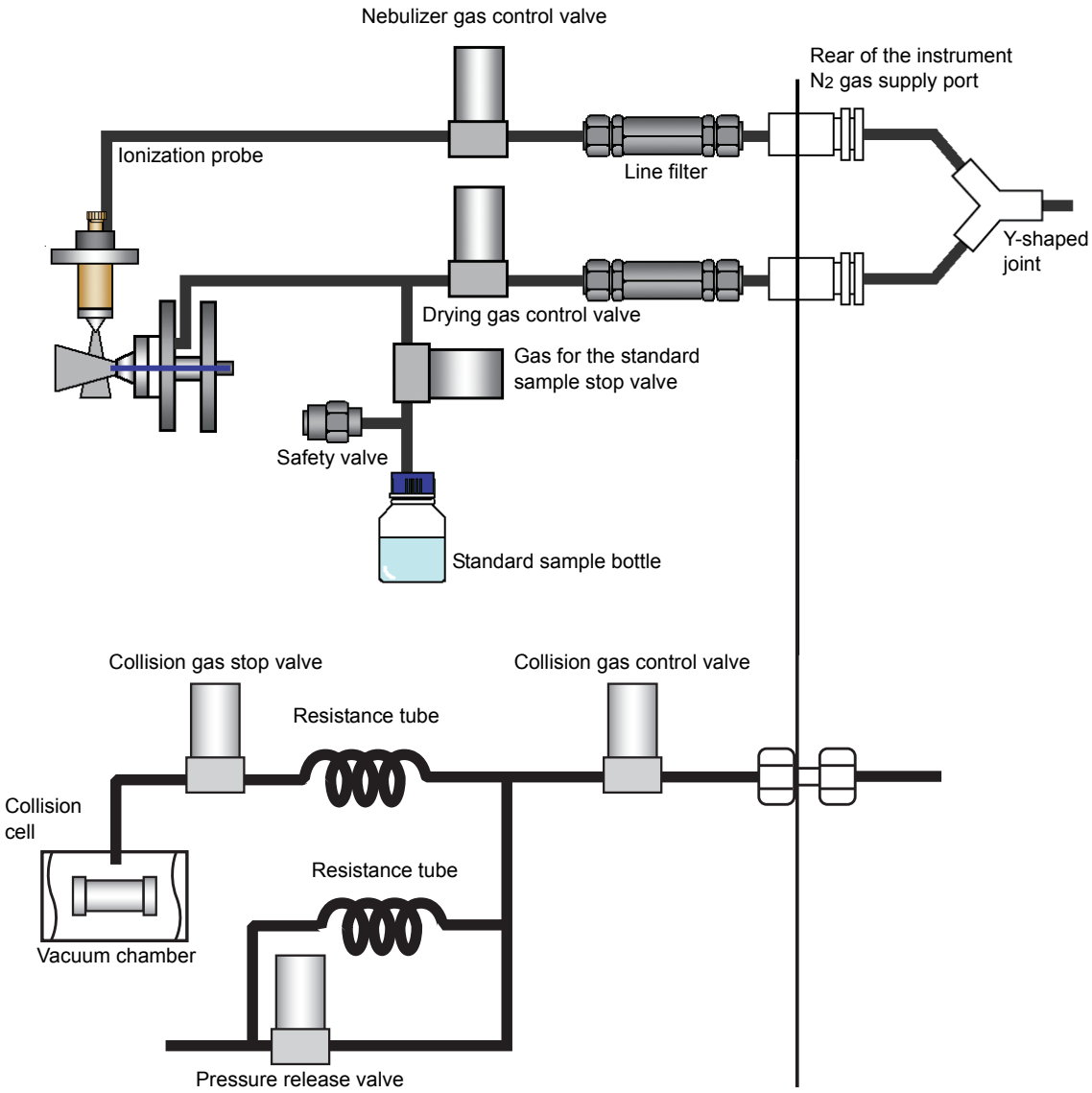


Fig. 2-35

2.12 Waste Drain

The waste drain comprises the drain that drains the solvent sprayed by the atmospheric pressure ionization probe (drain from the spray unit) and the drain from the leak tray.

The leak tray is equipped with a sensor that detects liquid leakage from the atmospheric pressure ionization probe and liquid leakage from the standard sample bottle.

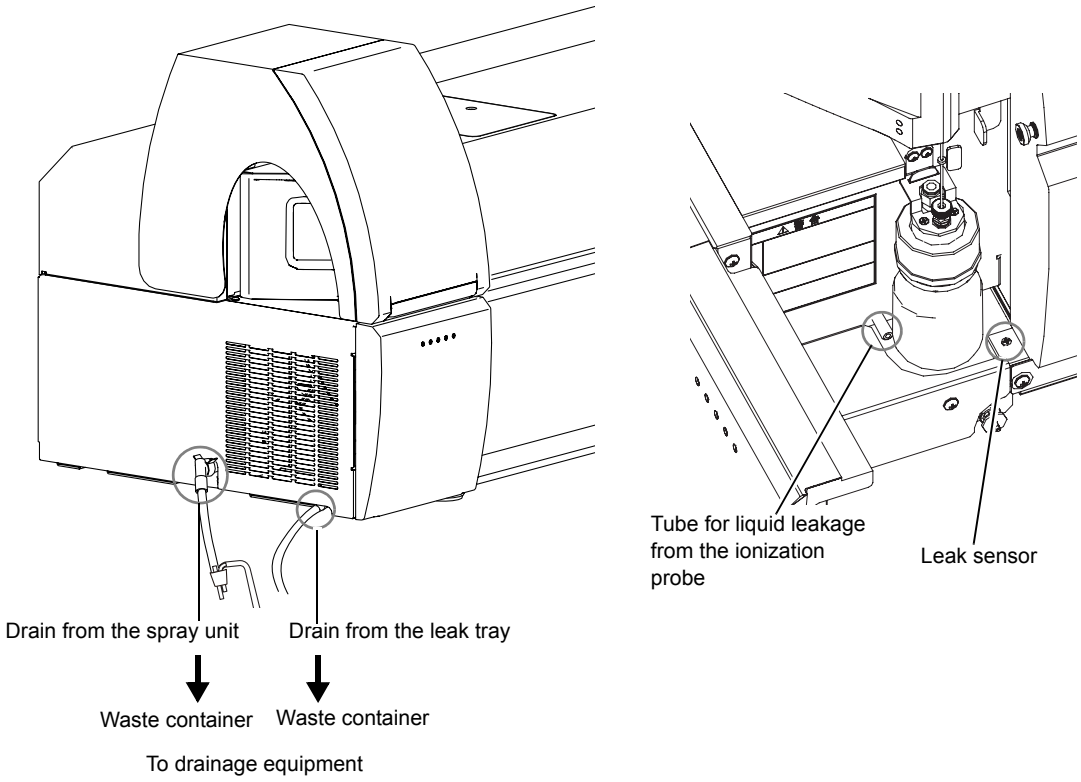


Fig. 2-36

2.13 Indication Lamps (LEDs)

The status of the instrument is shown by indication lamps (LEDs) on the front of the instrument.

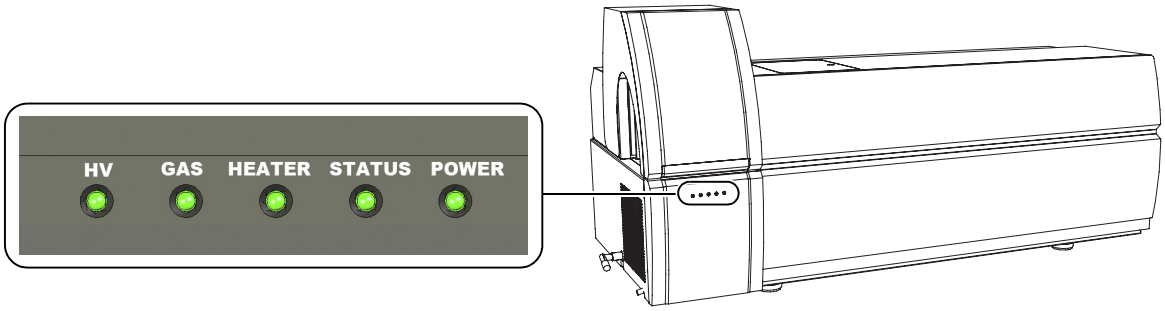


Fig. 2-37

Indication Lamps (LED)	LED Light Status	Operating Instrument Part	Instrument Status
HV	OFF	❶ Ionization voltage (probe voltage, needle voltage) ❷ Detector voltage (inside the instrument)	OFF
	Lit green	❶ Ionization voltage (probe voltage, needle voltage) ❷ Detector voltage (inside the instrument)	ON
GAS	OFF	❸ Nebulizer gas ❹ Drying gas	OFF
	Lit green	❸ Nebulizer gas ❹ Drying gas	ON
	Flashing green	❸ Nebulizer gas ❹ Drying gas	OFF
		❺ CID gas	ON
HEATER	OFF	❻ DL ❼ Heated block ❽ APCI heater (option)	OFF
	Lit green	❻ DL ❼ Heated block ❽ APCI heater (option)	ON
STATUS	OFF	Power supply to the instrument	OFF
	Lit green	❾ Rotary pump ❿ Triple inlet turbo molecular pump	Vacuum preparation complete
	Flashing green	❾ Rotary pump ❿ Triple inlet turbo molecular pump	Preparing for evacuation or in standby mode
	Flashing red	❾ Rotary pump ❿ Triple inlet turbo molecular pump	Vacuum error (triple inlet turbo molecular pump error)
POWER	OFF	Power supply to the instrument	OFF
	Lit green	Power supply to the instrument	ON

Note: The numbers ❶ to ❿ correspond to the operating parts in Fig. 2-38.

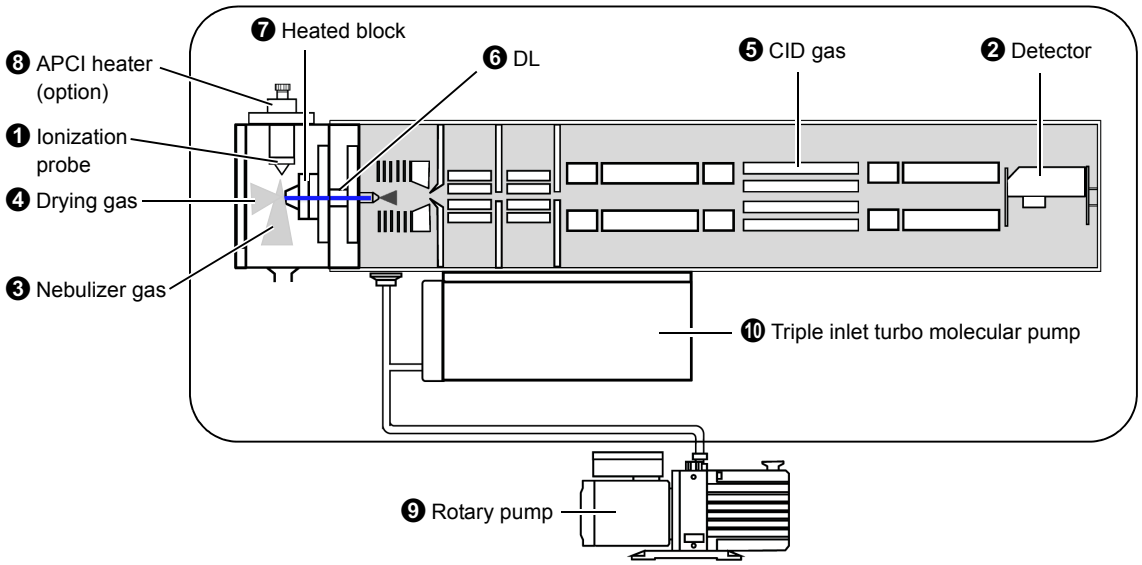


Fig. 2-38 LED Indications and Operating Parts

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3 Preparation

This chapter explains how to start and stop the instrument and the preparations to make before starting analysis.

Some parts of these explanations relate to the LabSolutions software. For more detail, refer to the "LabSolutions Software Instruction Manual". Also, operate each LC unit in accordance with the instruction manual provided for it.

3.1 Starting the Instrument

3.1.1 Turning the Power ON

1 Turn ON the power to each of the LC and MS units.

The POWER indication lamp on the front of the LCMS-8030/LCMS-8040 will light in green and the STATUS indication lamp will flash in green.

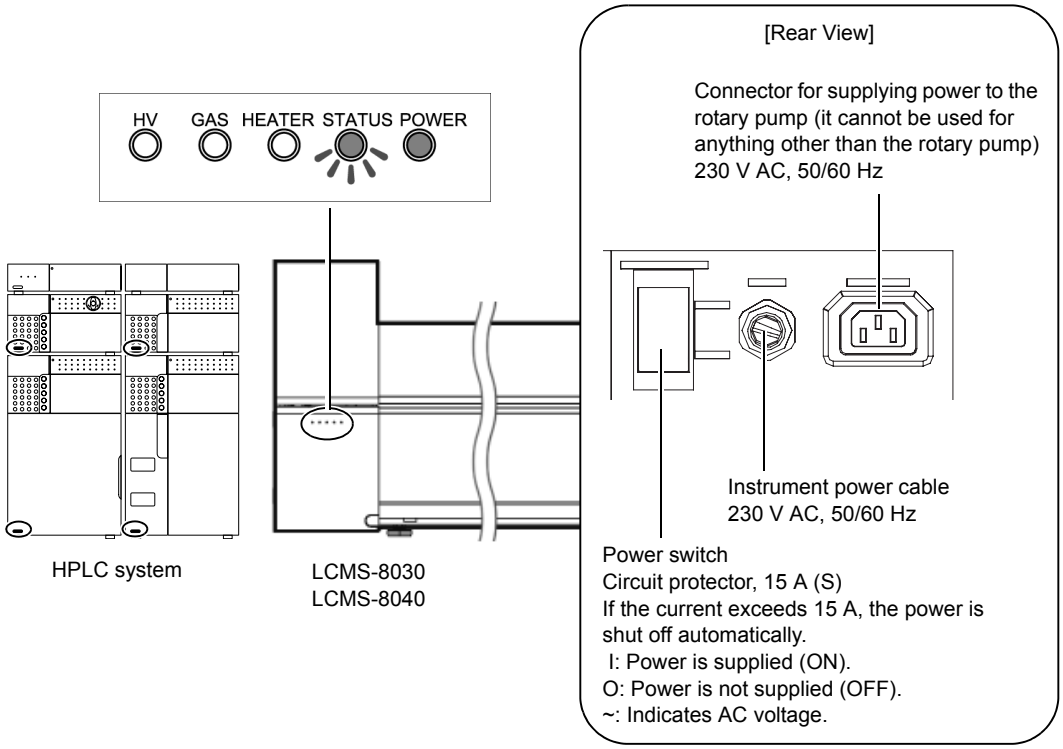


Fig. 3-1

2 Turn on the peripheral units (monitor, printer, etc.), turn on the power to the PC and start Windows.

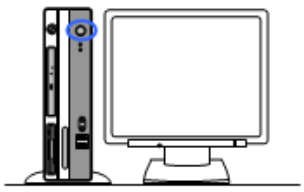
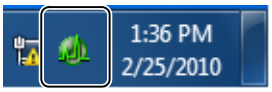


Fig. 3-2

3.1.2 Starting the Vacuum System

1 Open the valve of the CID gas cylinder.

2 Check that the [LabSolutions Service] icon is green.

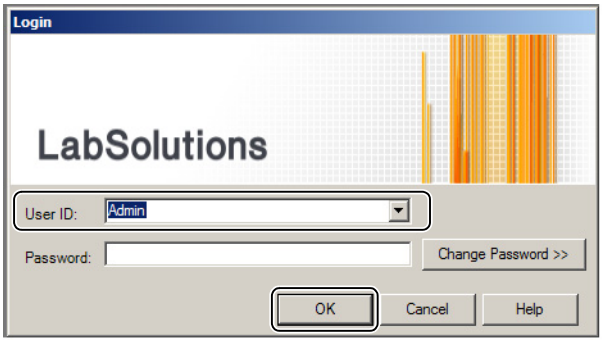


If this icon is yellow it means that the system is still starting up, so please wait a while.
If the icon is red, an error has occurred and you must restart the computer.

3 Double-click  on the desktop.

4 Log in.

Enter "Admin" at [User ID:], then click the [OK] button without entering anything in the [Password:] textbox.
To change the user or add a user, make the change you want to and log in.

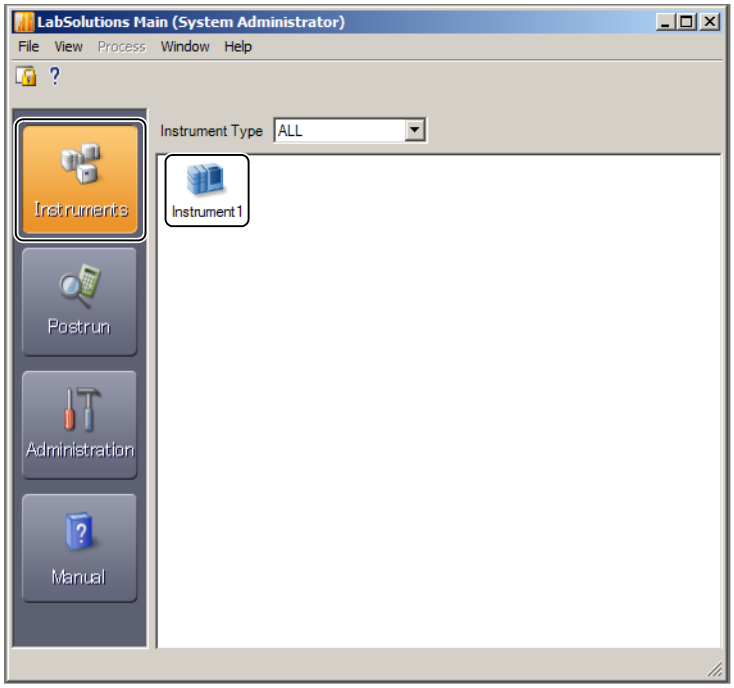


5 Start the analysis program.

Click 

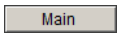
and then double-click 

.



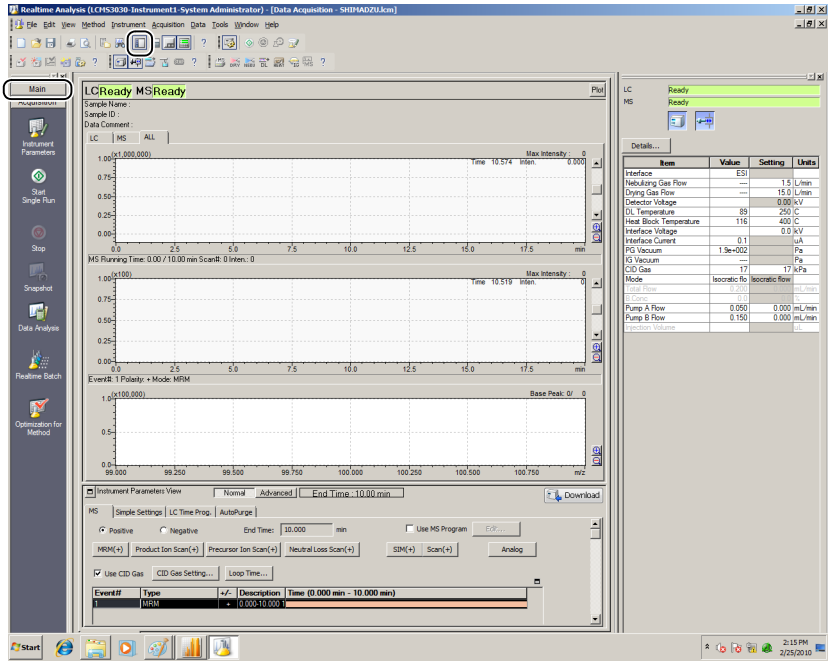
6 Open the [Data Acquisition] window and click 

(System Control).

Click 

(Main).

If the assistant bar is not displayed, click 
.



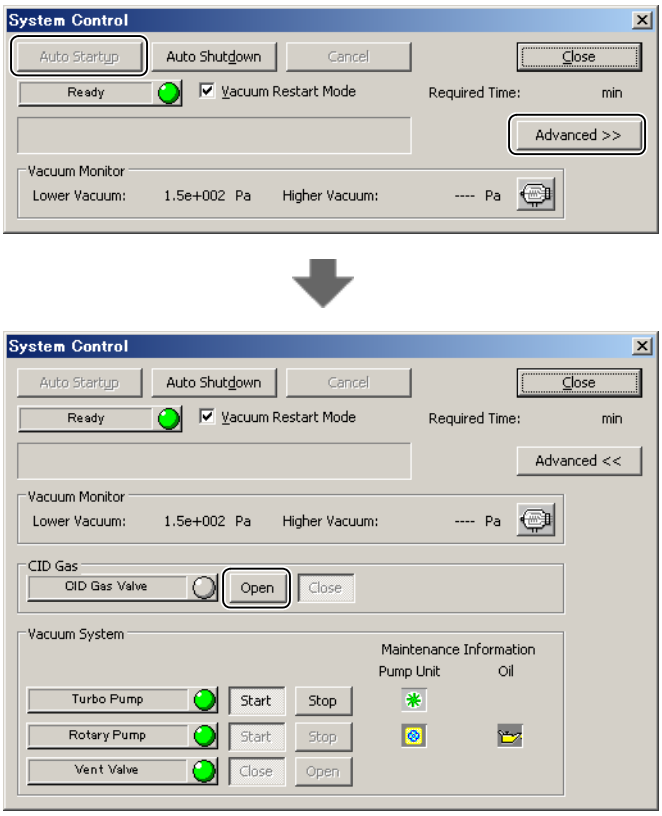
The instrument's [System Control] window will be displayed.

7 Click [Auto Startup].

The rotary pump will start, followed by the triple inlet turbo molecular pump.
Evacuation preparations are completed in about one hour, after which the "STATUS" indicator lamp lights up in green.
(If evacuation is stopped for an extended period of time, wait half to a whole day after performing evacuation prior to starting analysis.)

NOTE

If the system has been automatically started while the CID gas valve is closed, open the main cock on the CID gas cylinder, click [Advanced], and then click [Open] for [CID Gas valve].



