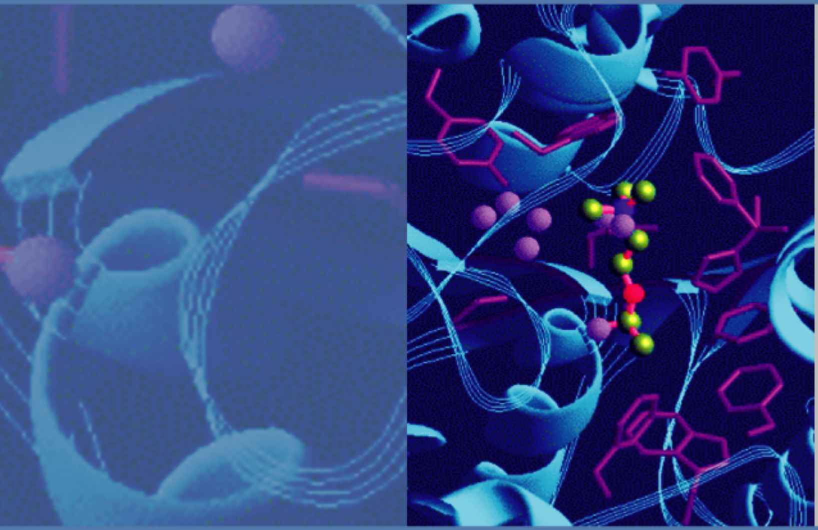

DSQ II

User's Guide

120299-0003 Revision D September 2, 2010

Thermo SCIENTIFIC

Ion Trap series refers to ITQ and PolarisQ instruments. DSQ series refers to all DSQ and DSQ II instruments. Information about the TRACE GC and FOCUS GC instruments is included in this document.

INSTRUMENT USAGE: Thermo Scientific systems operate safely and reliably under carefully controlled environmental conditions. If the equipment is used in a manner not specified by the manufacturer, the protections provided by the equipment may be impaired. If you maintain a system outside the specifications listed in this guide, failures of many types may occur. The repair of such failures is specifically excluded from the standard Warranty and service contract coverage.

Release history: Rev A, Aug 14, 2006. Rev B, Dec 4, 2008, Rev C November 11, 2009, Rev D September 2, 2010.

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Reader's Survey

Free Gift!

With every returned Reader's Survey

DSQ II User's Guide, 120299-0003, Revision D

Free gift for your returned Reader's Survey. Please help us improve the quality of our documentation by completing and returning this survey. Circle one number for each statement:

	Strongly Agree	Agree	Neutral	Disagree	Strongly Disagree
The manual is well organized.	1	2	3	4	5
The manual is clearly written.	1	2	3	4	5
The manual contains all the information I need.	1	2	3	4	5
The instructions are easy to follow.	1	2	3	4	5
The instructions are complete.	1	2	3	4	5
The technical information is easy to understand.	1	2	3	4	5
Examples of operation are clear and useful.	1	2	3	4	5
The figures are helpful.	1	2	3	4	5
I was able to operate the system using this manual.	1	2	3	4	5

If not, please comment below. Attach additional sheets if necessary.

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Customer Registration Card

Register now…and receive all the privileges associated with being a Thermo Fisher Scientific product user including customer support, application reports, and technical reports.

MY ORGANIZATION IS: **(Check only one)**

- ❏ Commercial (for profit) lab
- ❏ Government lab
- ❏ Hospital/Clinic
- ❏ Industrial lab
- ❏ Research Institute
- ❏ University/College
- ❏ Veterinary
- ❏ Other______________________

MY PRIMARY JOB FUNCTION IS**: (Check only one)**

- ❏ Administration
- ❏ Lab management
- ❏ Operator
- ❏ Other______________________

MY PRIMARY APPLICATION IS: **(Check only one)**

- ❏ Analytical
- ❏ Biomedical
- ❏ Clinical/Toxicology
- ❏ Energy
- ❏ Environmental
- ❏ Food/Agricultural
- ❏ Forensic/Toxicology
- ❏ Pharmaceutical
- ❏ Research/Education
- ❏ Other______________________

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Name ______________________________ Title ______________________________
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Regulatory Compliance

Thermo Fisher Scientific performs complete testing and evaluation of its products to ensure full compliance with applicable domestic and international regulations. When the system is delivered to you, it meets all pertinent electromagnetic compatibility (EMC) and safety standards as described below.

EMC Directive 89/336/EEC

EMC compliance has been evaluated by Professional Testing.

- PolarisQ, ITQ, and Ion Trap Series standards: EMC EN 55011:1998 + EN 50082-1:1998, Safety EN 61010-1:1990 + A1:1992 + A2:1995
- DSQ standards: EMC EN 61326-1:1998 + A1:1998. Safety EN 61010-1:1990 + A1:1992 + A2:1995
- DSQ II standards: EMC EN 61326-1:1997 + A1:1998 + A2:2001. Safety EN 61010-1:2001
- Direct Probe Controller (DPC) standards: EMC EN 55011:1991 + EN 50082-1:1992. Safety EN 61010-1:1994

Low Voltage Safety Compliance

This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001. Changes that you make to your system may void compliance with one or more of these EMC and safety standards. Changes to your system include replacing a part or adding components, options, or peripherals not specifically authorized and qualified by Thermo Fisher Scientific. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Fisher Scientific or one of its authorized representatives.

FCC Compliance Statement

Certifications, FCC part 15, Class A

This equipment has been tested and found to comply with the limits for a Class A digital device, pursuant to part 15 of the FCC rules. These limits are designed to provide reasonable protection against harmful interference when the equipment is operated in a commercial environment. This equipment generates, uses, and can radiate radio frequency energy. If it is not installed and used in accordance with the instruction manual, it may cause harmful interference to radio communication. Operation of this equipment in a residential area is likely to cause harmful interference. In this case, users will be required to correct the interference at their own expense. Detailed installation requirements are in the respective instrument's preinstallation guide.

WARNING Read and understand the various precautionary notes, signs, and symbols contained inside this manual pertaining to the safe use and operation of this product before using the device.

Notice on Lifting and Handling of Thermo Scientific Instruments

For your safety, and in compliance with international regulations, the physical handling of this Thermo Fisher Scientific instrument ***requires a team effort*** to lift and/or move the instrument. This instrument is too heavy and/or bulky for one person alone to handle safely.