CAUTION

Instructions

- Starting the rotary pump when the temperature is low

  When the instrument has been stopped for a long time when the ambient temperature is low, for example in the winter, the viscosity of the oil in the rotary pump increases.
  Starting the rotary pump under these conditions can impose an excessive load on the motor, actuating the breakers at the instrument and the distribution panel.
  If this happens, turn on the heating in the room and start the vacuum system once the temperature of the rotary pump (the temperature of the instrument's installation environment) has reached at least 18 °C.

- Supply CID gas to the instrument when starting the vacuum system.

  This enables the CID gas to flow and purge the ducts.

■ Using a DL plug for efficient evacuation

When starting the vacuum system you can shorten the starting time by sealing the DL with a DL plug.

The shutter can also protect the internal parts of the vacuum system from contamination when the instrument is not to be used for a long time.

⚠ WARNING

Instructions

- Before starting maintenance work, turn the heater OFF from the LabSolutions program and make sure that the temperature of the heated block has fallen to 50 °C or lower.
  The spray unit reaches high temperatures and could cause burns.
- Before starting maintenance work, turn the high-voltage switch OFF in the LabSolutions program and disconnect the high-voltage cable.
  If the high-voltage cable is not disconnected there will be a danger of electric shock.

1 Open the probe cover.

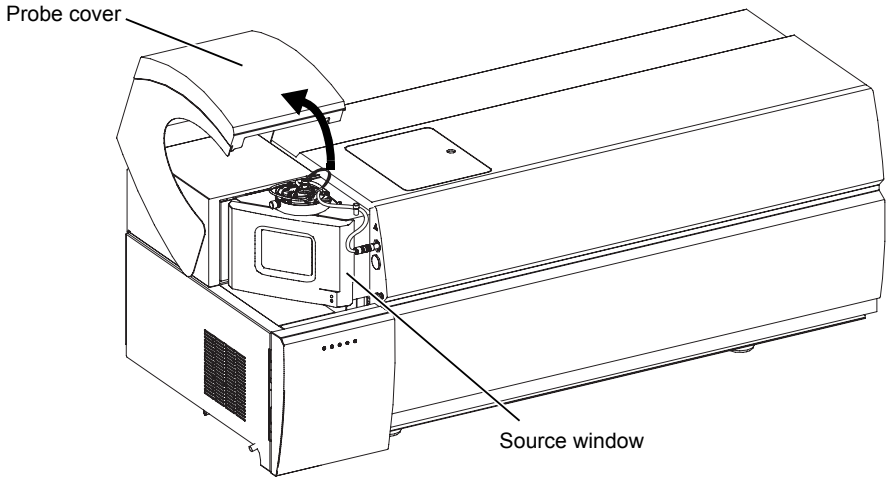


Fig. 3-3

2 Grip the lower right of the source window and pull towards you.

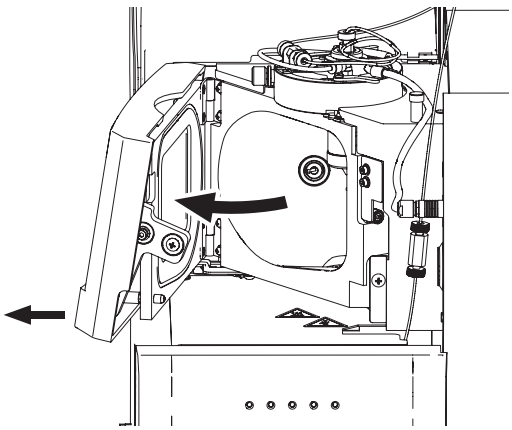


Fig. 3-4

3 Lift up the source window.

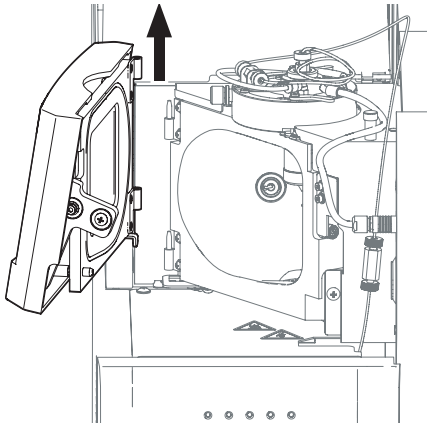


Fig. 3-5

4 Insert the DL plug into the DL center hole.

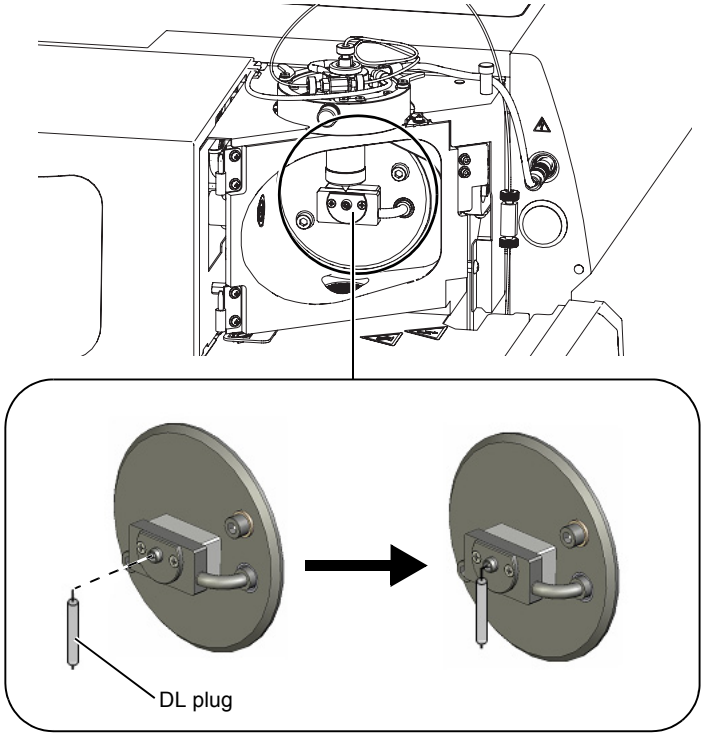


Fig. 3-6

5 Close the source window.

1 Replace the source window on its hinges.
2 Push the lower right of the source window.
This locks the source window in place.

6 Close the probe cover.

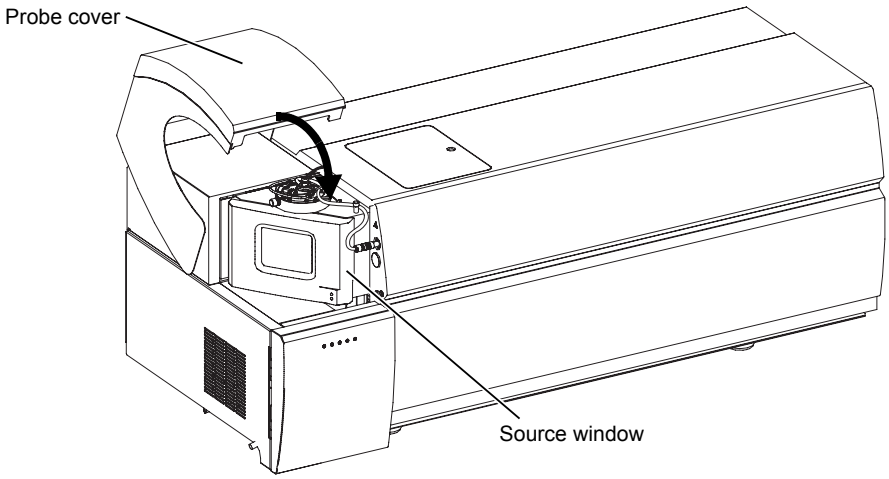


Fig. 3-7

NOTE

The DL plug must be removed before starting analysis.

3.2 Stopping the Instrument

This section describes the procedure for stopping the instrument's vacuum system and up to turning the power OFF.

Hint

The vacuum status affects the instrument's sensitivity. With the exception of situations where the instrument is not used for a long time, the instrument's vacuum system should be kept on in order to maintain a high vacuum in everyday use. (For details on daily shutdown of the instrument, see "3.4 Daily Shutdown" P.54.)

3.2.1 Stopping the Vacuum System

1 Open the [System Control] window.

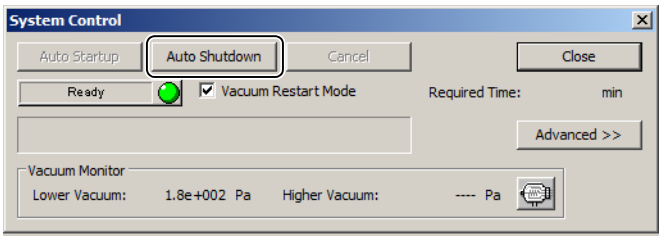
Reference

"3.1.2 Starting the Vacuum System" P.42

2 Click [Auto Shutdown].

If the temperature of the heated block and DL decreases below 100 °C, the triple inlet turbo molecular pump and the rotary pump will stop and the inside of the vacuum housing will be opened to atmospheric pressure.

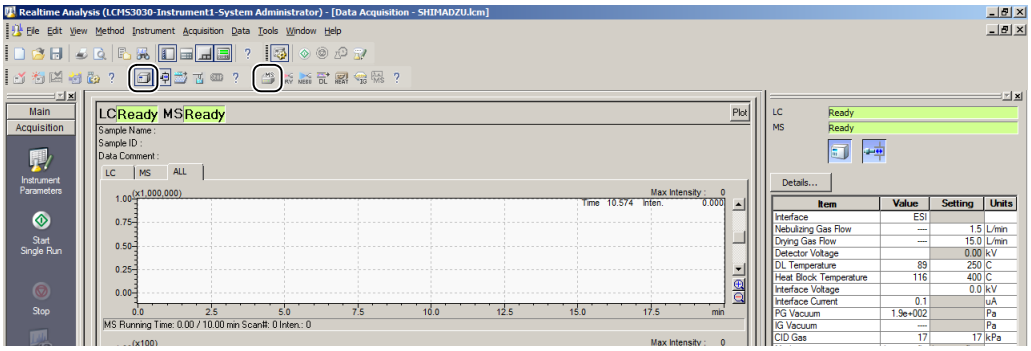
It takes approximately 3 minutes to equalize with atmospheric pressure.



3.2.2 Exiting LabSolutions

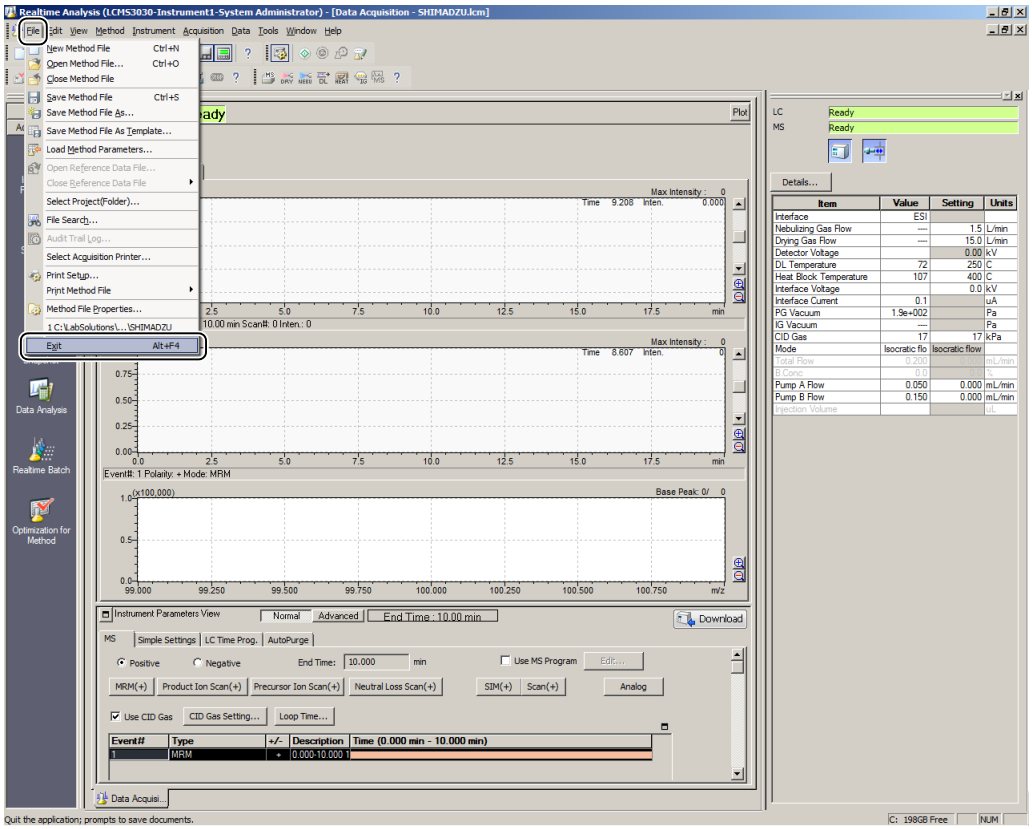
1 Turn off the operation of the LC and MS.

Click  and  .



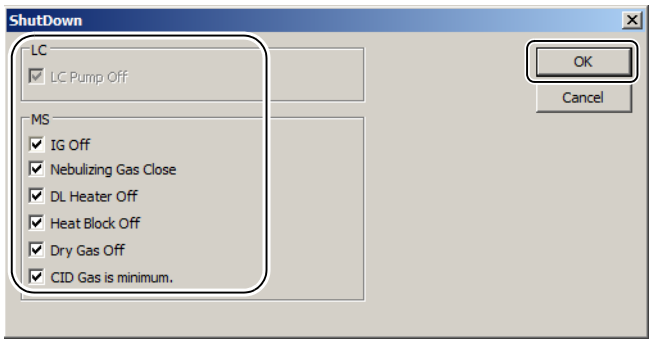
2 Close the open window.

Click the [File] menu and select [Exit].



The [ShutDown] window is displayed.

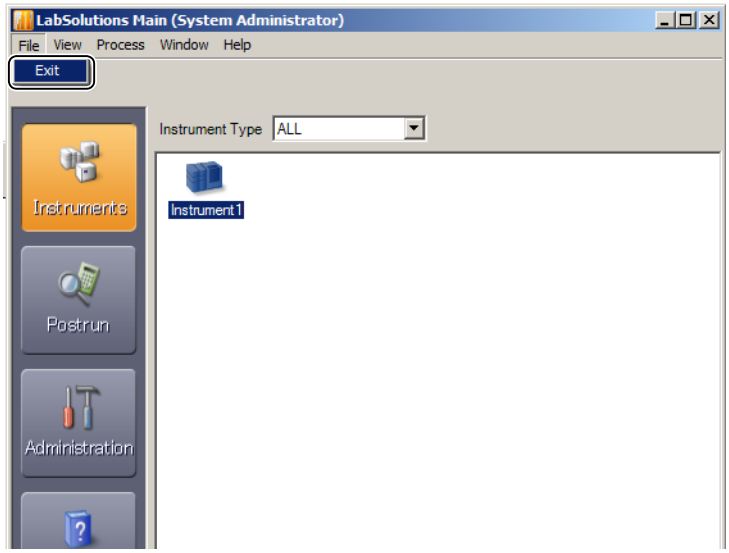
3 Select all the items and click [OK].



Shutdown processing will be performed.

4 Exit LabSolutions.

Click the [File] menu and select [Exit].



3.2.3 Turning the Power OFF

1 Turn off the power to each unit of the LC and MS.

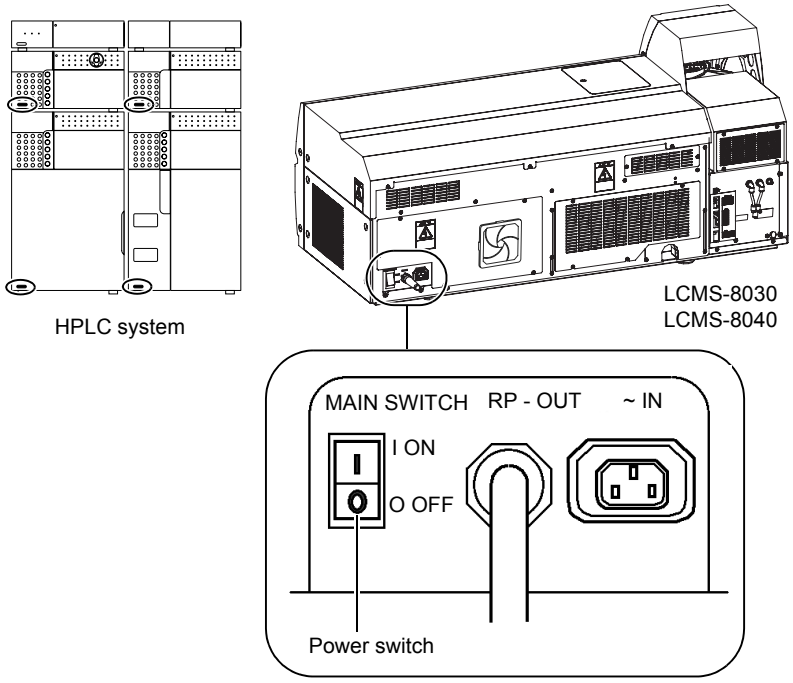


Fig. 3-8

Hint

In everyday operation, don't turn OFF the power to the LCMS-8030/LCMS-8040.

2 Close the valve of the CID gas cylinder.

3 Turn off the nitrogen gas generator.

3.3 Daily Startup

This section explains the procedure for everyday starting from the situation where the vacuum system of the LCMS-8030/LCMS-8040 has been started up (the power is ON).

1 Turn ON the power to every unit of the LC.

2 Check that the nitrogen gas generator is turned on and supply nitrogen gas to the MS.
Gas supply pressure: 690 to 800 kPa, purity: 97 % or more

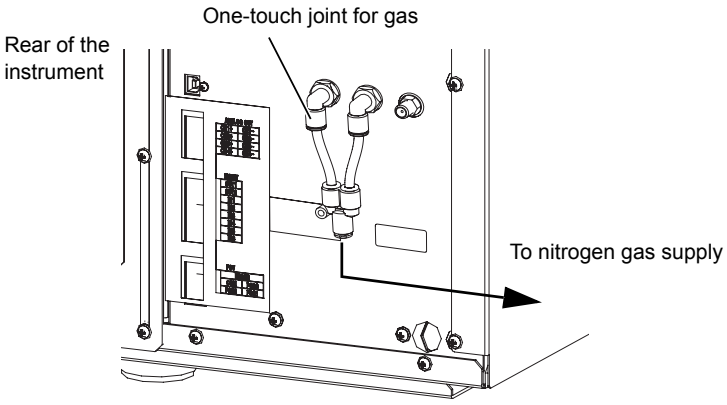


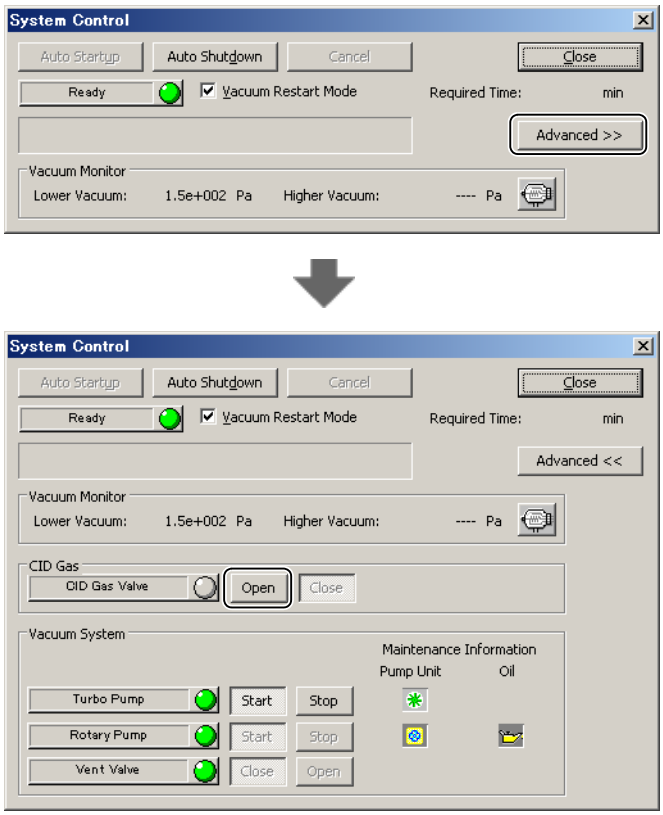
Fig. 3-9

3 Turn on the peripheral units (monitor, printer, etc.). Turn on the power to the PC and start Windows.

4 Start up LabSolutions.

5 Open the valve of the CID gas cylinder if it is closed.

In this case, click [Advanced], then click [Open] for [CID Gas valve].



6 Turn on the LC pump and oven, and the LCMS heated block, DL, and gas, and start operation.

3.4 Daily Shutdown

Hint

The vacuum status affects the instrument's sensitivity. With the exception of situations where the instrument is not used for a long time, the instrument's vacuum system should be kept on in order to maintain a high vacuum in everyday use.

1. Exit LabSolutions.

   Reference

   "3.2.2 Exiting LabSolutions" P.48

2. Stop the supply of nitrogen gas.

3. Turn OFF the power of every LC unit.

4. Mount the DL plug.

3.5 Preparation for ESI Analysis

3.5.1 Mounting the ESI Probe

1 Take the ESI probe ASSY out of its packing and check the projection length of the capillary tube.

Reference
"7.2 Maintenance of the ESI Probe" P.122

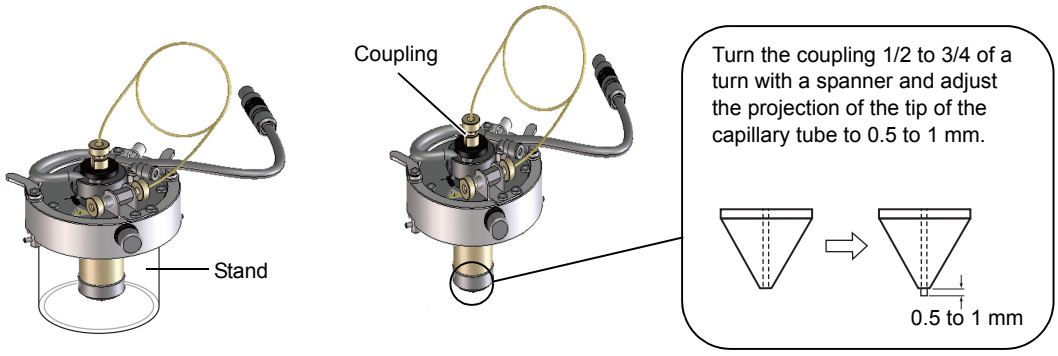


Fig. 3-10

CAUTION

Prohibitions

Do NOT knock the tip of the ESI probe against anything or contaminate it. This may reduce sensitivity.