Notice on the Proper Use of Thermo Scientific Instruments

In compliance with international regulations: Use of this instrument in a manner not specified by Thermo Fisher Scientific could impair any protection provided by the instrument.

Notice on the Susceptibility to Electromagnetic Transmissions

Your instrument is designed to work in a controlled electromagnetic environment. Do not use radio frequency transmitters, such as mobile phones, in close proximity to the instrument.

For manufacturing location, see the label on the instrument.

WEEE Compliance

This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2002/96/EC. It is marked with the following symbol:

Thermo Fisher Scientific has contracted with one or more recycling or disposal companies in each European Union (EU) Member State, and these companies should dispose of or recycle this product. See www.thermo.com/

WEEERoHS for further information on Thermo Fisher Scientific's compliance with these Directives and the recyclers in your country.

WEEE Konformität

Dieses Produkt muss die EU Waste Electrical & Electronic Equipment (WEEE) Richtlinie 2002/96/EC erfüllen. Das Produkt ist durch folgendes Symbol gekennzeichnet:

Thermo Fisher Scientific hat Vereinbarungen mit Verwertungs-/Entsorgungsfirmen in allen EU-Mitgliedsstaaten getroffen, damit dieses Produkt durch diese Firmen wiederverwertet oder entsorgt werden kann. Mehr Information über die Einhaltung dieser Anweisungen durch Thermo Fisher Scientific, über die Verwerter, und weitere Hinweise, die nützlich sind, um die Produkte zu identifizieren, die unter diese RoHS Anweisung fallen, finden sie unter www.thermo.com/WEEERoHS.

Conformité DEEE

Ce produit doit être conforme à la directive européenne (2002/96/EC) des Déchets d'Equipements Electriques et Electroniques (DEEE). Il est marqué par le symbole suivant:

Thermo Fisher Scientific s'est associé avec une ou plusieurs compagnies de recyclage dans chaque état membre de l'union européenne et ce produit devrait être collecté ou recyclé par celles-ci. Davantage d'informations sur la conformité de Thermo Fisher Scientific à ces directives, les recycleurs dans votre pays et les informations sur les produits Thermo Fisher Scientific qui peuvent aider la détection des substances sujettes à la directive RoHS sont disponibles sur www.thermo.com/WEEERoHS.

Contents

Preface

This guide describes how to install and configure the DSQ II system, set up methods, and run samples.

About Your System

Thermo Fisher Scientific systems provide the highest caliber gas chromatography/mass spectrometry (GC/MS) instrumentation available on today's market.

GC/MS represents a combination of two powerful analytical techniques: GC, which acts as a separation technique and MS, which acts as a detection technique. Complex mixtures of individual compounds can be injected into the GC, either manually or through the use of an optional autosampler, and then separated for presentation to the MS. The MS will then generate a mass spectrum of the GC eluent and its components, which can be used for qualitative identification, as well as accurate and precise quantification of the individual compounds present in the sample.

IMPORTANT Thermo Fisher Scientific systems are designed to optimize both the separation and detection capabilities of GC/MS techniques and combine them in a synergistic fashion to provide high performance analytical capabilities for both research and routine applications. More information on the use of this system can be found in related documentation sources and through the provided contact information.

WARNING Thermo Fisher Scientific systems operate safely and reliably under carefully controlled environmental conditions. If the equipment is used in manner not specified by the manufacturer, the protections provided by the equipment may be impaired. If you maintain a system outside the specifications listed in this guide, failures of many types, including personal injury or death, may occur. The repair of instrument failures caused by operation in a manner not specified by the manufacturer is specifically excluded from the Standard Warranty and service contract coverage.

Power Ratings

Mass Spectrometer (MS)
- 120 V ac +6/-10%, 50/60 Hz, 15 A max
- 230 V ac ±10%, 50/60 Hz, 10 A max

Gas Chromatograph (GC)
- 120 V ac +6%/-10%, 50/60 Hz, 20 A max
- 230 V ac ±10%, 50/60 Hz, 10 A max

Detailed instrument specifications are in the Product Specification or Product Brochure.

Safety Alerts and Important Information

Make sure you follow the precautionary notices presented in this guide. Safety and other special notices appear in boxes and include the following:

WARNING This is the general warning safety symbol and safety alert word to prevent actions that *could* cause personal injury. It highlights hazards to humans or the environment. Each WARNING safety alert is preceded with this safety symbol and another appropriate safety symbol (see "Safety Symbols and Signal Words" on page xiii.) Then it is followed with an appropriate safety precautionary message. When you see a safety alert on your instrument or in the publications, please carefully follow the safety instructions before proceeding.

CAUTION This is the safety alert word to prevent actions that *may* cause personal injury or instrument damage. We use it to highlight information necessary to prevent personal injury or damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal system performance. A CAUTION safety alert is always preceded with an appropriate safety symbol (see "Safety Symbols and Signal Words" on page xiii.) Then it is followed with an appropriate safety precautionary message. When you see a safety alert on your instrument or in the publications, please carefully follow the safety instructions before proceeding.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Emphasizes important information about a task.

Tip Helpful information that can make a task easier.

Safety Symbols and Signal Words

All safety symbols are followed by **WARNING** or **CAUTION**, which indicates the degree of risk for personal injury and/or instrument damage. Cautions and warnings are following by a descriptor, such as **BURN HAZARD**. A **WARNING** is intended to prevent improper actions that *could* cause personal injury. Whereas, a **CAUTION** in intended to prevent improper actions that *may* cause personal injury and/or instrument damage. The following safety symbols may be found on your instrument and/or in this guide:

	**BURN HAZARD.** This symbol indicates a hot surface that *could* or *may* cause burn injuries.
	**ELECTRICAL SHOCK HAZARD.** This symbol indicates that an electrical shock *could* or *may* occur.
	**FIRE HAZARD.** This symbol indicates a risk of fire or flammability, or that fire/flammability damage *could* or *may* occur.
	**FLAMMABLE GAS HAZARD.** This symbol alerts you to gases that are compressed, liquefied or dissolved under pressure and can ignite on contact with an ignition source. This symbol indicates this risk *could* or *may* cause physical injury.
	**GLOVES REQUIRED.** This symbol indicates that you must wear gloves when performing a task or else physical injury *could* or *may* occur.
	**HAND AND CHEMICAL HAZARD.** This symbol indicates that chemical damage or physical injury *could* or *may* occur.
	**INSTRUMENT DAMAGE.** This symbol indicates that damage to the instrument or module *may* occur. This damage may not be covered under the standard warranty.
	**LIFTING HAZARD.** This symbol indicates two or more people are required to lift the object to prevent a physical injury that *could* or *may* occur.
	**MATERIAL AND EYE HAZARD.** This symbol indicates that eye damage *could* or *may* occur.
	**RADIOACTIVE.** This symbol indicates the presence of radioactive material *could* or *may* occur.
	**READ MANUAL.** This symbol alerts you to carefully read your instrument's operational instructions before usage to ensure your safety and the instrument's operational ability. Failing to carefully read the instructions *could* or *may* put you at risk for a physical injury.
	**TOXIC SUBSTANCES HAZARD.** This symbol indicates that exposure to a toxic substance *will*, *could*, or *may* cause personal injury or death.
	This is the general warning symbol that the ISO 3864-2 standard refers to as the general warning signal to prevent personal injury. It is a triangle with an exclamation mark that precedes the **WARNING** safety alert word. In the vocabulary of ANSI Z535 signage, this symbol indicates a possible personal injury hazard exists if the instrument is improperly used or if unsafe actions occur. We use this symbol and another appropriate safety symbol to alert to an imminent or potential hazard that *could cause personal injury*.

Contacting Us

There are several ways to contact Thermo Fisher Scientific.

❖ To contact Technical Support

Phone	800-532-4752
Fax	561-688-8736
E-mail	US.Techsupport.Analyzer@thermofisher.com

Find software updates and utilities to download at http://mssupport.thermo.com.

❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
Web site	http://www.thermo.com/com/cda/resources/resources_detail/1,,12512,00.html

❖ To suggest changes to documentation or to Instrument Help

- Fill out a reader survey online at www.thermo.com/lcms-techpubs.
- Send an e-mail message to the Technical Publications Editor at techpubsaustin@thermofisher.com.

Related Documentation

In addition to this guide, Thermo Scientific provides the following documents for the DSQ II. These documents are also available on a “Print-By-Request” basis.

DSQ II Document Set, PN 120299

- *DSQ II Preinstallation Guide*, PN 120299-0001
- *DSQ II Hardware Manual*, PN 120299-0002
- *DSQ II User’s Guide*, PN 120299-0003
- *Instrument Help* is available from within the DSQ II Tune software.

To suggest ways we can improve the documentation, use your browser to complete our documentation survey.

Setting Up the DSQ II System

This chapter describes how to install and set up the DSQ II system. It is to be used by factory-trained Field Service Engineers or experienced users that need to set up the instrument.

Contents

DAY ONE:

DAY TWO:

Getting the Right Tools

The following table contains the tools and parts you will need to install the DSQ II system. However, keep in mind some items are included with the system.

Table 1. DSQ II System Installation Tools

Tools Needed
Aluminum plug (PN 290 326 55)
Brass back ferrules, Swagelok (PN A0101-02500)
Brass front ferrules, Swagelok (PN A0101-08500)
Brass nuts, Swagelok (PN A0101-15500)
Cable, PC to DSQ II, 15 ft Ethernet crossover (PN 76396-0052)
Cable, Serial, PC to TRACE GC Ultra (PN 230 980 00)
Cable, GC to DSQ II remote start (PN 76396-0050)
Capillary column, TR5MS, 15 m, 0.25 mm i.d., 0.25 µm (PN 76317-3015)
CI Ion Volume (PN 119650-0230), if applicable
Column measuring tool (PN 119640-0550)
Copper tubing, clean (PN 76381-0041, 1/8-in. o.d., 0.030-in. wall)
Digital voltmeter (Fluke model 77 or equivalent)
Dusting spray containing tetrafluoroethane (Falcon® Dust-Off®, MicroCare® MicroBlast™, or equivalent)
Flashlight, small hand-held
Flow meter (Thermo Scientific GFM Pro PN 66002-010 or equivalent)
Forceps (PN 76360-0400)
Gas filter, helium (PN A0950-01600)
Gloves, clean, lint and powder-free (medium PN 23827-0008, large PN 23827-0009)
Hex nut driver, 5.5 mm
Injector ferrule for 0.25 mm column (PN 290 134 88)
Injector nut (PN 350 324 23)
Ion volume tool (PN 119270-0001)
I/R tool and guide bar, if applicable
Leak detector (Thermo Scientific GLD Pro PN 66002-001 or equivalent)
Magnifying glass
Methanol or other suitable solvent
Potentiometer adjustment tool

Table 1. DSQ II System Installation Tools, continued

Tools Needed
Power cords with appropriate plugs
Preinstallation Guide (PN 120299-0001)
Scoring wafer (or sapphire scribe) to cut capillary column
Screwdriver, flat blade
Screwdriver, Phillips #1
Screwdriver, Phillips #2
Syringe, 10 µL, 70 mm needle (PN 3650-0103)
Tape measure
Teflon® thread tape
Tissue, lint-free
Tubing cutter
Test mix, octafluoronaphthalene and benzophenone (PN 120150-TEST)
Transfer line ferrule, 0.4 mm i.d. (PN A0101-18100)
Wrench, (adjustable) 12-in.
Wrench, (Allen) 1/16-in.
Wrench set, (Allen) 5, 2, 2.5, 3, 4, 5 mm (PN 3812-0100)
Wrench set, (open-ended) 5–17 mm
Wrench set, (open-ended) 1/4-in., 5/16-in., 7/16-in. (2), 9/16-in.,1/2-in.

Verifying Site Preparation

To verify the customer's site has been properly prepared, you will need:

- Digital voltmeter (Fluke model 77 or equivalent)
- Preinstallation checklist
- Preinstallation Guide
- Tape measure

Review the customer's Preinstallation Checklist with these items in mind:

- The customer is responsible for providing a completed Preinstallation Checklist prior to installation.
- All preinstallation requirements are listed in the *DSQ II Preinstallation Guide*, so you only need to double-check that the proper workbench, power outlets, power cords, temperature, and gases are available.

Unpacking the Instruments

To unpack the instruments, you will need:

- Original purchase order
- Packing slip
- Installation report (supplied by service organization)

1. Unpack the instruments to confirm that each item the customer ordered arrived without incident.

WARNING - LIFTING HAZARD. Use proper lifting techniques with heavy instruments to prevent bodily injury.

2. Check carefully for obvious damage. For example, look for tip indicators displaying a tipped condition or evidence of rough handling. If external damage is apparent, note this fact on the installation report and describe the extent of the damage. Have the customer sign or initial your comments.

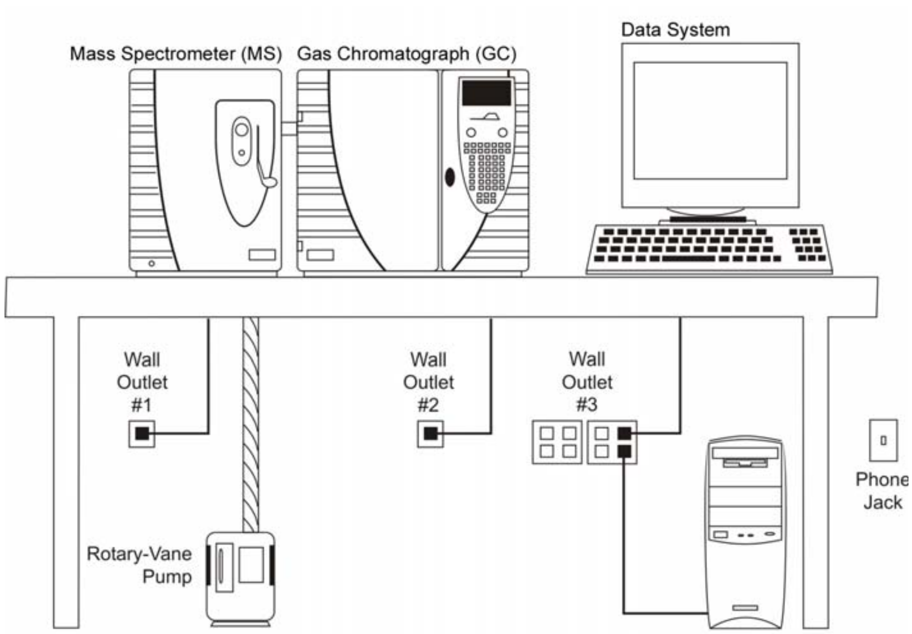
3. Confirm that the shipment is complete.

   a. Open and carefully remove all items from the shipping containers. The packing list is located in the installation packet.

   b. Verify that each item listed on the customer's purchase order and packing list is included with the shipment. If any items are missing, make a note on the installation report and immediately contact your local representative.

4. Set up the instruments.

Figure 1. DSQ II System Layout (Front View)



Work bench weight = 119 kg (292 lbs). Work bench length = 2 m (6 ft).

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a. Place the instruments from left to right in this order: DSQ II, TRACE GC Ultra or FOCUS GC, and the computer monitor with the mid-tower CPU beside the monitor or under the bench.

b. Check the computer CPU power indicator to make sure it is set for the correct line voltage.

c. Place the rotary-vane pump on the floor. If placed on the bench, excessive vibration could affect instrument performance.

> **Note** Install optional accessories, such as an autosampler, *after* the installation and qualification tests are complete.

5. Inspect and store the shipping containers.

   a. Carefully inspect ALL boxes and packing materials for missed items.

   b. Put packing materials back into shipping crates and store the empty boxes.

Connecting the Gas Lines

To connect the gas lines, you will need:

- Brass back ferrules, Swagelok
- Brass front ferrules, Swagelok
- Brass nuts, Swagelok
- Copper tubing, clean
- Gas filter, helium
- Leak detector (Thermo Scientific GLD Pro PN 66002-001 or equivalent)
- Teflon® thread tape
- Tubing cutter
- Wrench, (adjustable) 12-in.
- Wrench, (open-ended) 7/16-in.
- Wrench, (open-ended) 1/2-in.
- Wrench, (open-ended) 9/16-in.

> **Tip** To insure safe, leak-tight connections, read "Assembling Swagelok Fittings" on page 78 before assembling the Swagelok fittings.
>
> Leave enough slack in the tubing so the DSQ II and GC may be moved at least 40 cm (16-in.) away from each other. This ensures that column connections and system maintenance are easily performed.
>
> Forming shock loops with the tubing helps to dampen vibrations that can loosen the fittings.

Connecting the Carrier Gas

Carrier gas connection begins with supply lines to the GC carrier gas, to the gas filter, then to the GC carrier gas connection.

1. Connect one end of the supply line to the GC carrier gas and to the gas filter.

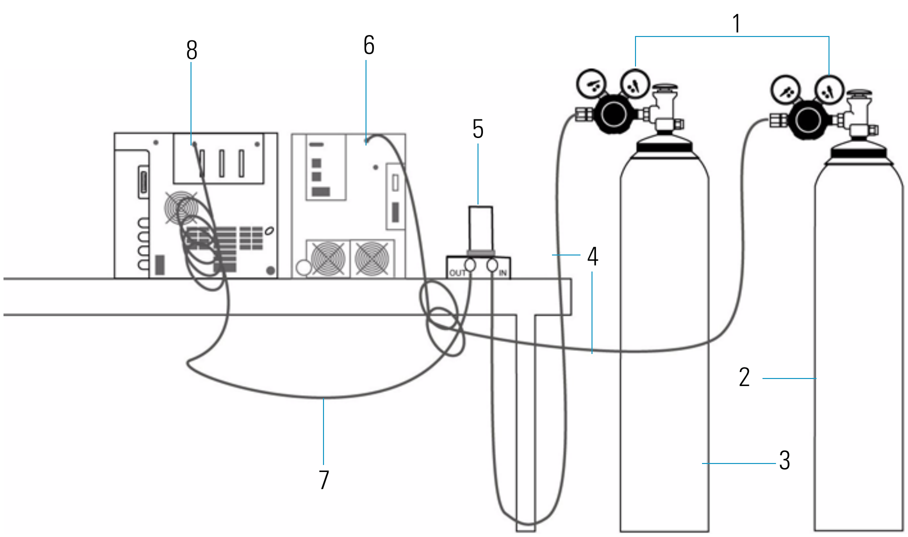
   a. Connect the carrier gas regulator to the carrier gas tank.

   b. Set the gas filter as close as possible to the GC. It should be easy to access since it must be changed regularly. Do not put it behind the GC where hot air from the exhaust vents will hit the gas filter. Mount it to the side of the GC or DSQ II or on top of one of the instruments. Instructions are included with the gas filter kit.