2 Open the probe cover and mount the ESI probe on the instrument.
Mount the probe with the position adjustment knob facing toward you.

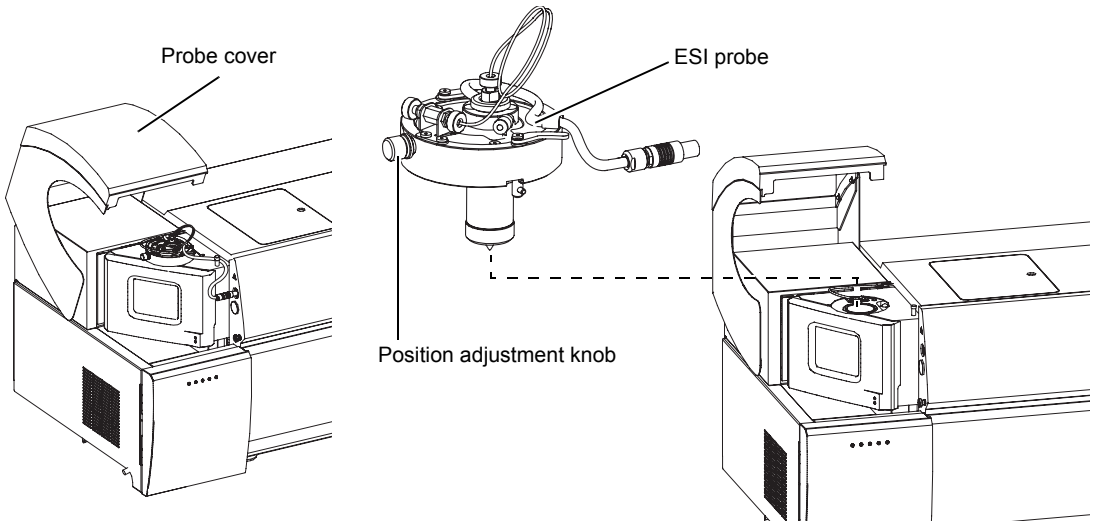


Fig. 3-11

3 Lock the ESI probe clamping levers.

Move the clamping levers to the positions indicated by the broken lines, insert the ESI probe, then push the clamping levers in the direction indicated by the arrows to clamp the probe.

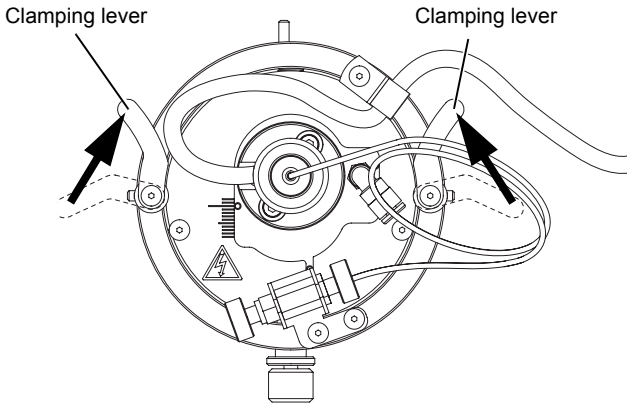


Fig. 3-12

4 Check the position of the ESI probe.

Adjust the position of the probe by tightening the locking screw in the counter-clockwise direction and turning the adjustment knob as necessary.
After adjustment, turn the locking screw in the clockwise direction to lock the adjustment knob.

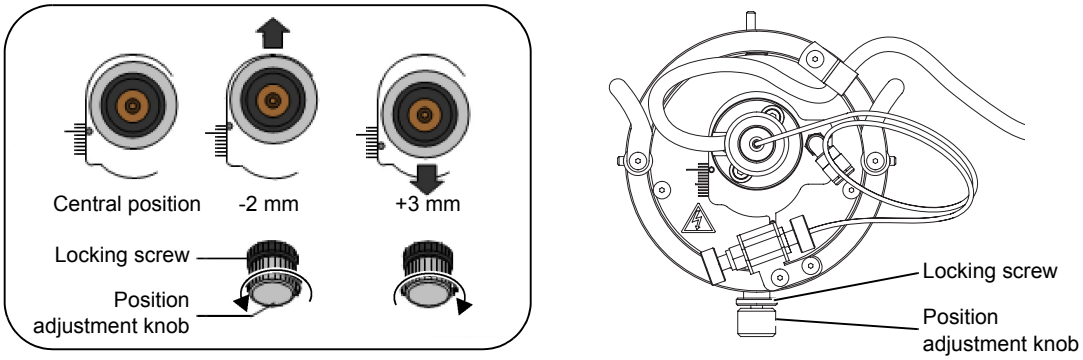


Fig. 3-13

Hint

Guide to ESI probe position

ESI analysis	0.2 mL/min to 0.5 mL/min → 0 to +2 mm
	1 mL/min → +3 mm
DUIS analysis	-1 to +1 mm
Auto tuning	+1.5 mm

5 Connect the nebulizer gas tube, tubing, and high-voltage cable.

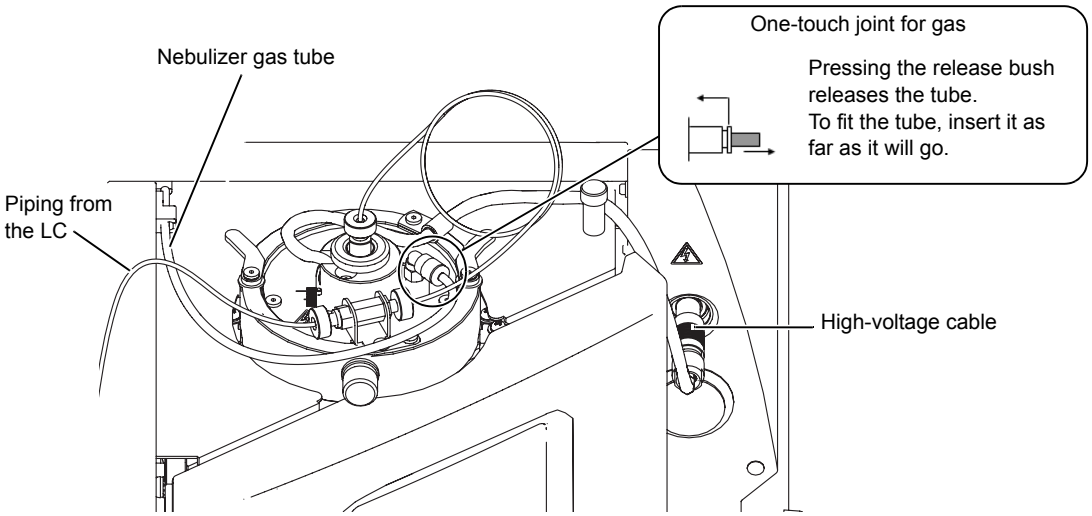


Fig. 3-14

WARNING

Instructions

Turn the high voltage supply OFF from LabSolutions before connecting to the instrument.

If you do not turn it OFF there will be a risk of electric shock.

Reference
"4.1 Turning the High Voltage ON/OFF" P.93

6 Close the probe cover.

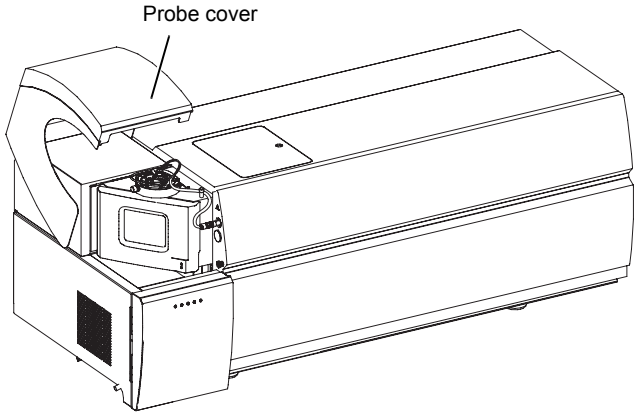


Fig. 3-15

3.5.2 Removing the ESI Probe

1 Open the probe cover and remove the high-voltage cable.

Unplug the connector.

WARNING

Instructions

Turn the high-voltage supply OFF from LabSolutions before connecting or disconnecting the high-voltage cable.

If you do not turn it OFF there will be a risk of electric shock.

Reference
"4.1 Turning the High Voltage ON/OFF" P.93

2 Disconnect the tubing.

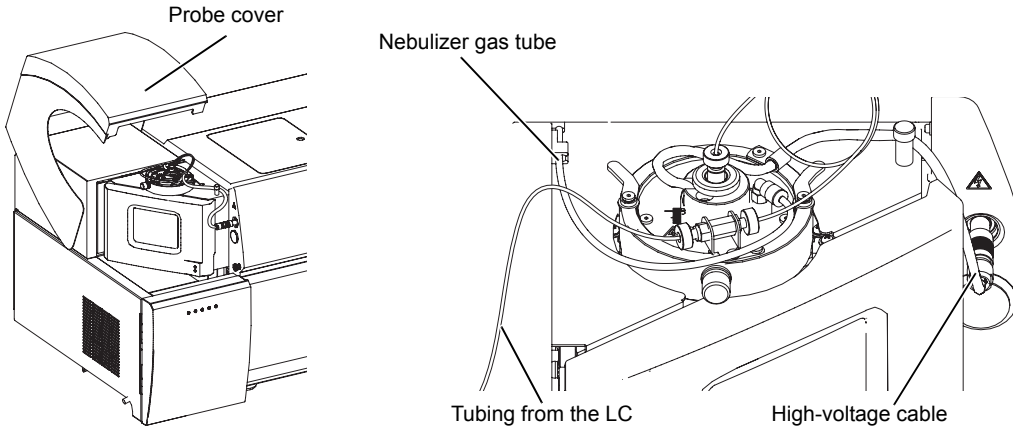


Fig. 3-16

3 Disconnect the nebulizer gas tube.

One-touch joint for gas

Pressing the release bush releases the tube.
To fit the tube, insert it as far as it will go.

CAUTION

Instructions

Turn the gas OFF from LabSolutions before connecting or disconnecting the nebulizer gas tube.

Reference
"4.3 Gas ON/OFF Status and Flow Rate Monitor" P.96

4 Unlock the ESI probe clamping levers.

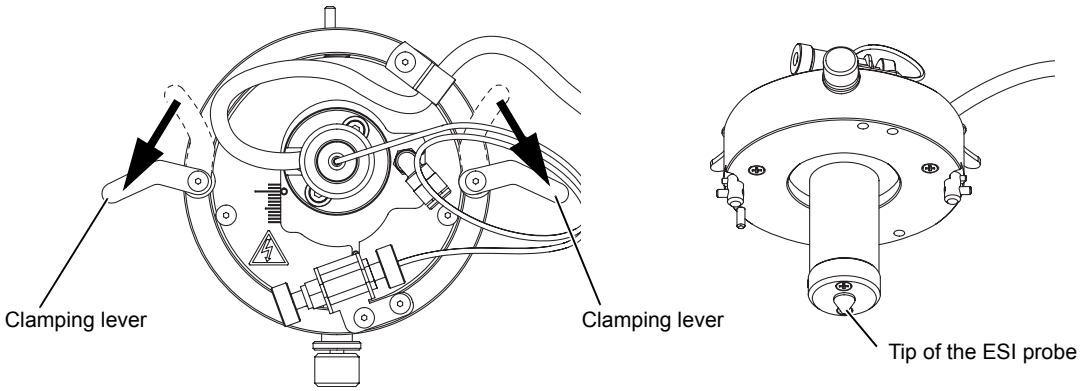


Fig. 3-17

CAUTION

Prohibitions

Do NOT knock the tip of the ESI probe against anything or contaminate it. This may reduce sensitivity.

5 Remove the ESI probe.

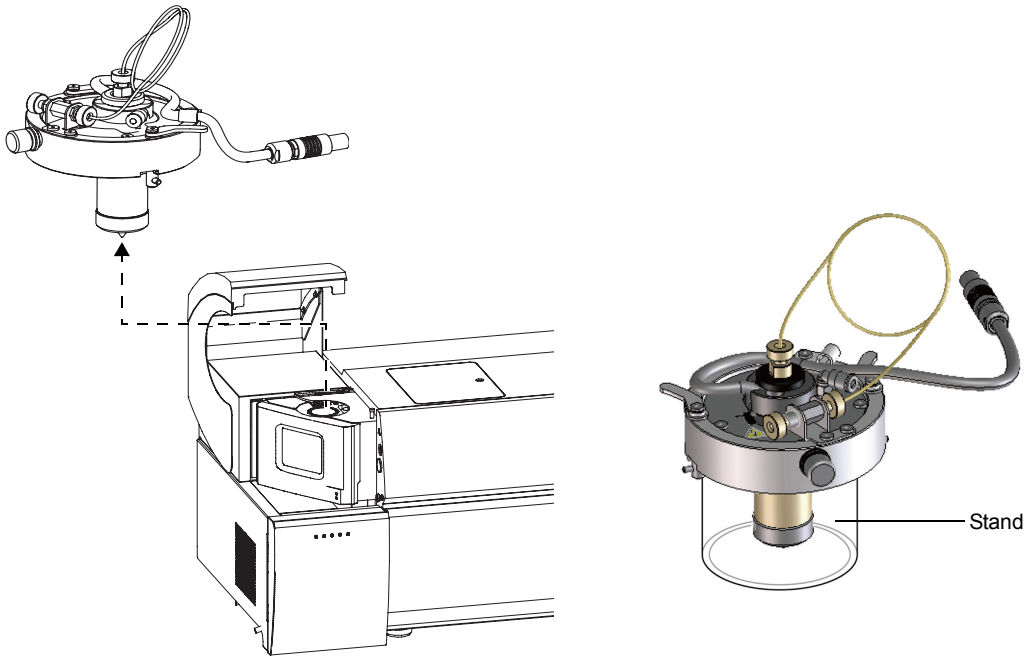


Fig. 3-18

Hint

Once you have taken the ESI probe out, rest it on its stand.

3.6 Preparation for APCI Analysis

3.6.1 Mounting the Corona Needle for APCI

WARNING

Disconnect the high-voltage cable before starting this work.

If it is not disconnected there will be a danger of electric shock.

Instructions

Reference

"4.1 Turning the High Voltage ON/OFF" P.93

1 Open the probe cover.

2 Open the source window.

WARNING

Check that the temperature of the DL and heated block has fallen to 50 °C or lower before proceeding with the work.

The ion source unit reaches high temperatures. Turn the heater OFF from LabSolutions before starting the work.

If you proceed with the work while the temperature is still high, you may sustain burns.

Instructions

Reference

"4.2 Heater ON/OFF Status and Temperature Monitor" P.94

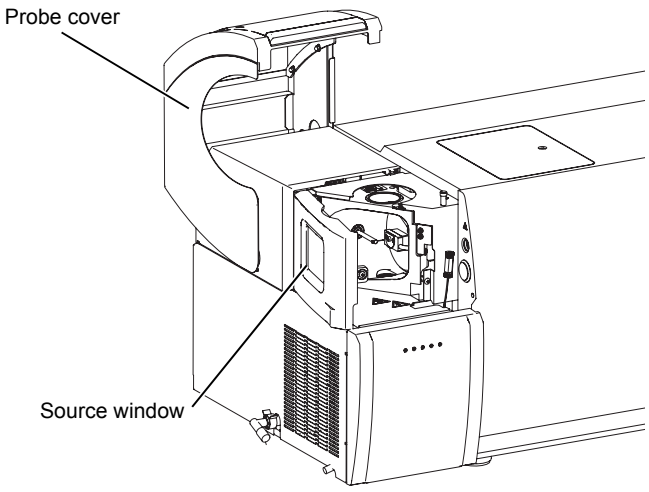


Fig. 3-19

3 Set the needle unit.

If a corona needle plug is used in the socket, remove the plug and then insert the needle as far as it will go into the socket, ensuring that the pin is aligned with the notch.
Make sure that the tip of the needle unit is positioned in the center of the DL tube.

⚠ CAUTION

Take care because the tip of the APCI needle is sharp.

Instructions

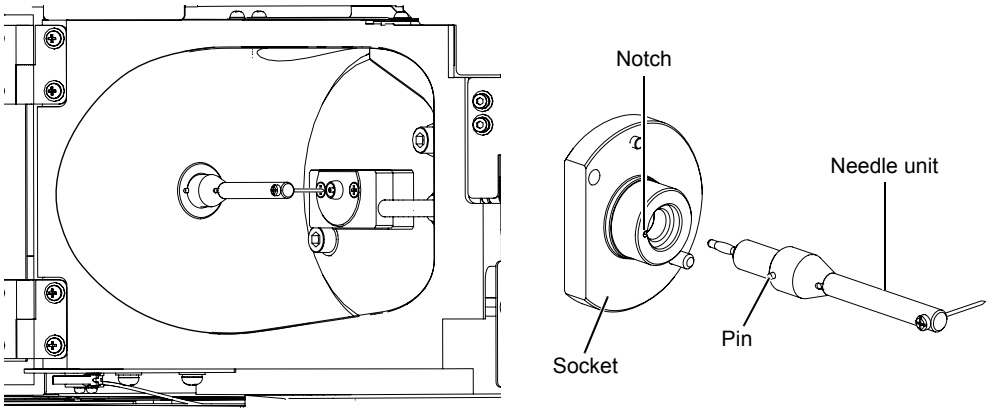


Fig. 3-20

Hint

Check that the tip of the APCI needle is not bent by using the needle alignment tool.

Check that the needle is contained within the range of the slit and repair the needle if it is bent.

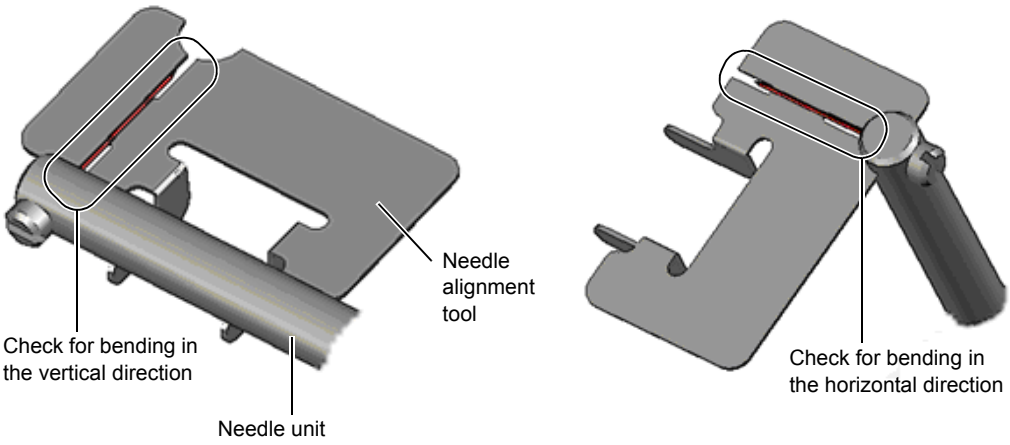


Fig. 3-21

4 Close the source window.

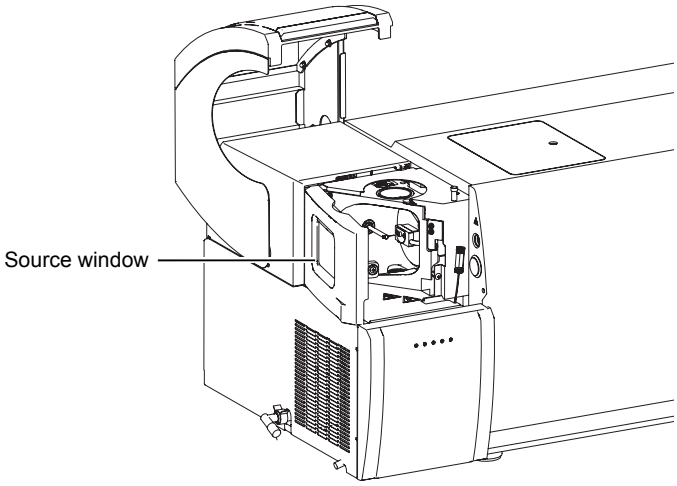


Fig. 3-22

5 Connect the APCI high-voltage cable connector.

WARNING

Instructions

Turn the high-voltage supply OFF from LabSolutions before connecting or disconnecting the high-voltage cable.

If you do not turn it OFF there will be a risk of electric shock.

Reference

"4.1 Turning the High Voltage ON/OFF" P.93

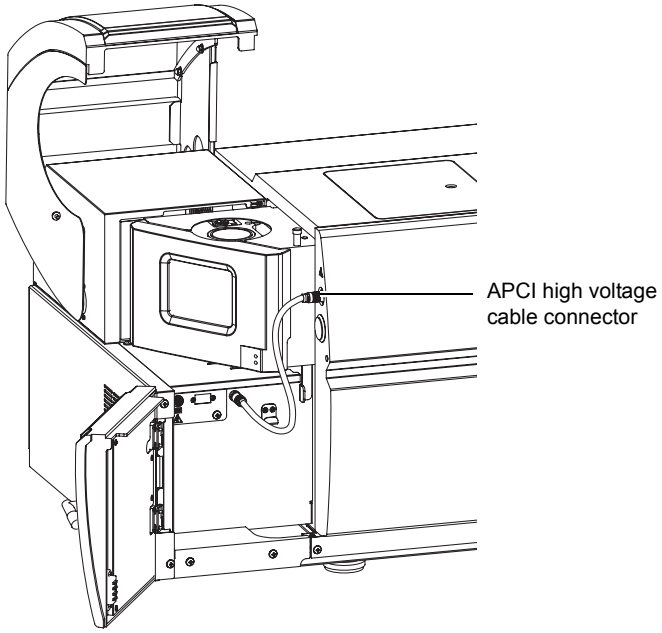


Fig. 3-23

3.6.2 Mounting the APCI Probe

CAUTION

Instructions

When performing APCI analysis in which a halogenated mobile phase additive is used, note the following:

In the APCI method, the analyte is heated to high temperatures. If the mobile phase contains a halogenated compound such as chloroform, a corrosive gas will be produced. Even a small percentage concentration of halogens in the mobile phase can cause corrosion.

Use SUS tubes to connect the high performance liquid chromatograph to the instrument. PEEK resin tubes do not have sufficient strength and should they rupture, solvent may blow out.

Black particles may build up on the APCI probe or inside the probe holder.

Because of exposure to corrosive gases, you may need to replace the following parts at a shorter interval than specified.

Part Name	Part No.
APCI pipe ASSY	S225-15845-91
Nebulizer joint ASSY	S225-15788-91
Heater unit ASSY	S225-15619-41
Adapter	S225-04993
Ferrule (LCMS-2020)	S225-03748-03
Nut	S225-15739
Heater flange	S225-15486-91
Needle unit	S225-15921-92
DL	S225-15718-91

1 Take the APCI probe out of its packaging.

NOTE

Remove the stand from the probe before mounting it on the instrument.

The probe can be removed by opening out the clamping levers.

2 Place the APCI probe onto the instrument from above as shown in Fig. 3-24.

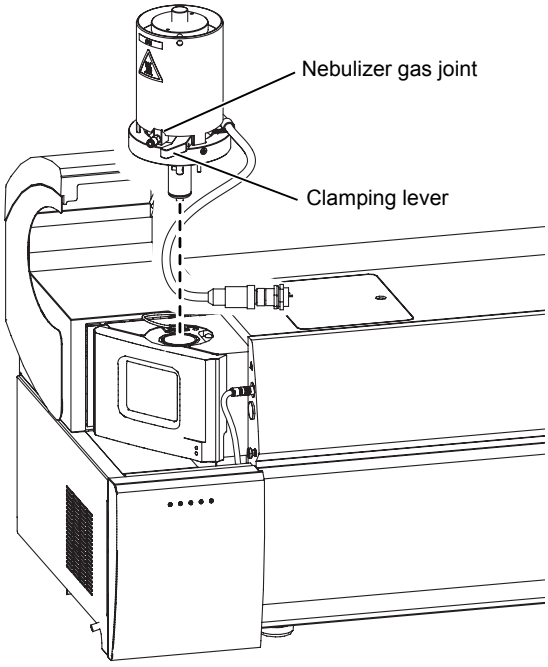


Fig. 3-24

3 Lock the APCI probe clamping levers.

Move the clamping levers to the positions indicated by the broken lines, insert the APCI probe, then push the clamping levers in the direction indicated by the arrows to clamp the probe.

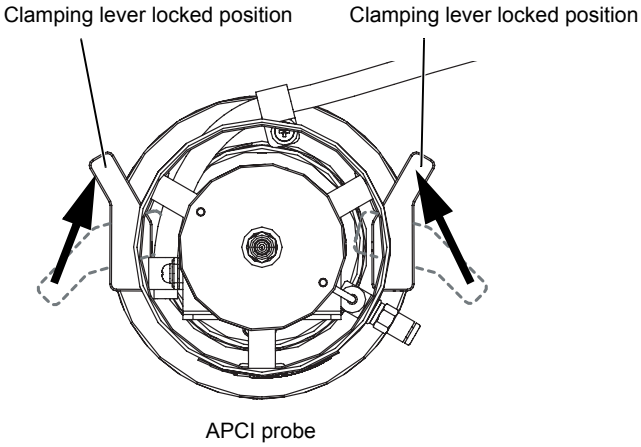


Fig. 3-25

4 Connect the heater cable.

Insert the connector with its notch positioned at the top left and turn it clockwise.

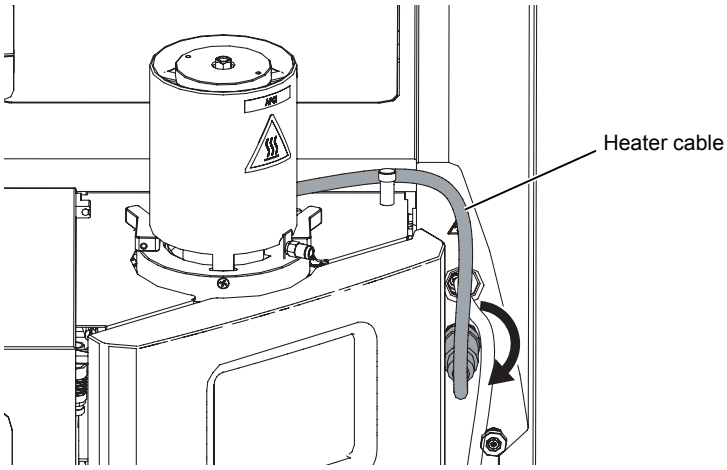


Fig. 3-26

5 Connect the nebulizer gas tube.

6 Connect the tubing.

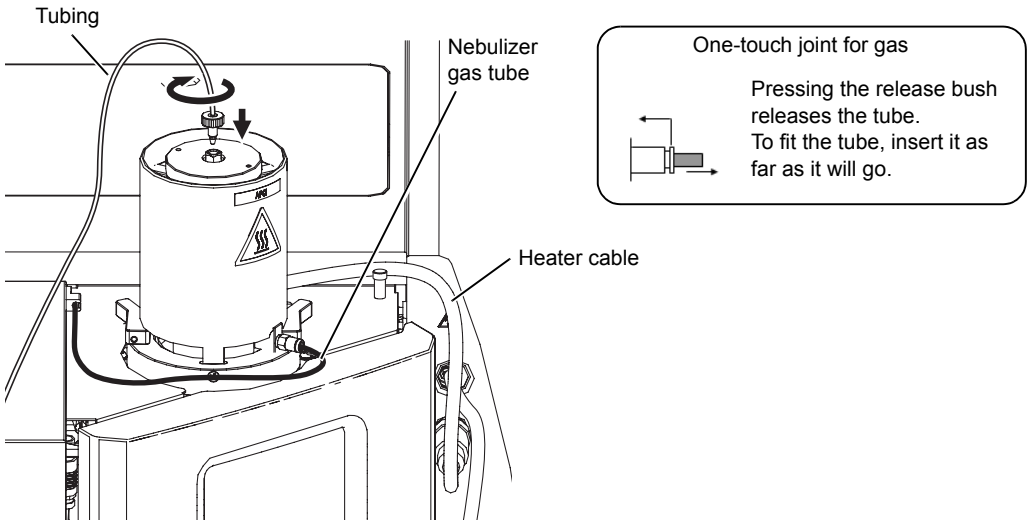


Fig. 3-27

3.6.3 Removing the APCI Probe

WARNING

Instructions

Check that the temperature of the APCI probe has fallen below 50 °C before attempting removal.

The APCI probe reaches high temperatures. You could sustain burns. Turn the heater OFF from LabSolutions before starting removal.

Reference

"4.2 Heater ON/OFF Status and Temperature Monitor" P.94

1 Open the probe cover.

2 Disconnect the tubing.

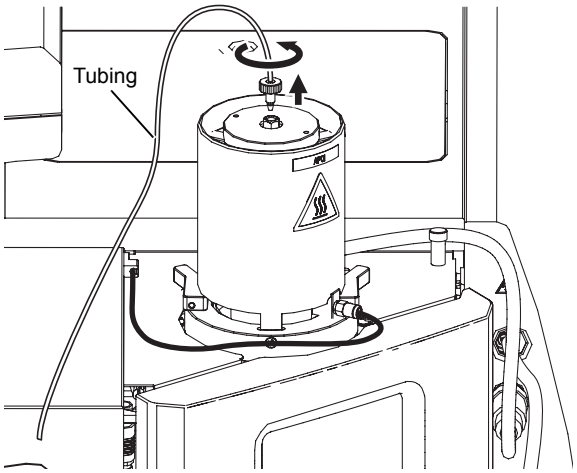


Fig. 3-28

3 Disconnect the nebulizer gas tube.

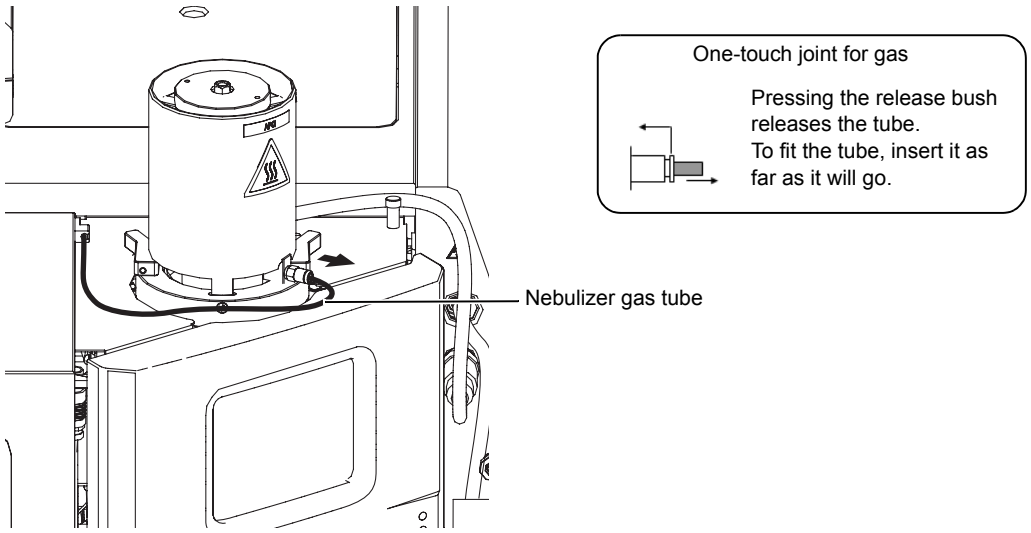


Fig. 3-29

CAUTION

Turn the gas OFF from LabSolutions before connecting or disconnecting the nebulizer gas tube.

Instructions

Reference
"4.3 Gas ON/OFF Status and Flow Rate Monitor" P.96

4 Disconnect the heater cable.

Turn the connector counter-clockwise.

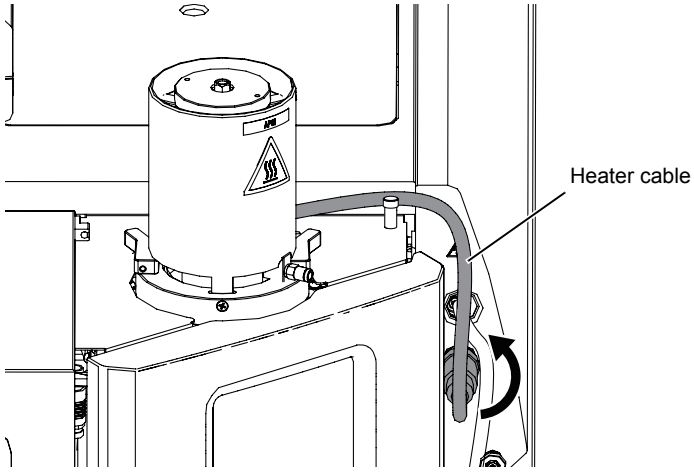


Fig. 3-30

5 Unlock the APCI probe clamping levers.

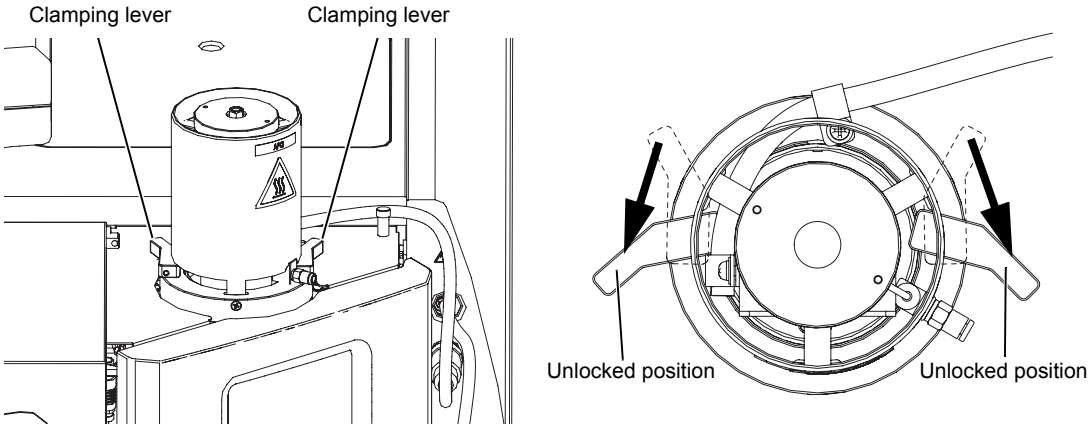


Fig. 3-31

6 Remove the APCI probe.

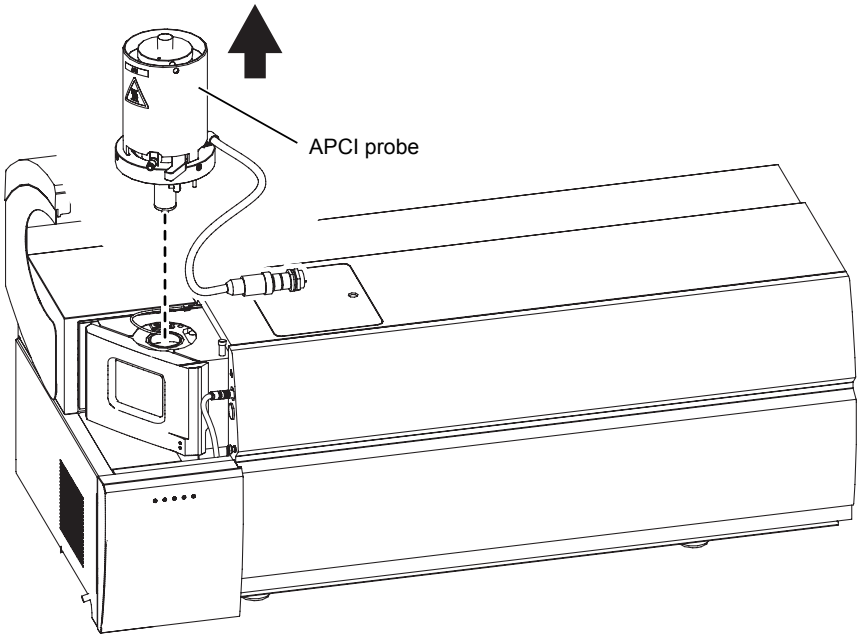


Fig. 3-32

7 Disconnect the APCI high-voltage cable.

WARNING

Instructions

Turn the high-voltage supply OFF from LabSolutions before connecting or disconnecting the high-voltage cable.

If you do not turn it OFF there will be a risk of electric shock.

Reference
"4.1 Turning the High Voltage ON/OFF" P.93

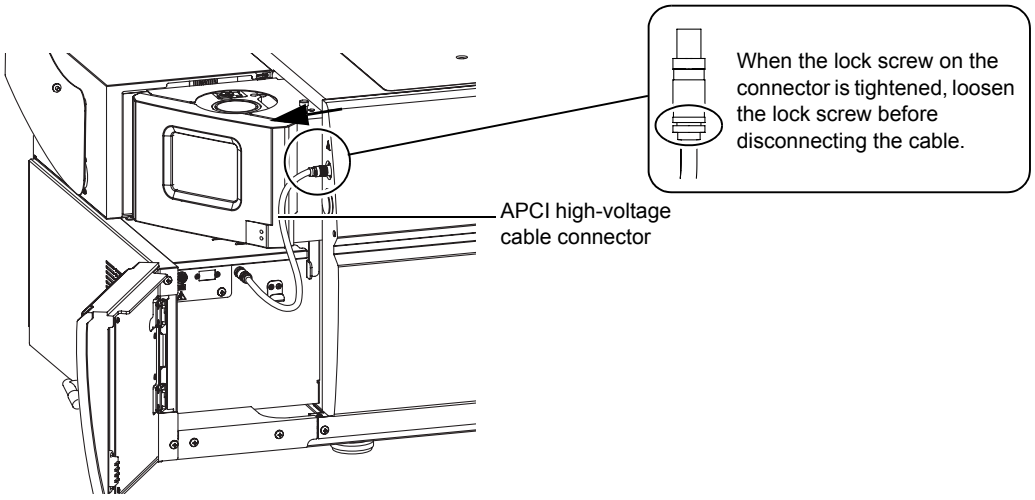


Fig. 3-33

3.6.4 Removing the Corona Needle for APCI

WARNING

Instructions

Turn the high-voltage supply OFF from LabSolutions before connecting or disconnecting the high-voltage cable.

If you do not turn it OFF there will be a risk of electric shock.

Reference
"4.1 Turning the High Voltage ON/OFF" P.93

1 Open the source window.

WARNING

Instructions

Check that the temperature of the DL and heated block has fallen to 50 °C or lower before proceeding with the work.

The ion source unit reaches high temperatures. You could sustain burns. Turn the heater OFF from LabSolutions before starting removal.

Reference
"4.2 Heater ON/OFF Status and Temperature Monitor" P.94

2 Remove the needle unit.

Remove it in the direction indicated by the arrow.

WARNING

Instructions

Disconnect the high-voltage cable before starting this work.

If it is not disconnected there will be a danger of electric shock.

CAUTION

Instructions

Take care because the tip of the APCI needle is sharp.

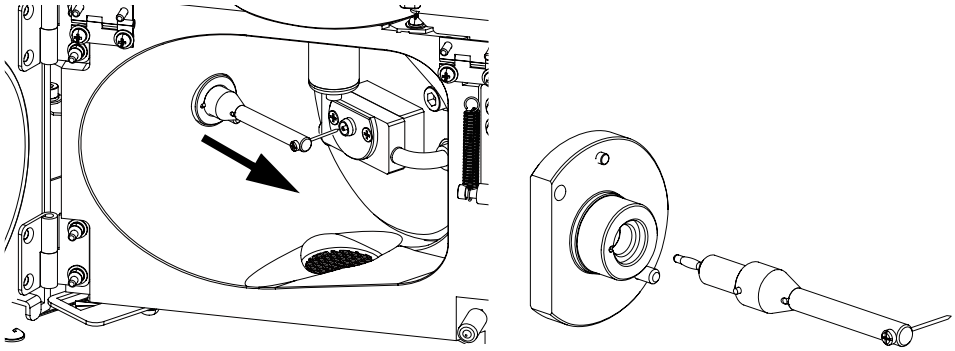


Fig. 3-34

Hint

When carrying out measurement in the ESI mode with the corona needle removed, fit the corona needle plug in order to prevent contamination of the parts where high voltages are applied.

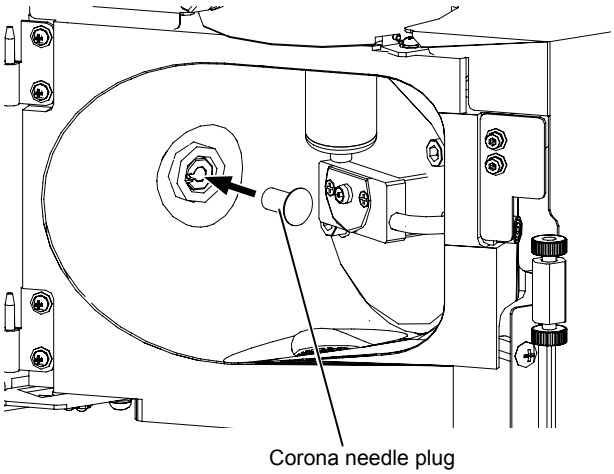


Fig. 3-35

3 Close the source window.

4 Close the probe cover.

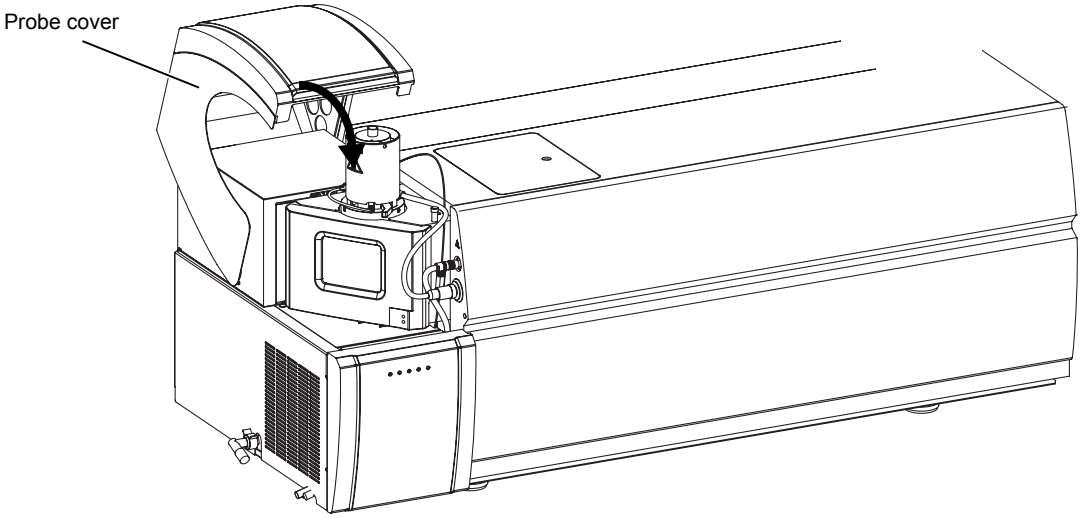


Fig. 3-36

3.7 Preparation for DUIS Analysis

3.7.1 Mounting the Corona Needle for DUIS

1 Open the probe cover.

2 Open the source window.

WARNING

Instructions

Check that the temperature of the DL and heated block has fallen to 50 °C or lower before proceeding with the work.

The ion source unit reaches high temperatures. You could sustain burns. Turn the heater OFF from LabSolutions before starting this work.

Reference
"4.2 Heater ON/OFF Status and Temperature Monitor" P.94

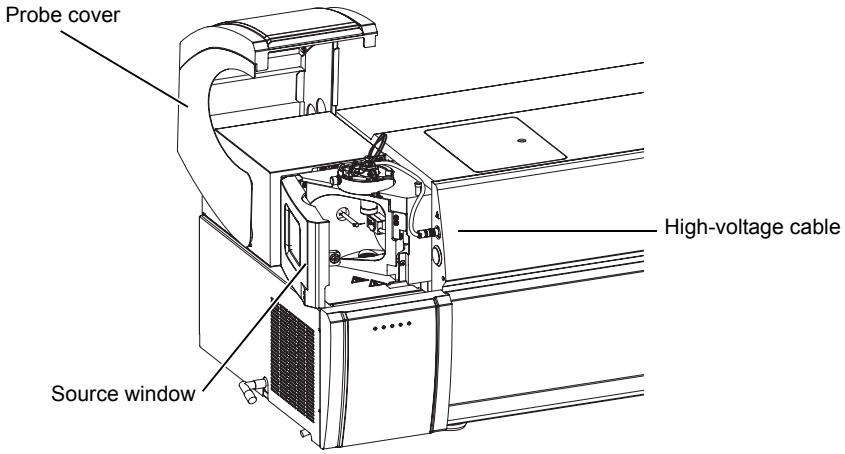


Fig. 3-37

3 Set the needle unit.

If a corona needle plug is used in the socket, remove the plug and then insert the needle as far as it will go into the socket, ensuring that the pin is aligned with the notch.