CAUTION - INSTRUMENT DAMAGE. To avoid contaminating the filter, do not loosen or remove caps from the gas filter until PURGED lines are connected.

   c. Notice that the gas filter has an IN and an OUT connection.

Figure 2. GC Carrier Gas Connections (View of the Back of System)



1	Gas Regulators	5	Gas Filter (IN and OUT Fittings)
2	CI Reagent Gas (Methane, Isobutane, or Ammonia 10 psi-70 kPa)	6	MS Reagent Gas Connection
3	Carrier Gas (Helium 60-100 psi, 400-700 kPa)	7	Shock Loops
4	Carrier Gas Supply Lines	8	GC Carrier Gas Connections

2. Prepare the carrier gas supply lines.
   a. Run a supply line from carrier gas regulator to the IN connection located on the gas filter, but do not remove the gas filter caps.
   b. Assemble the lines from the gas filter OUT connection to the GC. However, do not remove the caps from the GC.
   c. Include shock loops to isolate vibration and allow enough tubing to move the GC at least 40 cm (16-in.)
3. Purge the carrier gas supply line.
   a. Turn the carrier gas on and set to 5 psi.
   b. Purge the supply line for two minutes.
   c. While purging the lines, remove the cap from the gas filter IN connection and connect the carrier gas supply to the filter.
   d. Purge the gas filter and supply lines to the GC for 10 minutes.
4. Connect the carrier gas supply lines to the DSQ II and GC.
   a. Remove the carrier gas caps located on the GC carrier gas connection and connect the purged carrier gas supply lines.
   b. Tighten all fittings 3/4-in. turn past hand tight.
   c. If the GC is equipped with a left-side OCI or LVOCI inlet, and a right-side SSL injector, use a cross or tee to plumb to both right and left positioned DPFCs.
5. Reset the carrier gas regulator to a pressure of 100 psi (690 kPa). The nominal pressure is 80 psi (560 kPa).

CAUTION - INSTRUMENT DAMAGE. Do not set the carrier gas regulator pressure in excess of the maximum rated pressure of the DPFC.

Connecting the Reagent Gas (Optional Upgrade)

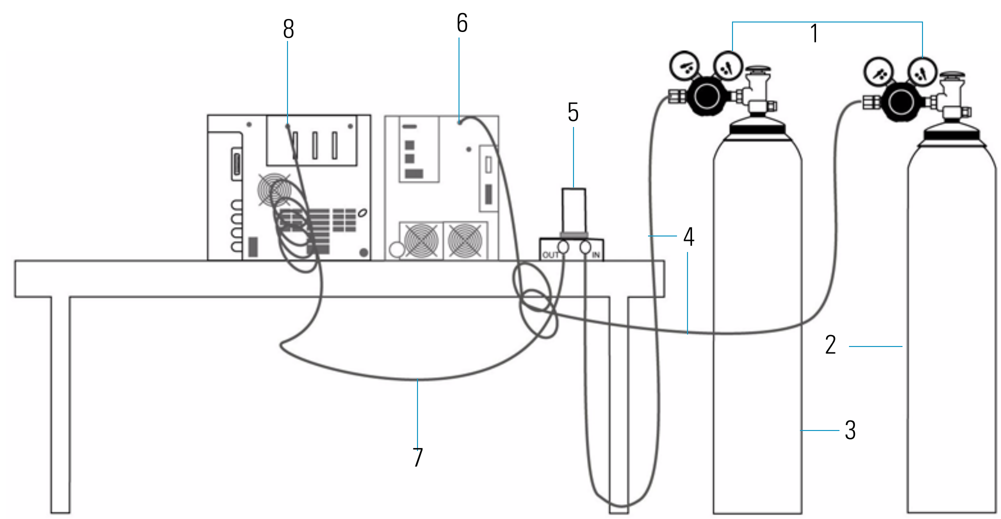
If you are using reagent gas and have a system equipped with the chemical ionization (CI) option, you must connect CI reagent gas. Methane is the most common CI reagent gas. You must connect the supply line to the reagent gas source.

1. Connect the reagent gas regulator to the reagent gas tank.

WARNING - FLAMMABLE GAS HAZARD. CI reagent gases are often flammable or corrosive, so you must vent the gas to a fume hood or other suitable exhaust. The CI reagent gas supply line must be leak tight.

2. Plumb a supply line to the CI reagent gas regulator and connect it to the regulator, but DO NOT remove the input cap from the DSQ II.

Figure 3. Reagent Gas Connections (View of the Back of System)



1	Gas Regulators	5	Gas Filter (IN and OUT Fittings)
2	CI Reagent Gas (Methane, Isobutane, or Ammonia 10 psi-70 kPa)	6	MS Reagent Gas Connection
3	Carrier Gas (Helium 60-100 psi, 400-700 kPa)	7	Shock Loops
4	Carrier Gas Supply Lines	8	GC Carrier Gas Connections

3. Turn on the CI reagent gas and set to 30 psi for purging.

CAUTION - INSTRUMENT DAMAGE. To avoid damaging the CI reagent gas flow controller, do not exceed 35 psi.

4. Prepare the reagent gas supply line.
   a. Run a supply line from the reagent gas regulator to the CI reagent gas input on the DSQ II, but do not connect it yet.
   b. Include a shock loop on the reagent gas supply line to isolate vibration and allow enough tubing to move the DSQ II at least 40 cm (16-in.)
   c. To allow for the collection of condensates, make sure the shockloop is below the level of the reagent gas regulator and the DSQ II reagent gas filter (if installed) input.
5. Purge the reagent gas supply line.
   a. Route the supply line to a vent hood or other suitable exhaust.
   b. Turn on the reagent gas supply and set the regulator to 30 psi (200 kPa).
   c. Purge the line for about 15 seconds to remove air and debris.
   d. Set the reagent gas regulator to 10 psi (70 kPa). Lower supply pressures produce more stable CI reagent gas flows.
   e. Turn off the reagent gas supply.
6. Connect the reagent gas supply line to the DSQ II.
   a. Attach the supply line to the CI reagent gas input on the DSQ II.
   b. Turn on the reagent gas supply.