WARNING

Instructions

Disconnect the high-voltage cable before starting this work.

If it is not disconnected there will be a danger of electric shock.

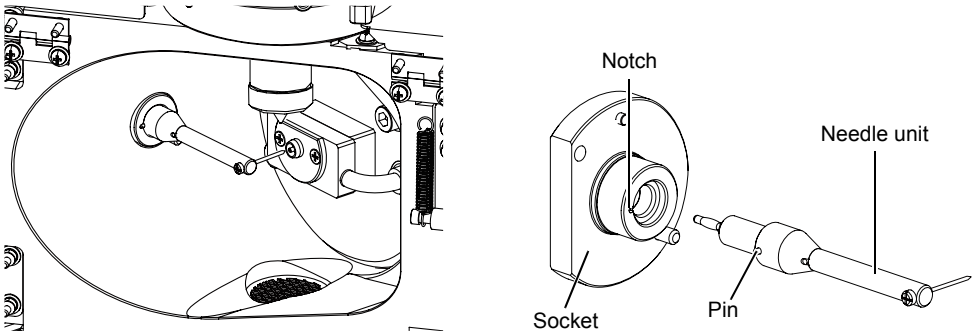


Fig. 3-38

CAUTION

Instructions

Take care because the tip of the DUIS needle is sharp.

NOTE

When setting the needle unit, check that the DUIS needle is not bent in either the vertical or horizontal direction.

Hint

Check that the tip of the DUIS needle is not bent by using the needle alignment tool.

Check that the needle is contained within the range of the slit and repair the needle if it is bent.

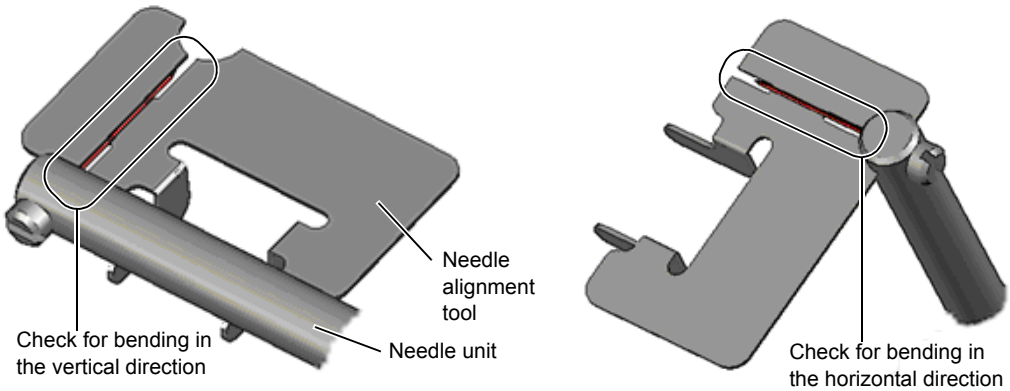


Fig. 3-39

4 Close the source window.

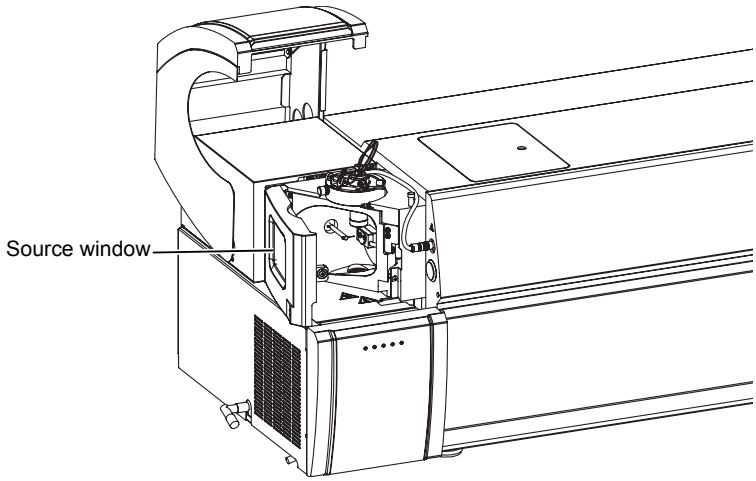


Fig. 3-40

5 Open the front door and connect the DUIS high-voltage cable connector to the instrument.

WARNING

Instructions

Turn the high-voltage supply OFF from LabSolutions before connecting or disconnecting the high-voltage cable.

If you do not turn it OFF there will be a risk of electric shock.

Reference

"4.1 Turning the High Voltage ON/OFF" P.93

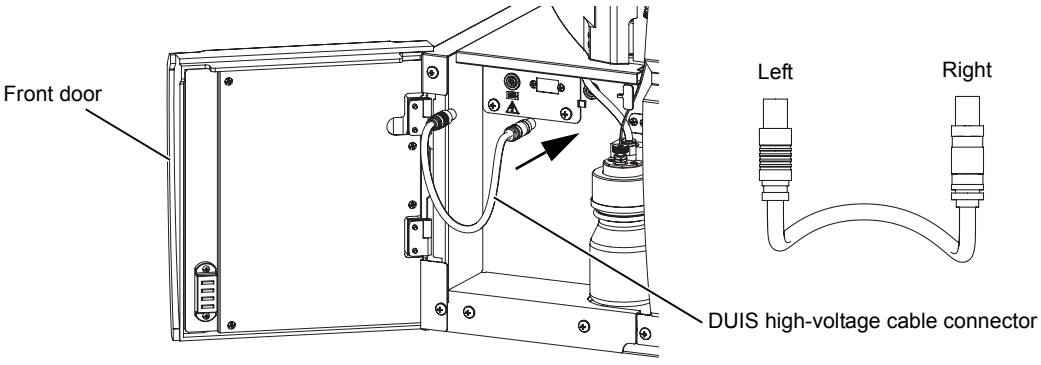


Fig. 3-41

6 Close the front door and probe cover.

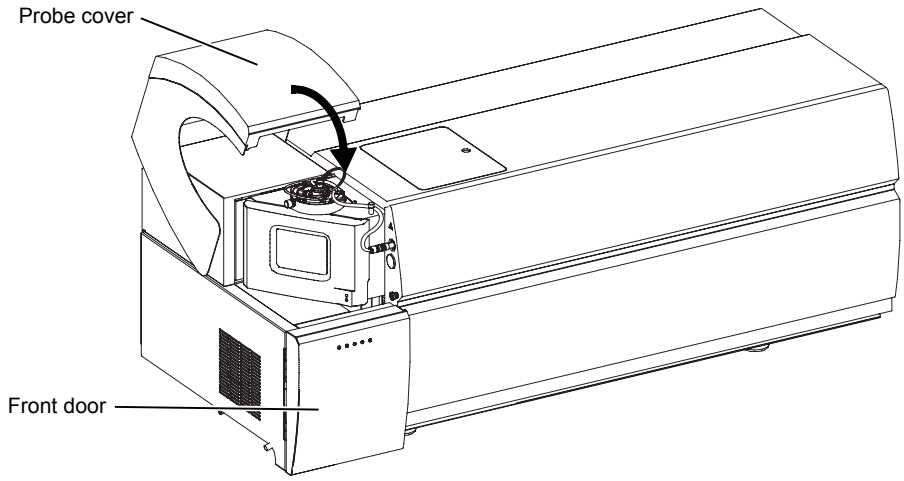


Fig. 3-42

3.7.2 Mounting the ESI Probe

Reference
"3.5.1 Mounting the ESI Probe" P.55

1 Check the position of the ESI probe.

Adjust the position of the ESI probe by turning the position adjustment knob.
After adjustment, turn the locking screw to lock the knob.
For DUIS analysis, adjust the probe to the +2 mm position.

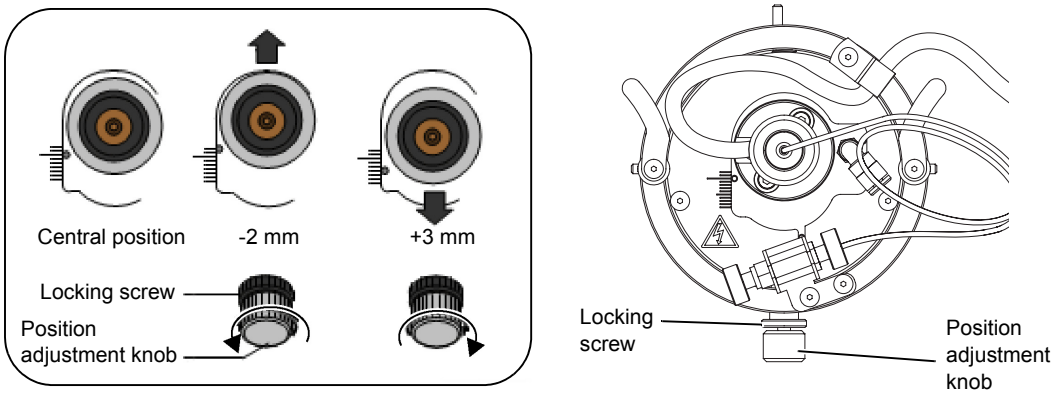


Fig. 3-43

3.7.3 Removing the ESI Probe

Reference
"3.5.2 Removing the ESI Probe" P.58

■ Removing the needle unit from the instrument

1 Open the probe cover.

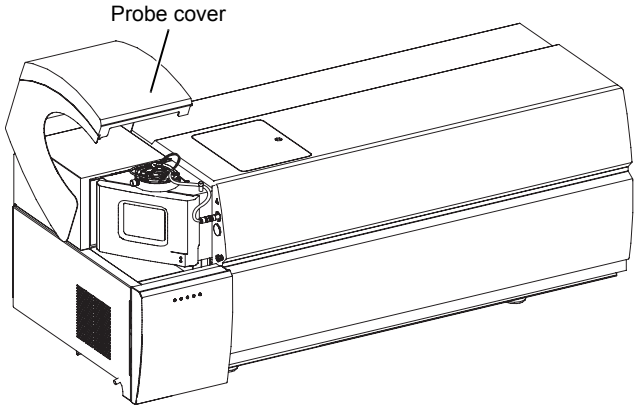


Fig. 3-44

2 Open the front door and remove the DUIS high-voltage cable connector.

WARNING

Instructions

Turn the high-voltage supply OFF from LabSolutions before connecting or disconnecting the high-voltage cable.

If you do not turn it OFF there will be a risk of electric shock.

Reference
"4.1 Turning the High Voltage ON/OFF" P.93

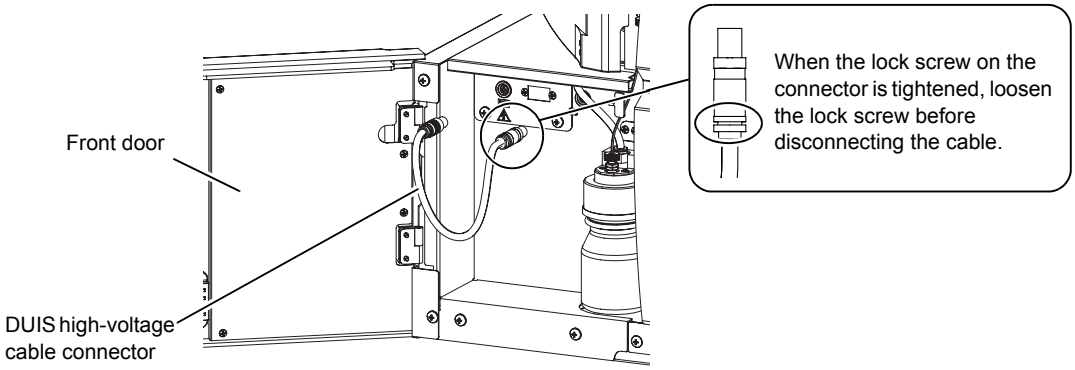


Fig. 3-45

3 Close the front door.

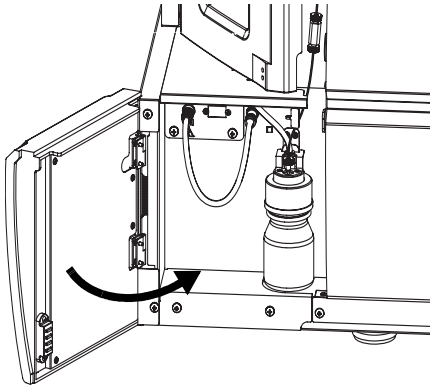


Fig. 3-46

4 Open the source window.

WARNING

Instructions

Check that the temperature of the DL and heated block has fallen to 50 °C or lower before proceeding with the work.

The ion source unit reaches high temperatures. You could sustain burns. Turn the heater OFF from LabSolutions before starting this work.

Reference

"4.2 Heater ON/OFF Status and Temperature Monitor" P.94

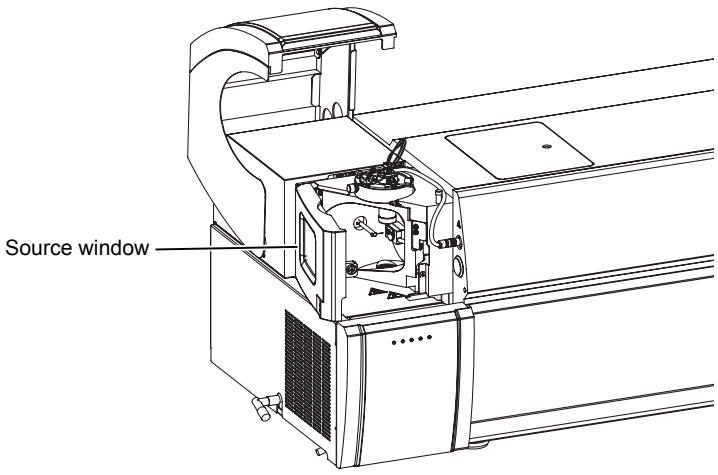


Fig. 3-47

5 Remove the needle unit.

WARNING

Instructions

Disconnect the high-voltage cable before starting this work.
If it is not disconnected there will be a danger of electric shock.

CAUTION

Instructions

Take care because the tip of the DUIS needle is sharp.

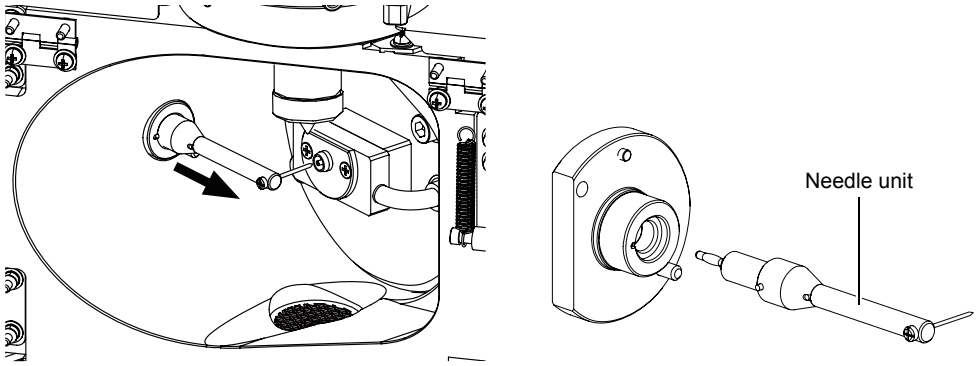


Fig. 3-48

6 Close the source window.

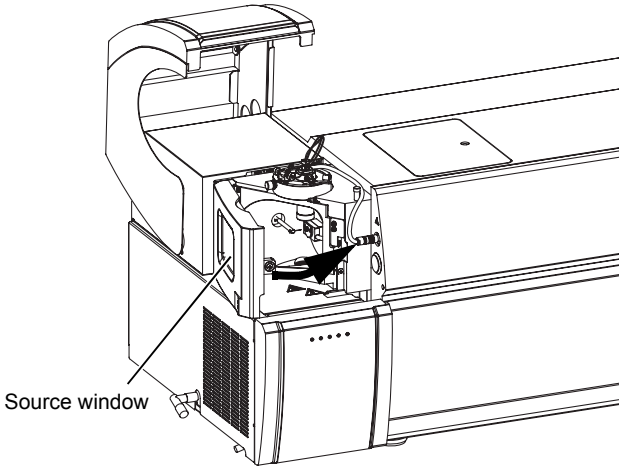


Fig. 3-49

7 Close the probe cover.

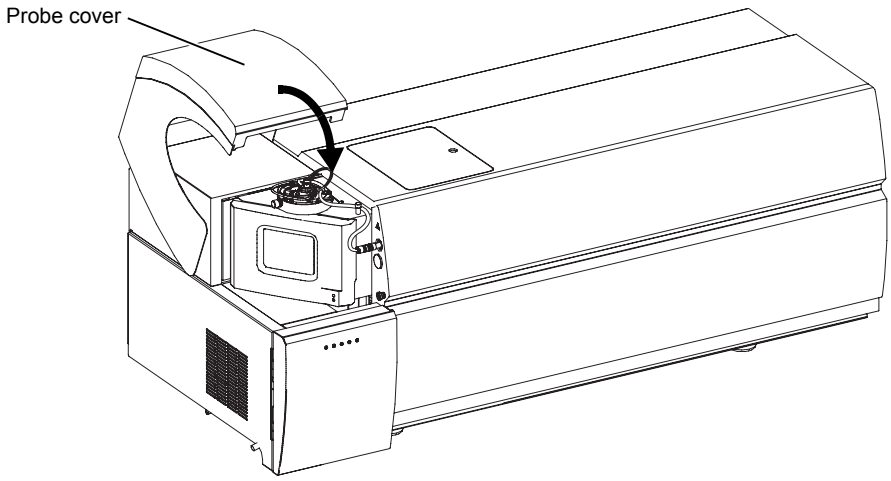


Fig. 3-50

Hint

When carrying out measurement in the ESI mode with the corona needle removed, fit a corona needle plug in order to prevent contamination of the parts where high voltages are applied.

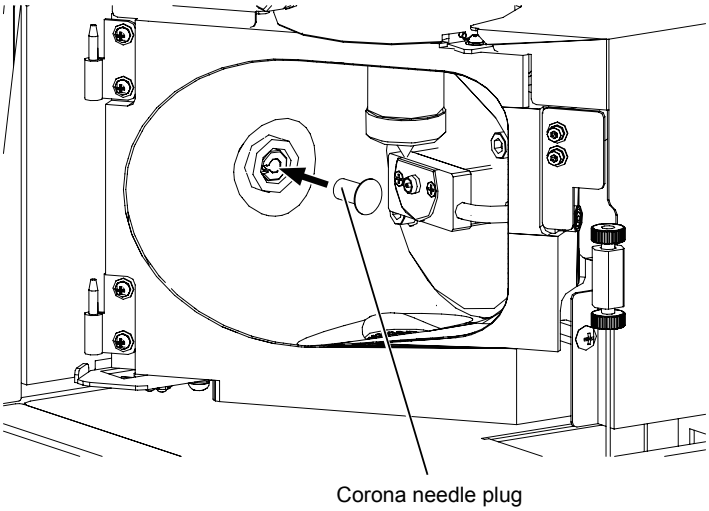


Fig. 3-51

3.8 Auto Tuning

Carry out auto tuning to adjust the voltage inside the instrument using ESI or DUIS ionization.

Perform auto tuning when you have stopped the vacuum system to carry out maintenance inside the instrument, when the instrument does not work correctly, or when the instrument has not been operated for a long period of time.

NOTE

- Remove the corona needle before performing auto tuning in the DUIS mode.
- Always perform auto tuning after replacing the detector.

Reference

"Removing the needle unit from the instrument" P.76

3.8.1 Preparing the Standard Sample

Prepare the standard sample before starting auto tuning such as sensitivity adjustment, resolution adjustment, or mass calibration of the instrument.

1 Open the front door and check the standard sample solution in the standard sample bottle.

If the tubing projects above the surface of the liquid it means that sample pumping is not possible. As a guide, check that there is 40 to 80 mL in the bottle. One execution of auto tuning uses approximately 1 mL.

Reference

"7.6 Maintenance of the Standard Sample Introduction Unit" P.154

"8.3 Standard Sample" P.213

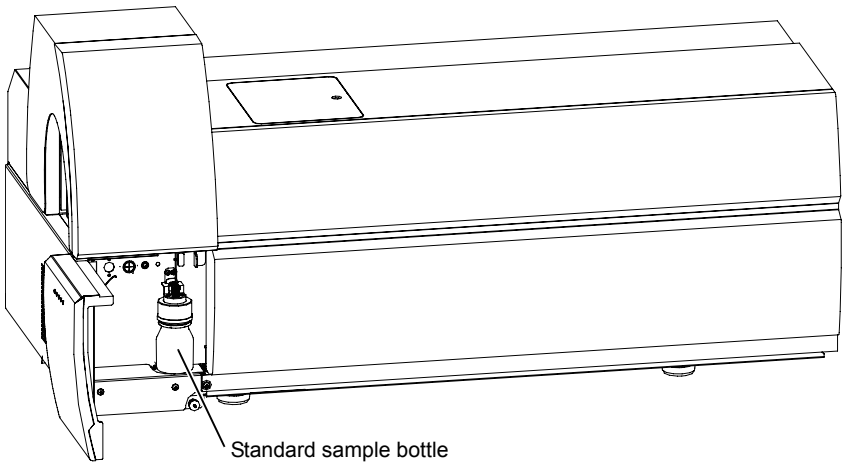


Fig. 3-52

2 Connect the tubing.

1. Open the probe cover.
2. Stop the operation of the LC (pump).
3. Disconnect the tube that comes from the LC and connect the resistance tube that is supplied with the instrument from the standard sample bottle to the ESI probe.

NOTE

Take care not to bend the resistance tube too much.
Maintain a moderate bending radius of at least 40 mm while handling the tube.