CAUTION - INSTRUMENT DAMAGE. To avoid damaging the CI reagent gas flow controller, do not exceed 35 psi.

Checking for Leaks

To check for leaks:

1. Use an electronic hand-held leak detector (sensitivity: helium 0.01 mL/min) to check all gas fittings for leaks.

CAUTION - INSTRUMENT DAMAGE. Do not use liquid soap leak detectors (such as Snoop) to check for leaks. They may contaminate your system.

2. Leak check the carrier gas supply line.
3. Leak check the reagent gas supply line.

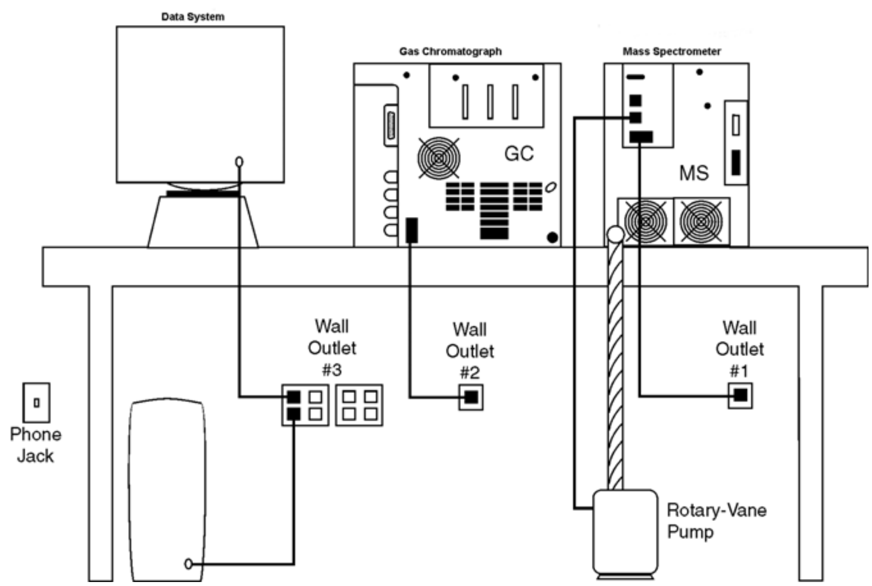
Installing the Data System

To install the data system (computer and Xcalibur software), you will need a 15 ft Ethernet crossover cable that connects the PC to the DSQ II and a serial cable that connects the PC to the GC.

To install the data system:

1. Set up power to the data system.

Figure 4. Data System Power Connections (View of the Back of System)



   a. Plug the power cords for the computer, monitor, and printer (optional upgrade) into wall outlet #3.

   b. Confirm the computer voltage setting is correct.

CAUTION - INSTRUMENT DAMAGE. If the computer voltage setting does not match the supplied line voltage, the computer may be damaged.

   c. Set up and connect the keyboard, mouse, monitor cable, and printer cable if applicable.

2. Connect the serial cable and Ethernet cables.

   a. Connect the GC serial cable to the computer's COM1 port.

   Note Be sure you use the supplied shielded, crossover cable to connect to the instrument. If you need a longer cable, connect a standard **Category 5 Ethernet cable** between the computer and the supplied cable.

   b. Connect the DSQ II's Ethernet cable one of the computer's Ethernet ports. The Ethernet port on a card is for the instrument, whereas the Ethernet port built into the motherboard may be used for a local area network.

3. Turn on the computer, monitor, and printer.
   a. Set the time and date.
   b. Set up passwords, if desired.
   c. Test the printer and install drivers. Without a printer driver, you cannot print Tune reports.

   Computers purchased from the factory have been fully set up and tested with the Xcalibur data system software. However, if you experience a situation where you need to reinstall software on a new computer or new hard drive, see "Reinstalling the Data System" on page 83.

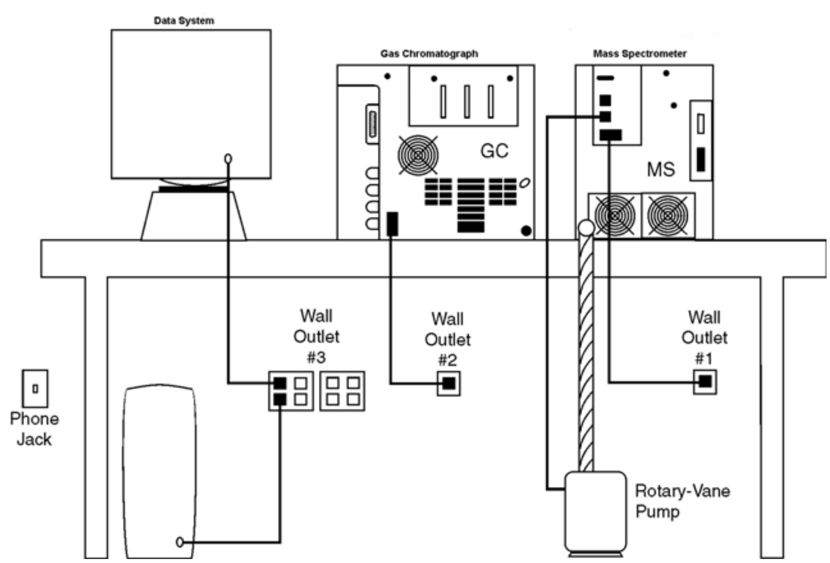
Installing the TRACE GC Ultra

To install the TRACE GC Ultra, you will need:

- Capillary column, TRACE TR-SQC, 15 m, 0.25 mm i.d., 0.25 µm
- Gloves, clean, lint- and powder-free
- Injector ferrule for 0.25 mm column
- Leak detector (Thermo Scientific GLD Pro PN 66002-001 or equivalent)
- Magnifying glass
- Methanol or other suitable solvent
- Scoring wafer (or sapphire scribe) to cut capillary column
- Tissue, lint-free
- Wrench, (open-ended) 6 mm

1. Use the sales order to verify the configuration of the TRACE GC Ultra.
2. Connect the transfer line cable to the left side of the TRACE GC Ultra.