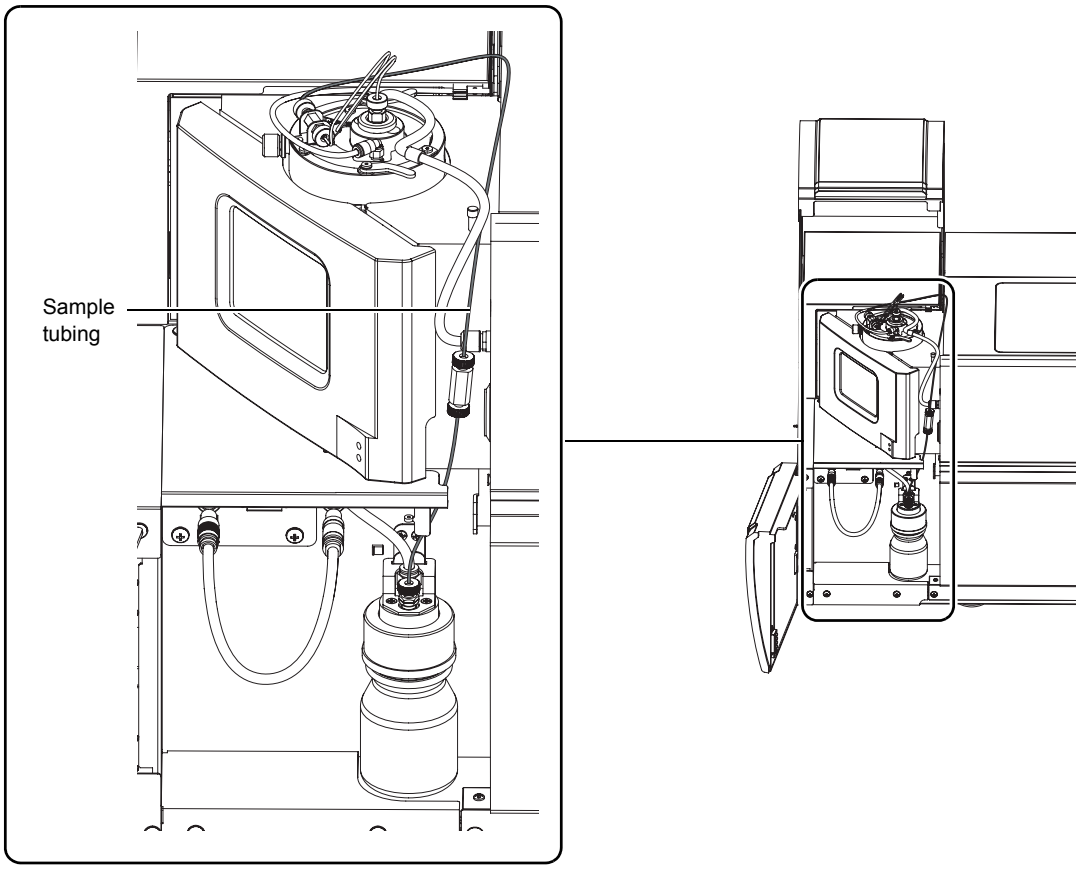


Fig. 3-53

3 Close the front door and probe cover.

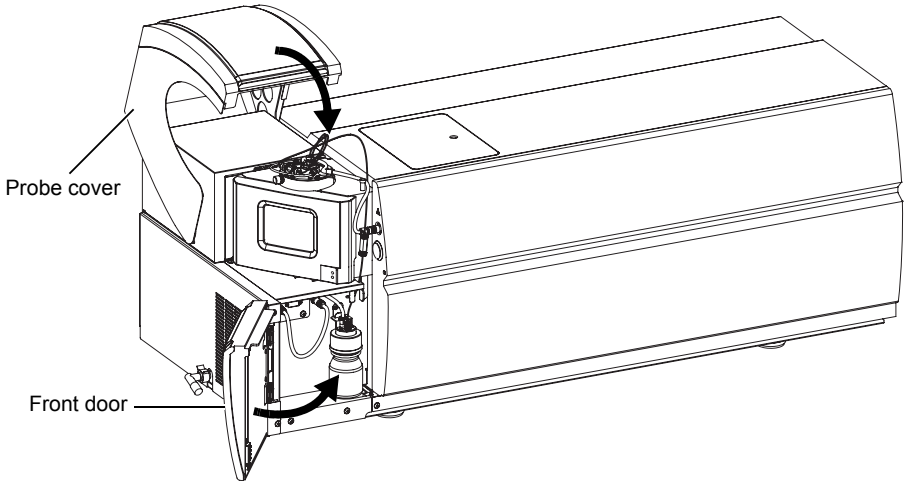


Fig. 3-54

CAUTION

Clean the sample tubing (resistance tube) with methanol after use.
Failure to clean the tubing may cause blockages to occur.

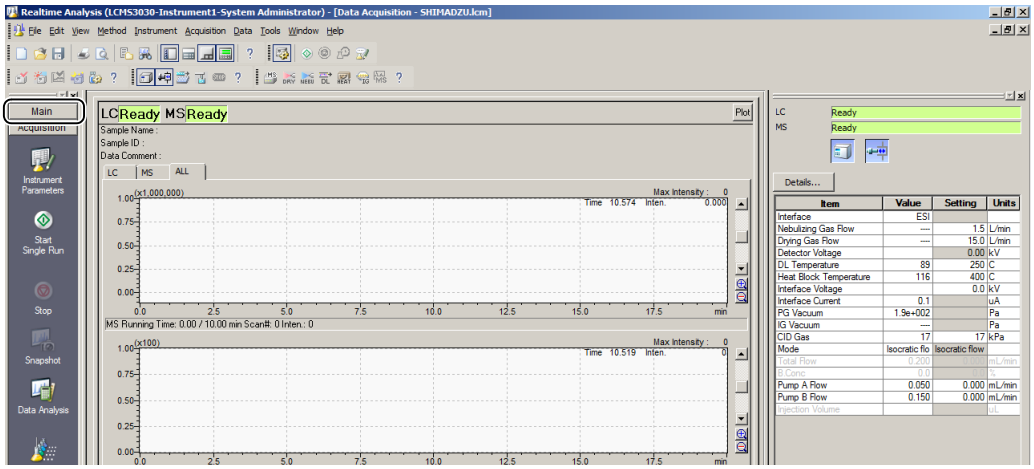
Instructions

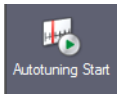
3.8.2 Starting Auto Tuning

1 Start up LabSolutions.

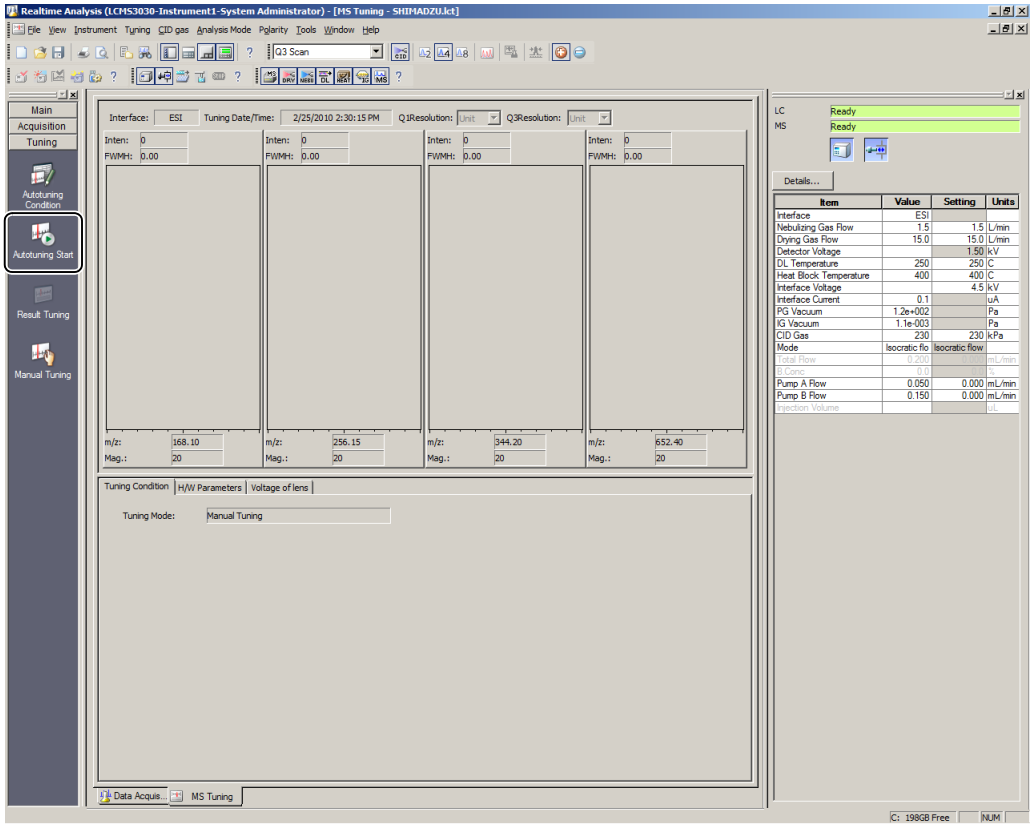
2 Click the Tuning (Tuning) icon.

If the [Tuning] icon is not displayed, click Main (Main) in the assistant bar.



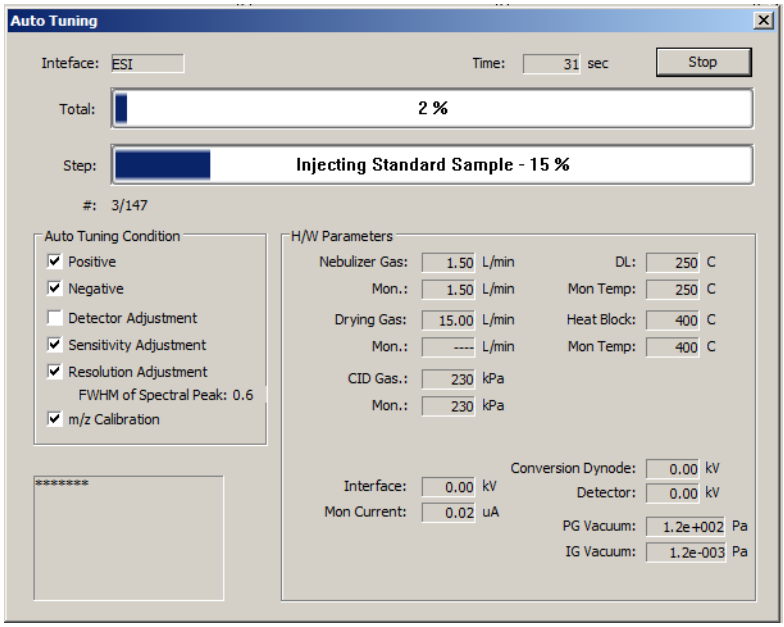
3 Click the 

(Autotuning Start) icon.



Hint

Screen shown during the execution of auto tuning



Auto tuning is executed as shown in Fig. 3-55 according to the analysis mode (Q1, Q3, MS/MS). Auto tuning is completed in about 40 minutes and the results are saved.

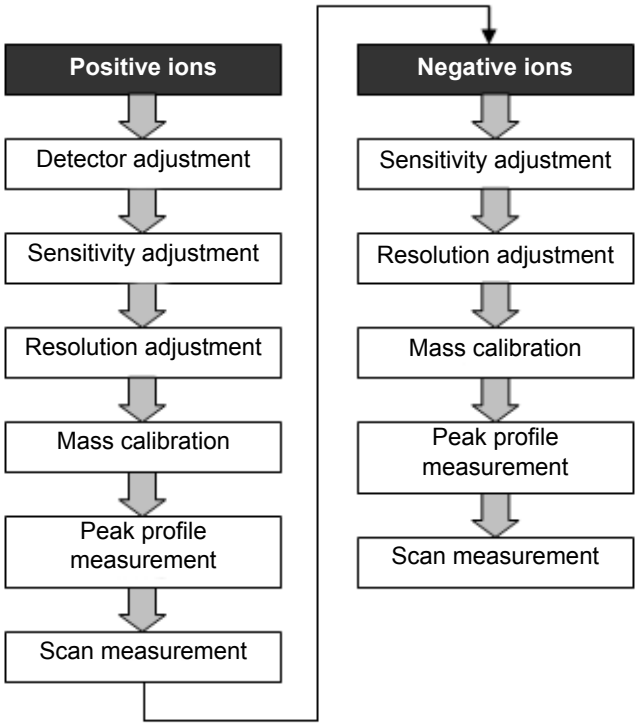


Fig. 3-55

■ Detector adjustment

The detector voltage is adjusted automatically.
The same detector voltage is used for all analysis modes.

■ Sensitivity adjustment

Optimize the lens voltage for each m/z.
Optimize the voltages of the Qarray, multipole and entrance lens for each analysis mode.

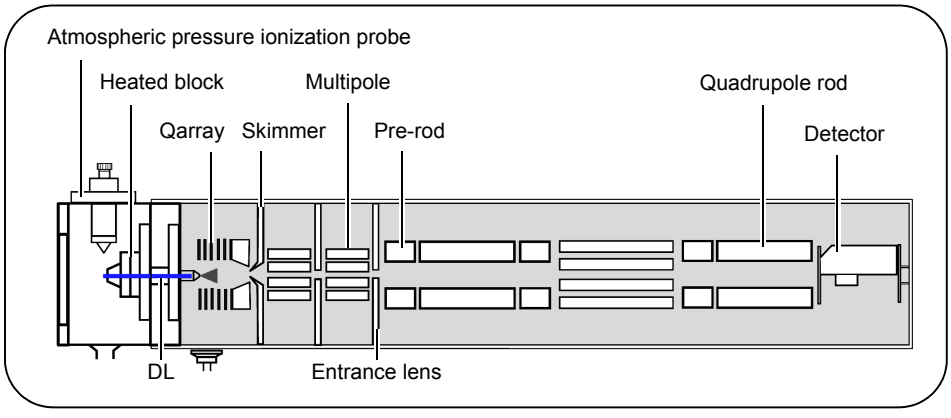


Fig. 3-56

■ Resolution adjustment

Adjust the FWHM of the peak profile to 0.6 u.

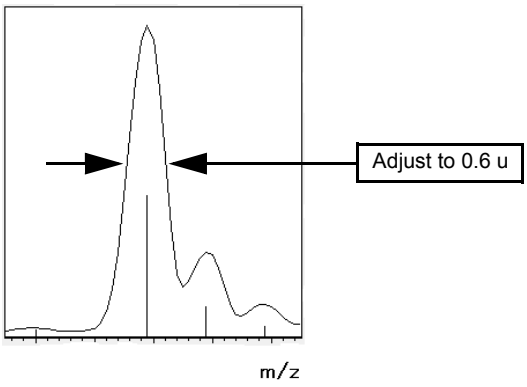


Fig. 3-57

■ Mass calibration

Calibrate the m/z based on the ions in the standard sample.

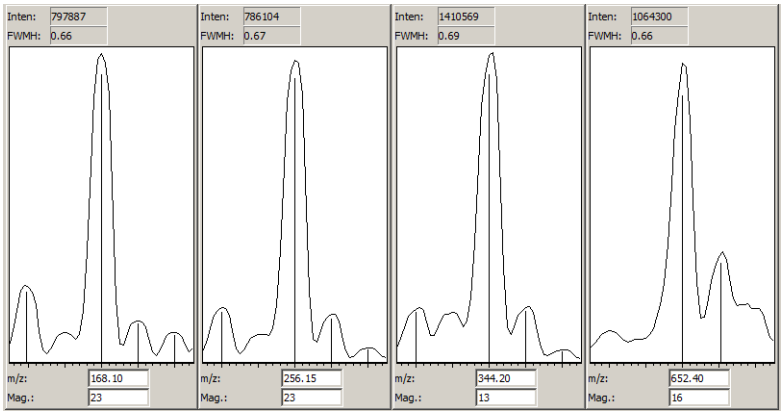


Fig. 3-58

■ Peak profile measurement

Measure the peak profile for displaying tuning results.

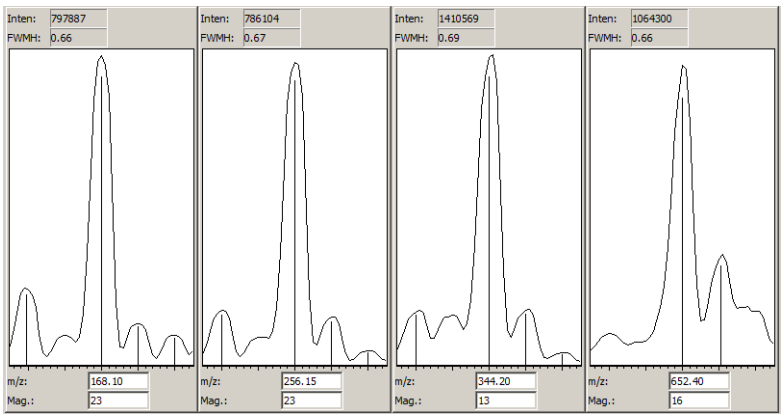


Fig. 3-59

■ Scan measurement

Measure the mass spectrum for displaying tuning results.

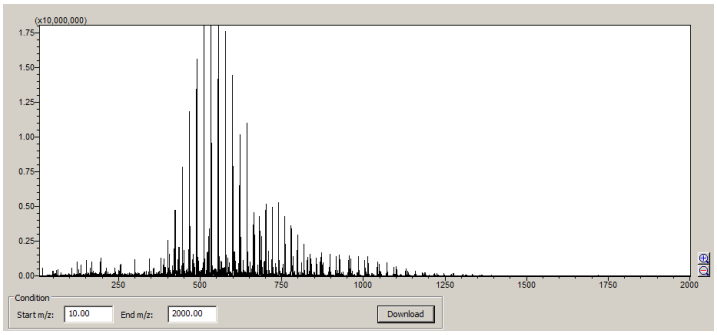
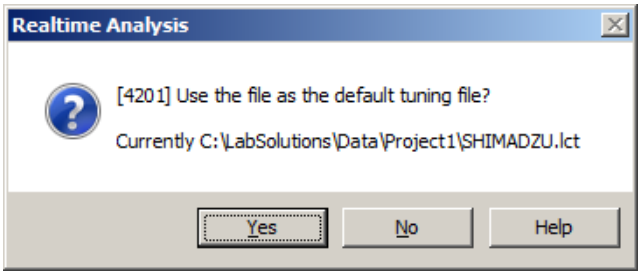


Fig. 3-60

4 Save the tuning file.

Select [Save Tuning File As] in the [File] menu and save the tuning file (*.lct). Next, select whether to set the tuning file as the default tuning file.



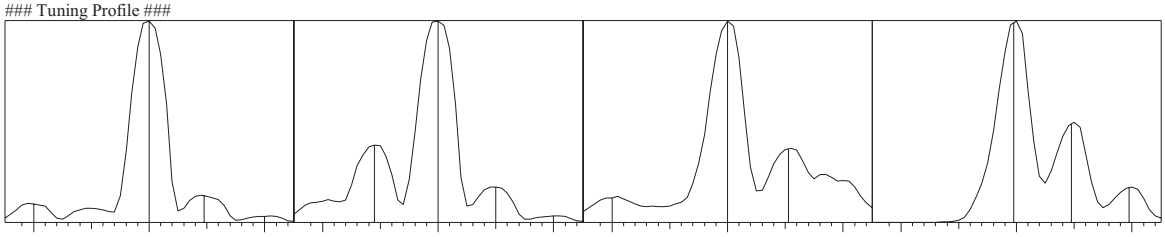
If [Yes] is selected, the saved tuning file will be set as the default tuning file. The new default tuning file will automatically be displayed from the next time the [Tuning] window is opened.
If [No] is selected, the saved tuning file will not be set as the default tuning file, and the existing default tuning file will be displayed when the [Tuning] window is opened.

Unless a tuning file to be used is specified at the start of analysis, the default tuning file will automatically be used.