Figure 5. Power Connections (View of the Back of System)

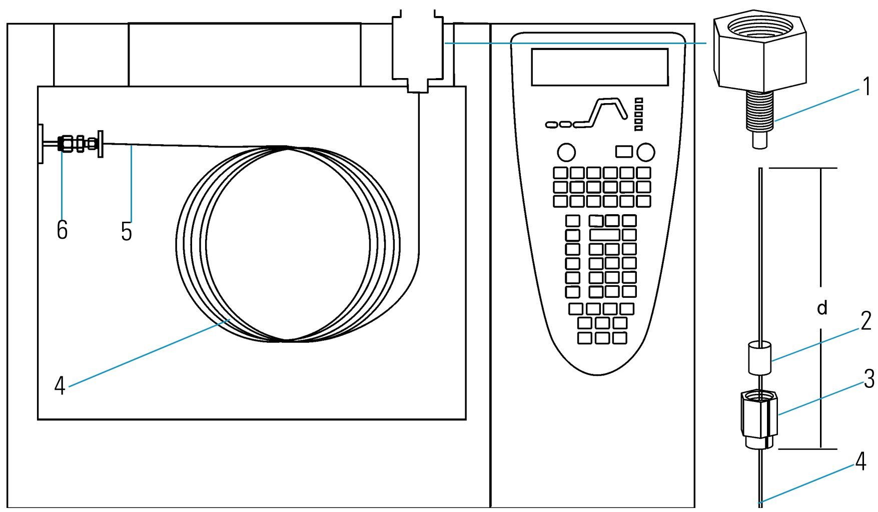


3. Plug the power cord into the back of the TRACE GC Ultra and then into wall outlet #2.

4. Connect the column to the injector. The test column is conditioned at the factory and requires no additional conditioning.

   If you are using a FOCUS GC, you must open Xcalibur on the computer, click **Instrument Setup** on the Home Page, and set the instrument parameters using the virtual keypad. Refer to the FOCUS GC documentation for instructions on using the keypad.

Figure 6. GC Injector (View of the Front of the TRACE GC Ultra)



1	Injector	4	Column
2	Injector Ferrule	5	Column Outlet
3	Injector Nut	6	Transfer Line

> **Note** Wear clean, lint and powder free gloves when you handle the column and injector ferrule.

a. Pressure test the inlet.

b. Unwind the column about a half-turn.

c. Wipe about 100 mm (4-in.) of the column with a tissue soaked in methanol.

d. Insert the column through the injector nut and ferrule open end up.

e. Wipe the column again with a lint-free tissue soaked in methanol.

f. Use the scoring wafer to score and break the column about 2.5 cm (1-in.) from the end. With the magnifying glass, check for an even, flat cut. Repeat if necessary.

> **Note** Sliding a septum on the column before the injector nut will help measure the proper distance between the nut and the end of the column. If you want to remove it later, cut the septum from the center to the edge.

   g. Insert the column into the injector so that the end of the column is the proper distance from the back of the injector nut. Proper distances are as follows: splitless = 64 mm, split = 40 mm, PTV = 30 mm.
   h. Finger-tighten the injector nut and then give it an additional 1/4-turn with the wrench.
5. Use the scoring wafer to score and break the column outlet about 2.5 cm (1-in.) from the end.
6. Power on the TRACE GC Ultra.
7. Set up the TRACE GC Ultra.
   a. Set the oven, injector, and transfer line temperatures to 30 °C.
   b. Set the injector flow to 1.0 mL/min.
   c. Turn the vacuum compensation off under the right or left carrier menu.
   d. Dip the column outlet in a small vial of methanol. Bubbles indicate there is flow through the column.
   e. Allow the column to purge for at least 10 minutes.
8. Install an injector nut with an aluminum plug onto the TRACE GC Ultra inlet.
9. Use a 6 mm wrench to tighten it.
10. Press the Left or Right Carrier button and put the inlet in constant pressure mode.
11. Move the septum purge and split vent valve to the OFF position.
   a. Press the Valve button that is located on the lower portion of the GC keypad.
   b. Select the left or right inlet.
   c. Scroll to each of the inlet valve selections and press the front panel OFF key.
   d. Allow several seconds after pressing the OFF button for the display to indicate OFF.
12. Press the Left or Right Inlet button and scroll to Pressure.
   a. Set the inlet pressure to 35 Psig (250 kPa) and allow the inlet several seconds to pressurize.
   b. Confirm the set point has been reached.
13. Turn the inlet pressure OFF and monitor the pressure. The pressure should not change more than 10 kPa in an hour. This is less than 2 kPa drop in 10 minutes.
14. Determine if there is a leak.
   a. Use a suitable leak detector if the pressure test indicates a gradual leak. The most likely place is the septum nut, septum purge or split vent, injector nut with plug, or at the terminal fitting for capillary column. It is not uncommon for a very small leak (approximately < 1 mL) to exit out the split or septum purge vent.

b. Test if a small leak at one of these vents is the reason for a decrease in pressure, hold a septum over the top of the vent, pressurize the inlet and allow several seconds for the vent fitting to pressurize, turn the pressure off and see if the pressure holds.

c. If the pressure holds, remove the septum and see if the pressure begins to decrease. A decrease greater than 1 psi (7 kPa) over three minutes may indicate a defective flow module.

15. After completing the pressure test, set the split vent and septum purge valve to ON.

a. Set the inlet pressure to 5 psi (35 kPa).

b. Press the Left or Right Inlet Carrier button and return the inlet to the constant flow mode.

16. Remove the injector nut with plug and continue installing the column.

17. Perform a column characterization.

a. Raise the oven and injector temperatures to 50 °C and allow them to stabilize.

b. Press the Column Eval key to characterize the column, which takes several minutes.

c. Expect a K-factor of about 0.7 – 0.9 for a 15 m, 0.25 mm i.d. column. If the column does not report a K-factor within this range or within 0.1 units of the previous stored value, check for a leak or broken column using the leak detector. The K-factor is a measured flow resistance for the column. A K-factor that is too low may indicate a leak in the system, while a K-factor that is too high may indicate a blockage.