Results of Auto Tuning

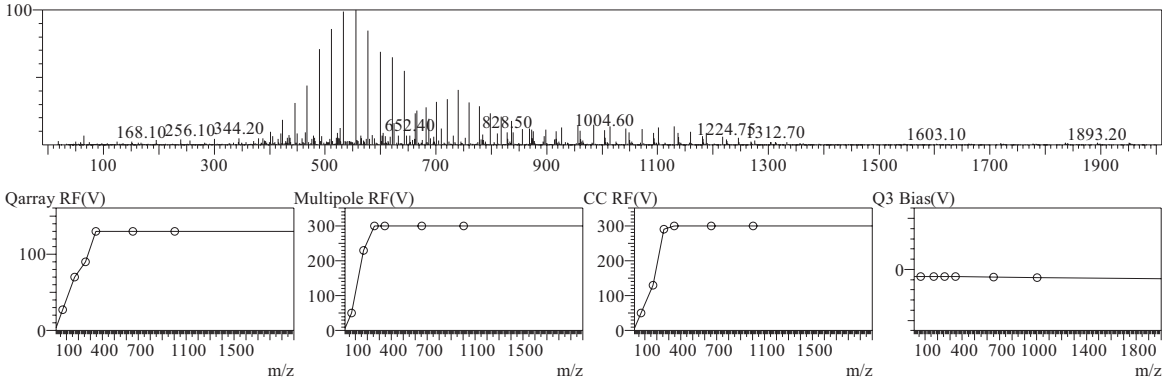
### Sample Information ###	
Sample Type:	PEG+PPG+Raffinose
### Tuning Condition ###	
Detector Adjustment:	On
Resolution Adjustment:	On
FWHM of Spectrum:	0.60
Sensitivity Adjustment:	On
Mass Calibration:	On
### Tuning Result ###	
Model:	LCMS-8030/LCMS-8040
Interface:	ESI
Polarity:	Pos
Tuning Mode:	Auto
Tuning Date:	5/11/2010 2:11:23 PM
Acquisition Mode:	Q3 Scan(Use CID Gas)
Nebulizing Gas Flow:	1.50(settings : 1.50) L/min
Drying Gas Flow:	0.00(settings : 15.00) L/min
CID Gas Flow:	230(settings : 230) kPa
Interface Bias:	+4.50 kV
Interface Current:	0.72 uA
DL Temp.:	249(settings : 250) C
Heat Block Temp.:	400(settings : 400) C
Q1 RF Gain:	---
Q1 RF Offset:	---
Q3 RF Gain:	5001
Q3 RF Offset:	5003
Q1 Post-rod Bias:	-5.0 V
CID CELL Exit Lens:	-3.4 V
Conversion Dynode:	-6.00 kV
Detector:	-1.96 kV
PG Vacuum:	8.2e+001 Pa
IG Vacuum:	1.7e-003 Pa

Tuning Profile



Int.: 334760	Int.: 615200	Int.: 734652	Int.: 1278527
FWHM: 0.67	FWHM: 0.70	FWHM: 0.68	FWHM: 0.65
m/z : 256.15	m/z : 344.20	m/z : 652.40	m/z : 1004.60
Mag.: 59	Mag.: 32	Mag.: 27	Mag.: 15

Scan Range: 10.00 - 2000.00 Scan Speed: 500 u/s Base Peak: 555.45 (12784371)



	65.05	168.10	256.15	344.20	652.40	1004.60
DL Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Qarray Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Qarray RF	+27.1	+70.0	+90.0	+130.0	+130.0	+130.0
Multipole RF	+50.0	+230.0	+300.0	+300.0	+300.0	+300.0
Multipole1 Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Multipole1 Lens	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Multipole2 Bias	-0.8	-0.8	-0.8	-0.8	-0.8	-0.8
Multipole2 Lens	-2.0	-2.0	-2.0	-2.0	-2.0	-2.0
Q1 Bias	-5.0	-5.0	-5.0	-5.0	-5.0	-5.0
CC Lens1	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
CC Lens2	-100.0	-100.0	-100.0	-100.0	-100.0	-100.0
CC Lens3	-20.0	-20.0	-20.0	-20.0	-20.0	-20.0

	65.05	168.10	256.15	344.20	652.40	1004.60
CC RF	+50.0	+130.0	+290.0	+300.0	+300.0	+300.0
CE	-5.0	-5.0	-5.0	-5.0	-5.0	-5.0
Q3 Bias	-7.0	-7.0	-7.1	-7.2	-7.6	-8.0

	107.15	1071.50
Q1 Pre Bias	-5.0	-50.0
Q3 Pre Bias	-5.0	-50.0

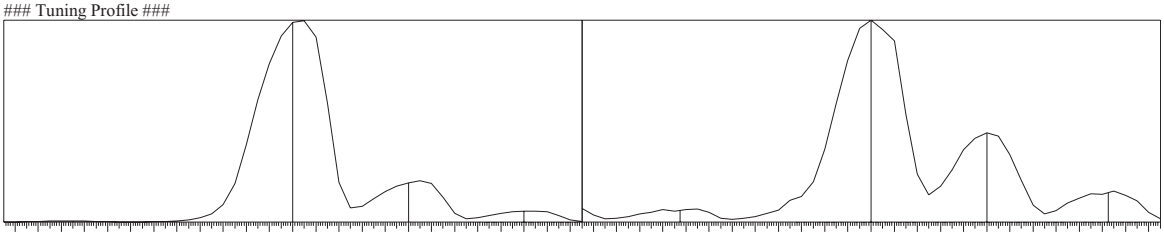
Fig. 3-61

Sample Information
Sample Type: PEG+PPG+Raffinose

Tuning Condition
Detector Adjustment: On
Resolution Adjustment: On
FWHM of Spectrum: 0.60
Sensitivity Adjustment: On
Mass Calibration: On

Tuning Result
Model: LCMS-8030/LCMS-8040
Interface: ESI
Polarity: Neg
Tuning Mode: Auto
Tuning Date: 5/11/2010 2:15:20 PM
Acquisition Mode: Q3 Scan(Use CID Gas)
Nebulizing Gas Flow: 1.50(settings : 1.50) L/min
Drying Gas Flow: 0.00(settings : 15.00) L/min
CID Gas Flow: 230(settings : 230) kPa
Interface Bias: -3.50 kV
Interface Current: 0.55 uA
DL Temp.: 250(settings : 250) C
Heat Block Temp.: 400(settings : 400) C
Q1 RF Gain: ---
Q1 RF Offset: ---
Q3 RF Gain: 5002
Q3 RF Offset: 5003
Q1 Post-rod Bias: 5.0 V
CID CELL Exit Lens: 3.4 V
Conversion Dynode: +6.00 kV
Detector: -1.96 kV
PG Vacuum: 8.2e+001 Pa
IG Vacuum: 1.7e-003 Pa

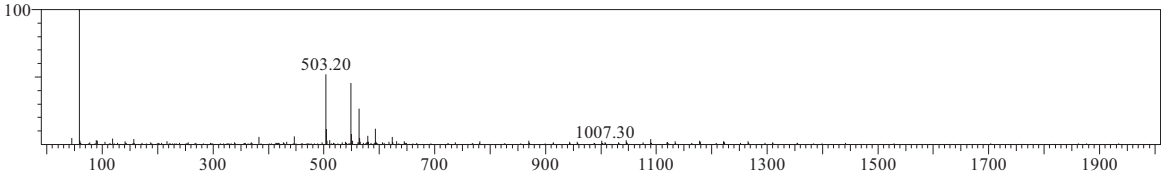
Tuning Profile

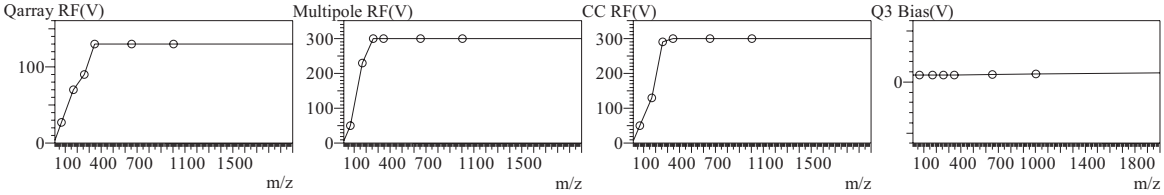


Int.: 1554545
FWHM: 0.67
m/z : 503.15
Mag.: 12

Int.: 53473
FWHM: 0.65
m/z : 1007.30
Mag.: 374

Scan Range: 10.00 - 2000.00 Scan Speed: 500 u/s Base Peak: 59.10 (3213194)





	65.05	168.10	256.15	344.20	652.40	1004.60
DL Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Qarray Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Qarray RF	+27.1	+70.0	+90.0	+130.0	+130.0	+130.0
Multipole RF	+50.0	+230.0	+300.0	+300.0	+300.0	+300.0
Multipole1 Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Multipole1 Lens	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Multipole2 Bias	+0.8	+0.8	+0.8	+0.8	+0.8	+0.8
Multipole2 Lens	+2.0	+2.0	+2.0	+2.0	+2.0	+2.0
Q1 Bias	+5.0	+5.0	+5.0	+5.0	+5.0	+5.0
CC Lens1	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
CC Lens2	+100.0	+100.0	+100.0	+100.0	+100.0	+100.0
CC Lens3	+20.0	+20.0	+20.0	+20.0	+20.0	+20.0

	65.05	168.10	256.15	344.20	652.40	1004.60
CC RF	+50.0	+130.0	+290.0	+300.0	+300.0	+300.0
CE	+5.0	+5.0	+5.0	+5.0	+5.0	+5.0
Q3 Bias	+7.0	+7.0	+7.1	+7.2	+7.6	+8.0

	107.15	1071.50
Q1 Pre Bias	+5.0	+50.0
Q3 Pre Bias	+5.0	+50.0

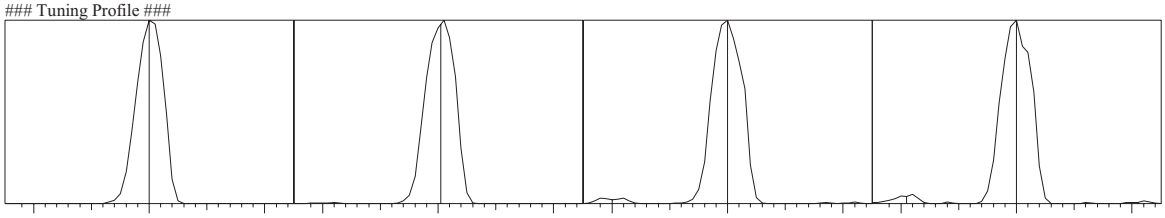
Fig. 3-62

Sample Information
Sample Type: PEG+PPG+Raffinose

Tuning Condition
Detector Adjustment: On
Resolution Adjustment: On
FWHM of Spectrum: 0.60
Sensitivity Adjustment: On
Mass Calibration: On

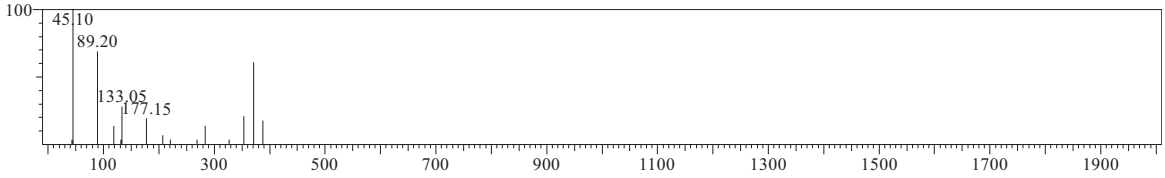
Tuning Result
Model: LCMS-8030/LCMS-8040
Interface: ESI
Polarity: Pos
Tuning Mode: Auto
Tuning Date: 5/11/2010 2:21:37 PM
Acquisition Mode: Product Scan
Nebulizing Gas Flow: 1.50(settings : 1.50) L/min
Drying Gas Flow: 0.00(settings : 15.00) L/min
CID Gas Flow: 230(settings : 230) kPa
Interface Bias: +4.50 kV
Interface Current: 0.71 uA
DL Temp.: 249(settings : 250) C
Heat Block Temp.: 400(settings : 400) C
Q1 RF Gain: 5000
Q1 RF Offset: 5000
Q3 RF Gain: 5001
Q3 RF Offset: 5007
Q1 Post-rod Bias: -5.0 V
CID CELL Exit Lens: -3.6 V
Conversion Dynode: -6.00 kV
Detector: -1.96 kV
PG Vacuum: 8.2e+001 Pa
IG Vacuum: 1.7e-003 Pa

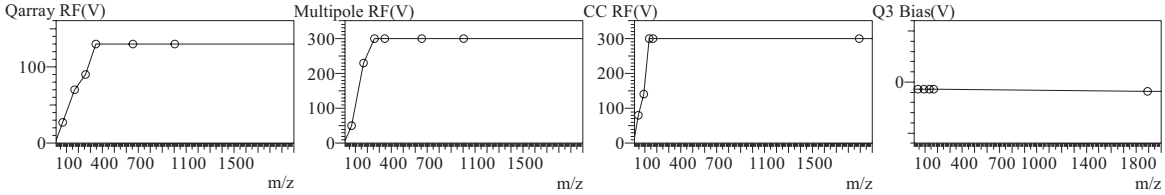
Tuning Profile



Int.: 46234 FWHM: 0.56 m/z : 45.05 Precursor of m/z: 168.10 Mag.: 432
Int.: 37954 FWHM: 0.62 m/z : 89.05 Precursor of m/z: 168.10 Mag.: 516
Int.: 27058 FWHM: 0.65 m/z : 133.10 Precursor of m/z: 388.25 Mag.: 739
Int.: 12247 FWHM: 0.65 m/z : 177.10 Precursor of m/z: 388.25 Mag.: 1633

Scan Range: 10.00 - 2000.00 Scan Speed: 500 u/s Base Peak: 45.10 (56403) Precursor of m/z: 388.25





	65.05	168.10	256.15	344.20	652.40	1004.60
DL Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Qarray Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Qarray RF	+27.1	+70.0	+90.0	+130.0	+130.0	+130.0
Multipole RF	+50.0	+230.0	+300.0	+300.0	+300.0	+300.0
Multipole1 Bias	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Multipole1 Lens	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
Multipole2 Bias	-0.8	-0.8	-0.8	-0.8	-0.8	-0.8
Multipole2 Lens	-2.0	-2.0	-2.0	-2.0	-2.0	-2.0
Q1 Bias	-5.0	-5.0	-5.0	-5.0	-5.0	-5.0
CC Lens1	+0.0	+0.0	+0.0	+0.0	+0.0	+0.0
CC Lens2	-100.0	-100.0	-100.0	-100.0	-100.0	-100.0
CC Lens3	-20.0	-20.0	-20.0	-20.0	-20.0	-20.0

	45.05	89.05	133.10	168.10	1893.40
CC RF	+80.0	+140.0	+300.0	+300.0	+300.0
CE	-25.0	-15.0	-15.0	-15.0	-15.0
Q3 Bias	-7.0	-7.0	-7.0	-7.0	-9.0

	107.15	1071.50
Q1 Pre Bias	-5.0	-50.0
Q3 Pre Bias	-5.0	-50.0

Fig. 3-63

Hint

Interpreting tuning results

A detector voltage of about -1.6 to -2.5 kV is normal.

The detector deteriorates at a rate that depends on its conditions of use and should be replaced around every two years.

As a guide, it should be replaced when the auto tuning result reaches about -2.7 kV.

The PG (Pirani gauge) indicates the pressure of the interface unit.

Normally, this is about 100 Pa. If it is lower than 50 Pa, check that the DL is not sealed with a DL plug.

If a DL plug is not present, the DL is most likely clogged. In this case, replace the DL.

Reference

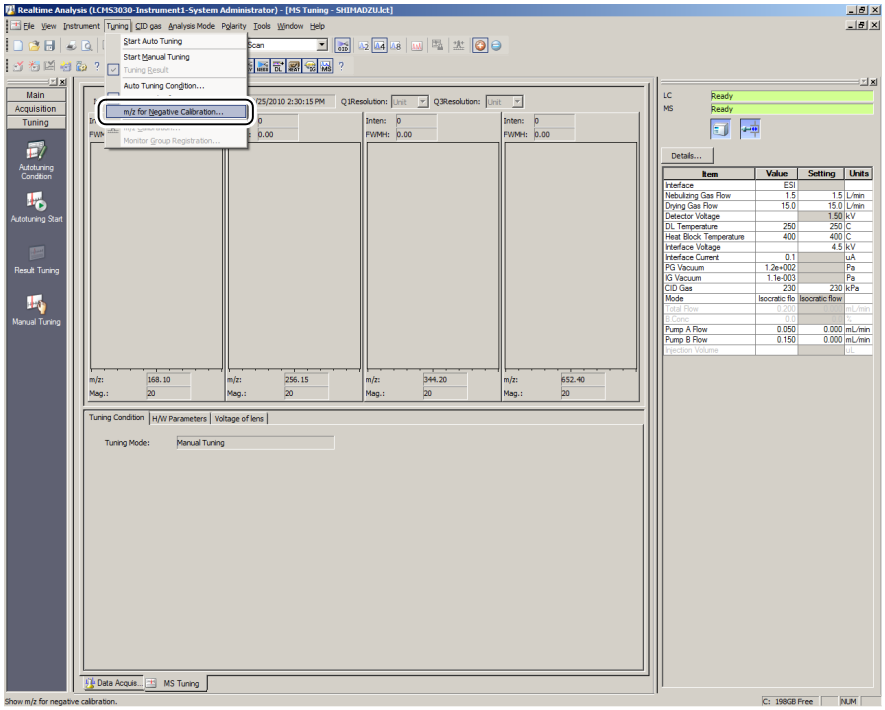
"7.9 Replacing the DL" P.163

NOTE

In negative tuning, the sensitivity of the raffinose peak used for mass calibration can drop substantially depending on the type of mobile phase. This is due to the fact that mobile phase derivatives are added to the raffinose.

If this happens, the mass used for mass calibration has to be changed.

Check the negative ions that are observed in "8.2 Manual Tuning" and enter the mass to be used for mass calibration.



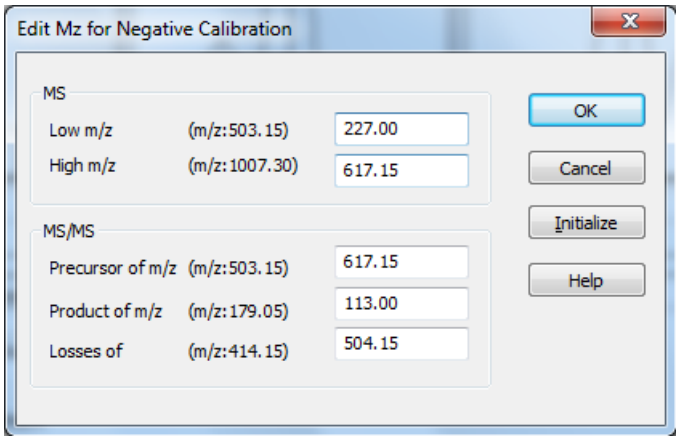
CAUTION

Prohibitions

When implementing regular auto tuning normally, do NOT change the mass used for mass calibration.

Typical example

	MS	MS/MS
When acetic acid is contained in the mobile phase	Low m/z: 119.05 High m/z: 563.20	Precursor of m/z: 563.20 Product of m/z: 179.05 Losses of: 384.15
When TFA (trifluoroacetic acid) is contained in the mobile phase	Low m/z: 227.00 High m/z: 617.15	Precursor of m/z: 617.15 Product of m/z: 113.00 Losses of: 504.15



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4 Basic Operation

This chapter explains the operations for turning the instrument's high voltage, heater and gas ON and OFF.

For information on data acquisition, refer to the LabSolutions Getting Started Guide and Operators Guide, or refer to the operation manual.

4.1 Turning the High Voltage ON/OFF

To ensure safety, turn the high voltage OFF before starting maintenance work on the instrument.

Turn OFF the atmospheric pressure ionization probe, corona needle, quadrupole and detector voltage by clicking the [MS detector] button in LabSolutions. The detector voltage cannot be turned ON when the nebulizer gas is OFF.

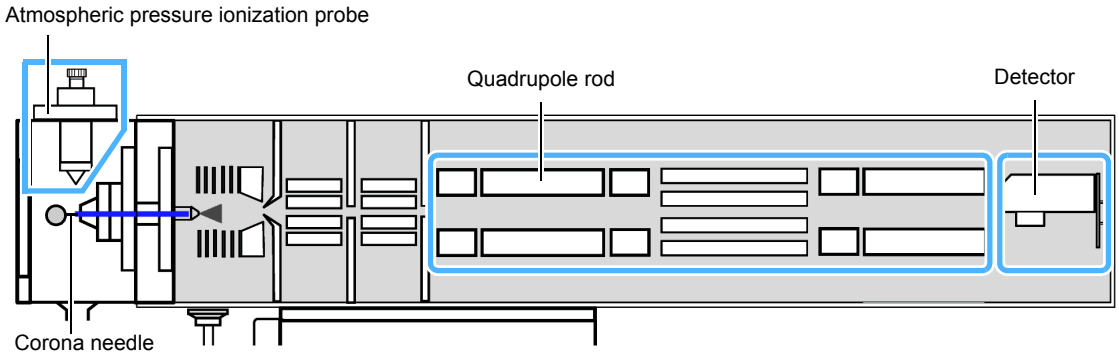
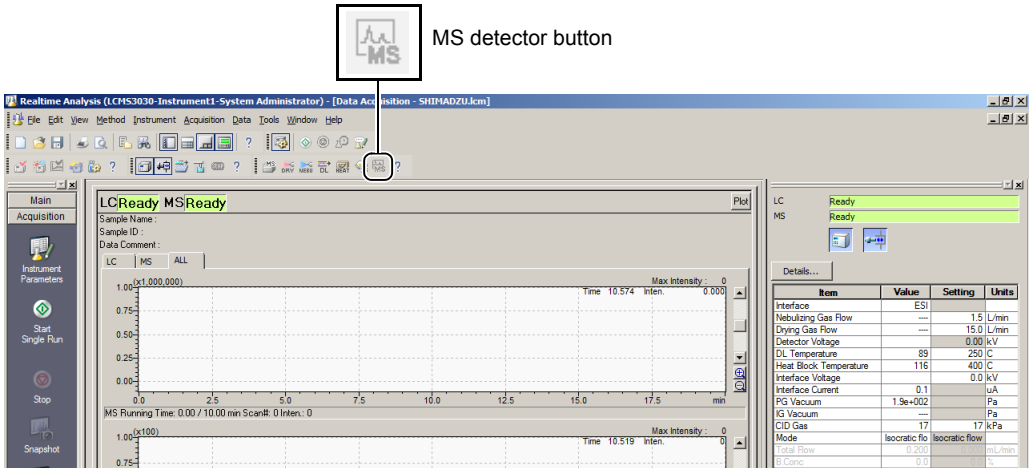


Fig. 4-1

1 Start up LabSolutions.

Click [MS detector] button to turn the high voltage ON or OFF.

Button	High Voltage ON	High Voltage OFF
MS detector		



4.2 Heater ON/OFF Status and Temperature Monitor

To ensure safety, turn the heater OFF and check that the temperature of all units has fallen below 50 °C before starting maintenance work on the instrument.

Turn the APCI heater (option), heated block and DL OFF.

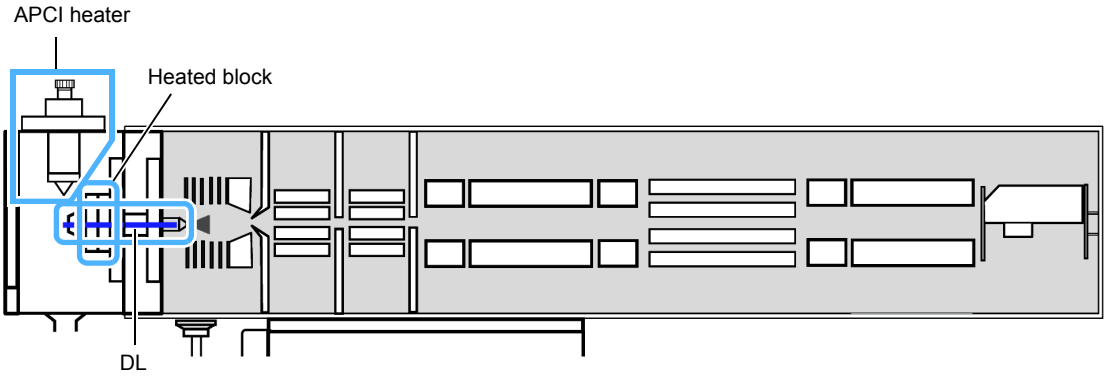
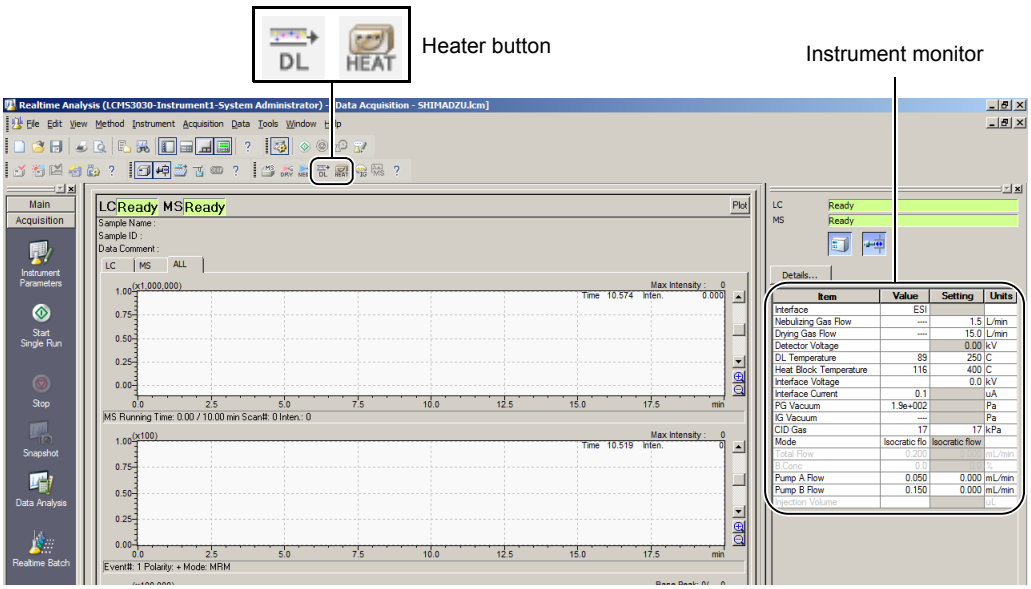


Fig. 4-2

1 Start up LabSolutions.

Click the buttons for each of the heaters to turn the heaters ON or OFF.

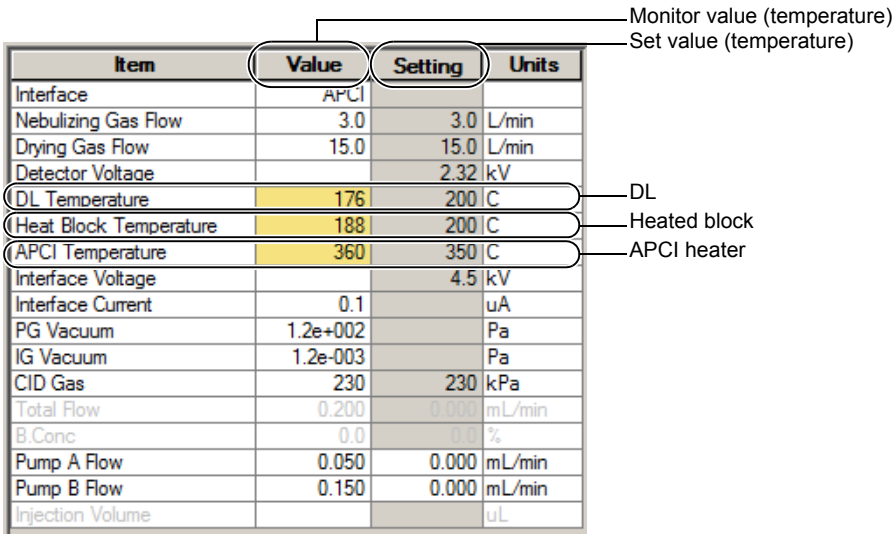
Button	ON	OFF
DL		
Heated block		
APCI heater (option)		



2 Check the temperature in the instrument monitor panel.

Reference

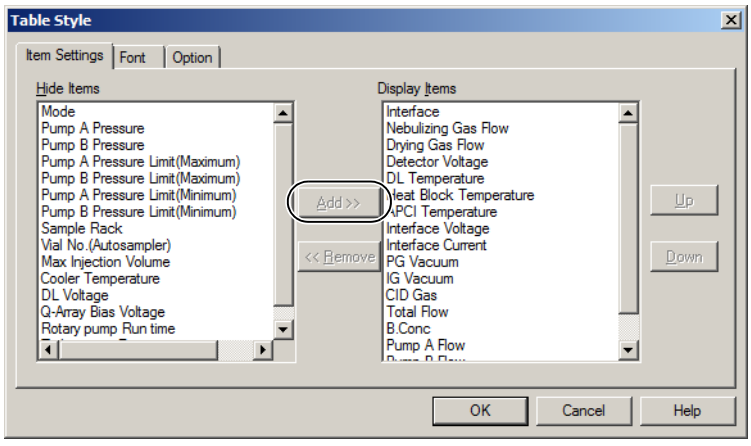
For initial values, see "8.2.3 Explanations of Parameters" P.208.



Item	Value	Setting	Units
Interface	APCI		
Nebulizing Gas Flow	3.0	3.0	L/min
Drying Gas Flow	15.0	15.0	L/min
Detector Voltage		2.32	kV
DL Temperature	176	200	C
Heat Block Temperature	188	200	C
APCI Temperature	360	350	C
Interface Voltage		4.5	kV
Interface Current	0.1		uA
PG Vacuum	1.2e+002		Pa
IG Vacuum	1.2e-003		Pa
CID Gas	230	230	kPa
Total Flow	0.200	0.000	mL/min
B.Conc	0.0	0.0	%
Pump A Flow	0.050	0.000	mL/min
Pump B Flow	0.150	0.000	mL/min
Injection Volume			uL

Hint

- If the instrument monitor panel is not displayed, display it by selecting [View] - [Instrument Monitor].
- If the heater temperature is not displayed in the instrument monitor panel
  Right click on the instrument monitor panel to display the [Table Style] window.
  Select [DL Temperature], [Heat Block Temperature] and/or [APCI Temperature] from the [Hide Items] list and click [Add >>].



4.3 Gas ON/OFF Status and Flow Rate Monitor

The LCMS-8030/LCMS-8040 uses nebulizer gas and drying gas.

To ensure safety, turn the gas OFF before starting maintenance work on the instrument.

Turn the gas OFF by clicking the buttons indicated below.

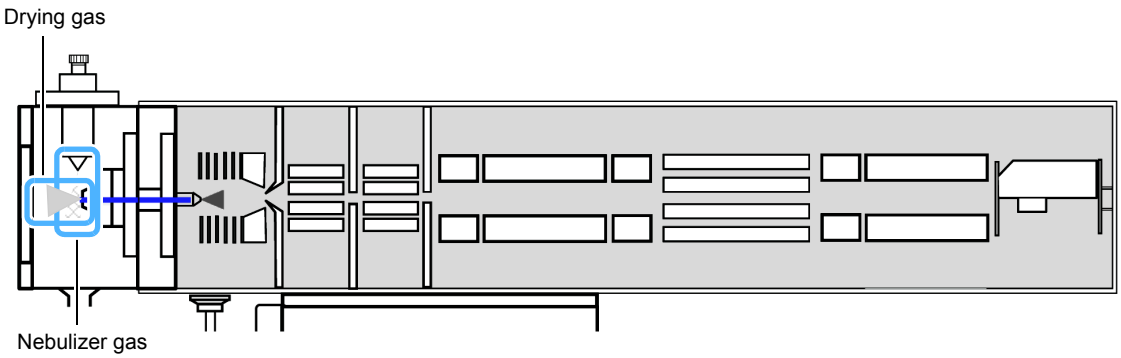
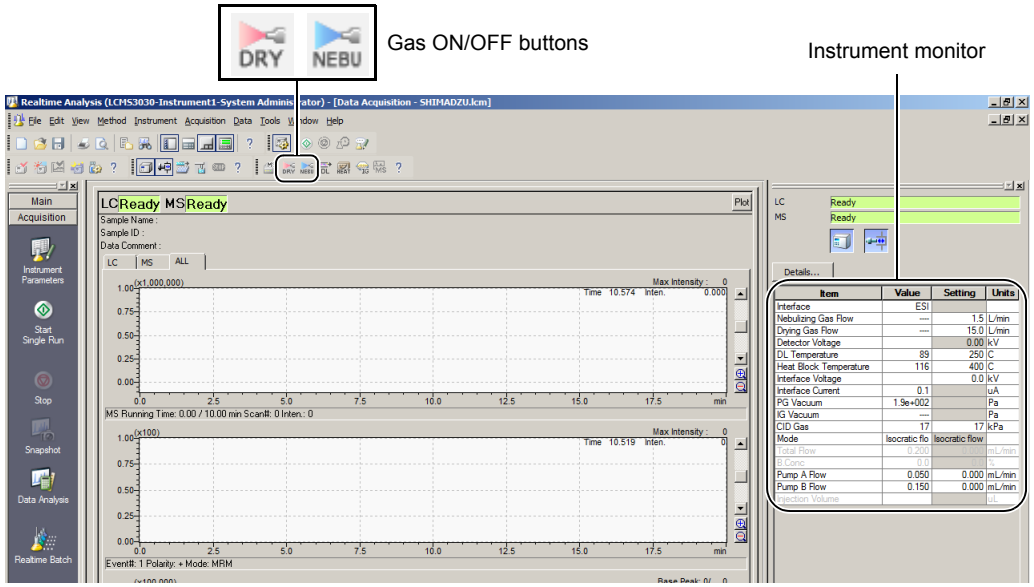


Fig. 4-3

1 Start up LabSolutions.

Click the gas buttons to turn the gas ON or OFF.

Button	ON	OFF
Nebulizer gas	NEBU	NEBU
Drying gas	DRY	DRY



2 Check the flow rate in the instrument monitor panel.

Reference

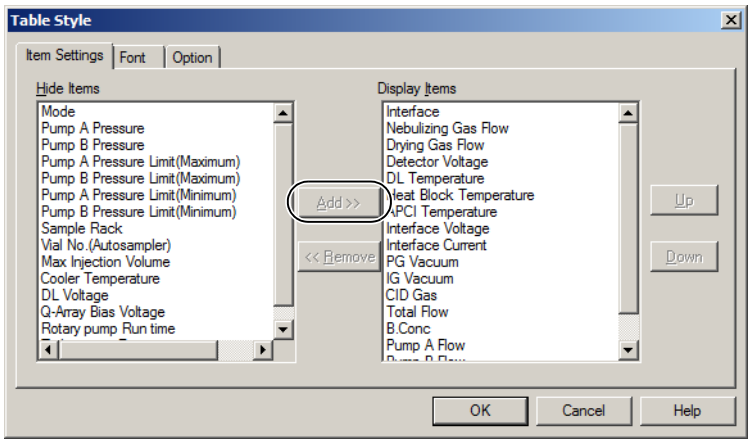
For initial values, see "8.2.3 Explanations of Parameters" P.208.

Item	Value	Setting	Units
Interface	APCI		
Nebulizing Gas Flow	1.5	1.5	L/min
Drying Gas Flow	15.0	15.0	L/min
Detector Voltage		2.32	kV
DL Temperature	176	200	C
Heat Block Temperature	188	200	C
APCI Temperature	360	350	C
Interface Voltage		4.5	kV
Interface Current	0.1		uA
PG Vacuum	1.2e+002		Pa
IG Vacuum	1.2e-003		Pa
CID Gas	230	230	kPa
Total Flow	0.200	0.000	mL/min
B.Conc	0.0	0.0	%
Pump A Flow	0.050	0.000	mL/min
Pump B Flow	0.150	0.000	mL/min
Injection Volume			uL

Monitor value (temperature)
Set value (temperature)
Nebulizer gas
Drying gas

Hint

- If the instrument monitor panel is not displayed, display it by selecting [View] - [Instrument Monitor].
- If the gas flow rate is not displayed in the instrument monitor panel:
  Right click on the instrument monitor panel to display the [Table Style] window.
  Select [Nebulizing Gas Flow] and/or [Drying Gas Flow] from the [Hide Items] list and click [Add >>].



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5 Analysis Modes

The LCMS-8030/LCMS-8040 is an analysis instrument that combines two quadrupole mass filters in order to obtain all kinds of mass spectra.

Needless to say, MS analysis is possible in addition to MS/MS analysis using the analysis mode of each quadrupole mass filter.

5.1 MS Analysis

MS analysis is possible using either Q1 or Q3 in the MS analysis mode. As with the LCMS-2020, scan analysis and SIM analysis are also possible. Notably, high speed scanning at 15,000 u/sec, which is the same as the LCMS-2020, can be performed in Q3 MS mode.

Analysis Mode	Q1	Collision Cell	Q3
Q1 MS	Resolution mode	Ion guide mode	
Q3 MS	Ion guide mode		Resolution mode

5.2 MS Scan Mode

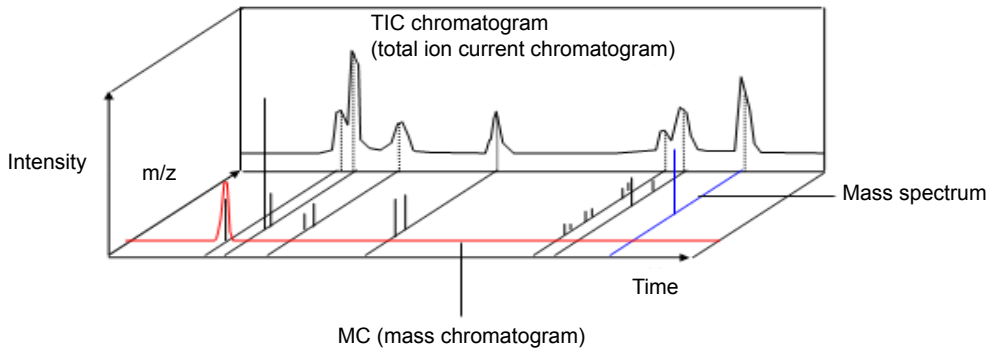


Fig. 5-1

Scan measurement is a method in which measurement is performed while scanning the mass range once every fixed interval (at the sampling rate). (I.e., a mass spectrum is obtained once every fixed interval.)

This method is mainly used for qualitative analysis.

Let's take the example of scanning from m/z 100 to 600:

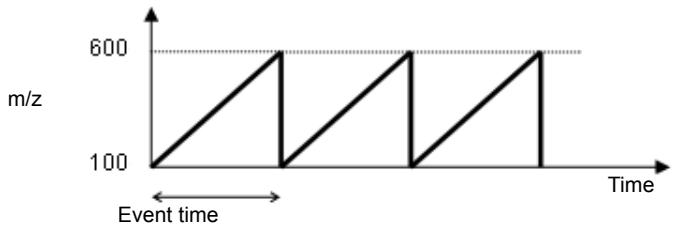


Fig. 5-2

As shown in Fig. 5-2, the m/z range is scanned.

If we make the scan time 1 second, this means that the range from m/z 100 to 600, which is an interval of 500, is scanned in 1 second.

This is called a scan speed of 500 u/sec.

The LCMS-8030/LCMS-8040 is capable of scan measurement at a maximum speed of 15,000 u/sec in Q3 MS mode. When performing high speed scan measurement, use Q3 MS mode as opposed to Q1 MS mode.

TIC chromatogram (total ion current chromatogram)

A TIC chromatogram is a chromatogram that is displayed using all of the detected ions.

MC (mass chromatogram)

This is a chromatogram that shows the change in the intensity of m/z over time for a selected ion with a specific mass.

5.3 SIM Mode

In scan measurement a mass spectrum is obtained continually. SIM is a method in which only ions with the target mass are selectively detected. Compared with scan measurement it enables high-sensitivity analysis with no detection time wasted on the detection of ions with masses that are not required.

Since the peak height and area are stable too, SIM is normally used for quantitative analysis.

An example where m/z 100, 200 and 600 are analyzed using SIM is shown below.

Up to 32 channels can be set for a single event.

512 events can be configured. (3 channels are set in the example below.)

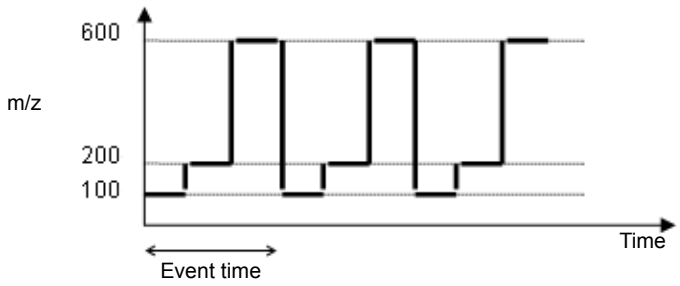


Fig. 5-3

5.4 MS/MS Analysis Mode

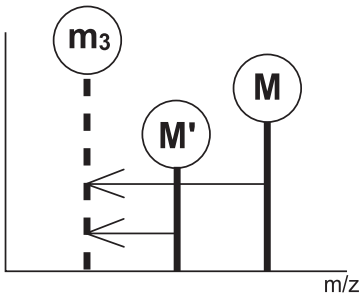
Specific ions are selected in the first quadrupole mass filter (Q1) in MS/MS analysis mode. These selected ions are referred to as precursor ions. The precursor ions are collided with inert gas in the collision cell (collision-induced dissociation, CID) to generate product ions. By measuring the product ions in the second quadrupole mass filter (Q3), we can obtain information regarding the structure of the precursor ions. This analysis method is referred to as MS/MS. Four types of analysis are possible by configuring either scan analysis or SIM analysis for Q1 and Q3.

Analysis Mode	Q1	Collision Cell	Q3
Precursor ion scan	Scan	Ion guide mode	SIM
Product ion scan	SIM		Scan
Neutral loss scan	Scan		Scan
MRM	SIM		SIM

5.5 Precursor Ion Scan Mode

The analysis method in this mode involves performing scanning in Q1, fixing Q3 to a specific m/z, and selectively analyzing the ions generated in the CID. This allows the examination of precursor ions with common product ions. This mode is suitable for screening ions with common substructures.

The horizontal axis of the displayed mass spectrum indicates the scale of Q1 and the vertical axis indicates the intensity of the product ions.



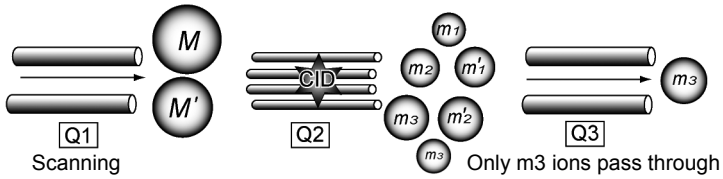


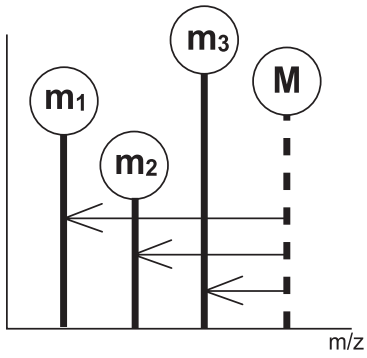
Fig. 5-4 Precursor Ion Mode Pattern Diagram

5.6 Product Ion Scan Mode

The analysis method in this mode involves fixing Q1 to a specific m/z and performing selective analysis on precursor ions selected in Q3 that were generated in the CID. As product ion spectra can be obtained, this mode is suitable for examining the structure of ions selected in Q1. The horizontal axis of the displayed mass spectrum indicates the scale of Q3.

Example of usage: MRM analysis condition examination - Product ion identification

Determining the amino-acid sequence of peptides and proteins



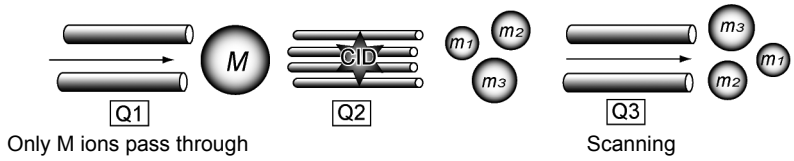
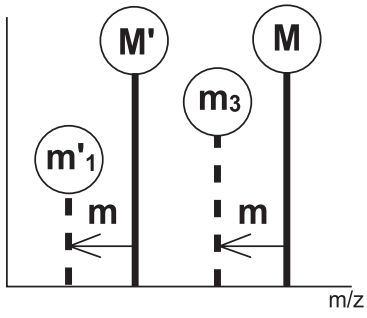


Fig. 5-5 Product Ion Mode Pattern Diagram

5.7 Neutral Loss Scan Mode

The analysis method in this mode involves maintaining the difference in the m/z for analysis in Q1 and Q3 while performing scan analysis. This allows the scanning of ions desorbed from common neutral fragments. As with the precursor ion scan mode, this mode is suitable for screening ions with common substructures (neutral fragments). Generally, the horizontal axis of the displayed spectrum indicates the scale of Q1 and the vertical axis indicates the intensity of the product ions.



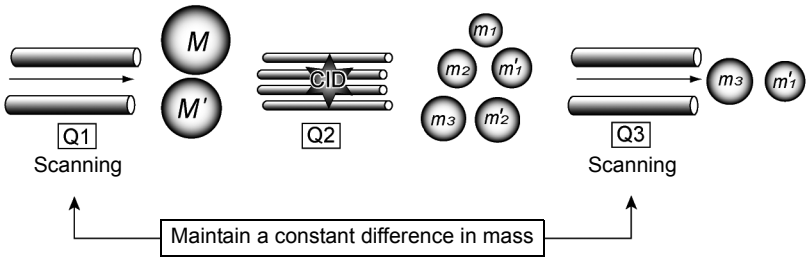
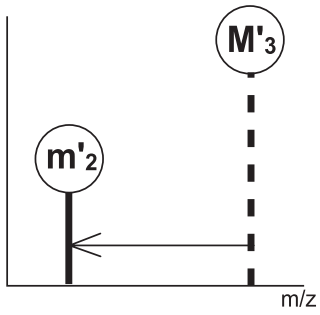


Fig. 5-6 Neutral Loss Mode Pattern Diagram

5.8 MRM Mode

The analysis method in this mode involves fixing both Q1 and Q3 to a specific m/z and selectively analyzing ions. Precursor ions are selected in Q1 and product ions that contain structural information generated in the CID are selected in Q3. As both precursor ions and product ions are specified and monitored, highly selective quantitative analysis that is low in unwanted substances can be achieved compared to SIM measurement. This means this mode is effective in determining the quantities of trace constituents contained in large matrix samples. Only chromatograms can be obtained in MRM mode as scanning is not performed.



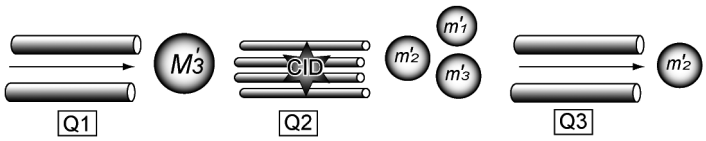


Fig. 5-7 MRM (Multiple Reaction Monitoring)

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