CAUTION - INSTRUMENT DAMAGE. Do not raise the oven temperature until you are sure the system is free of leaks. The column will be destroyed if it is exposed to oxygen at temperatures above 100 °C.

d. Raise the oven temperature to 150 °C and allow it to stabilize.

18. Perform a column leak check.

a. Run an automated leak check on the TRACE GC Ultra.

b. If the report indicates there is a leak, use the leak detector to fix leaks at all the fittings in the TRACE GC Ultra.

c. Repeat the column evaluation and leak check until there are no more leaks.

d. Raise the injector temperature to 220 °C.

Installing the DSQ II

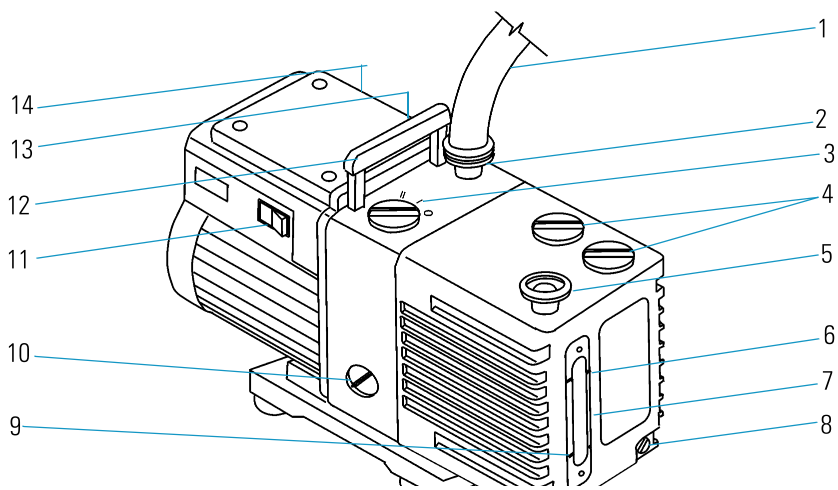
To install the DSQ II, you will need:

- Cable, GC to DSQ II remote start
- Column measuring tool
- Gloves, clean, lint- and powder-free
- Leak detector (Thermo Scientific GLD Pro PN 66002-001 or equivalent)
- Magnifying glass
- Methanol or other suitable solvent
- Potentiometer adjustment tool
- Scoring wafer (or sapphire scribe) to cut capillary column
- Tissue, lint-free
- Transfer line ferrule, 0.4 mm i.d.
- Wrench, open-ended 5/16-in.
- Wrench, open-ended 7/16-in.

1. Install the rotary-vane pump.

    a. Set the rotary-vane pump on the floor behind the system. The pump should not be placed on the workbench as it produces excessive vibration that may affect the performance of the system.

Figure 7. Rotary-Vane Pump Components



1	Foreline Vacuum Hose	8	Drain Plug
2	Inlet Port	9	MIN (minimum level mark)
3	Gas-Ballast Control	10	Mode Selector
4	Oil Filler Plugs	11	On/Off Switch
5	Outlet Port	12	Handle
6	MAX (maximum level mark)	13	Voltage Indicator
7	Oil-Level Sight-Glass	14	Electrical Inlet Connector

b. Check the voltage indicator to verify the rotary-vane pump is configured for the same voltage as the DSQ II.

CAUTION - INSTRUMENT DAMAGE. If the rotary vane pump is set to a different voltage than the DSQ II, the pump may be damaged when the power is turned on.

c. Remove one of the oil filler plugs.

d. Add oil to the oil filler plug opening half way between the MIN and MAX level marks.

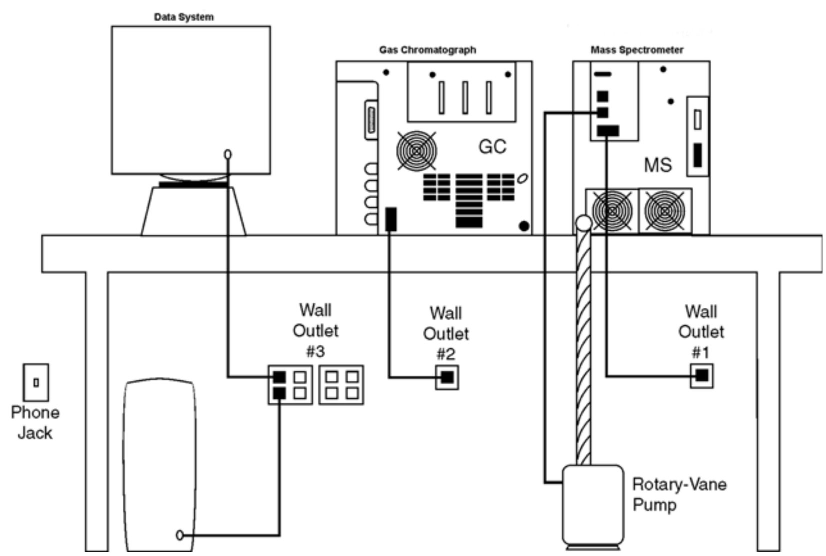
e. If the oil level goes above the MAX level mark, remove the drain plug and drain the excess oil from the pump.

f. Replace the oil filler plug.

g. Connect the foreline vacuum hose.

h. Connect the outlet port to a suitable exhaust.

Figure 8. Rotary-Vane Pump Power Connection (View of the Back of DSQ II)



i. Plug the power cord into the mechanical pump connection on the back of the DSQ II.

2. Repeat Step 1 if you are installing a second rotary-vane pump, which is included with the sample probe upgrade.

   a. Plug the second pump into the accessory start connection on the back of the DSQ II.

   b. Make sure the inlet valve vacuum hose exits the DSQ II just above the foreline vacuum hose.

3. Connect the transfer line, Ethernet, and remote start cables.

   a. Confirm the transfer line cable is plugged into the left side of the GC.

b. Carefully push the GC next to the DSQ II, making sure the transfer line extends into the GC.

c. Connect the Ethernet cable leading from the computer to the back of the DSQ II.

d. Connect the remote start cable from the GENERIC HANDSHAKE port located on the GC to the GC START port located on the DSQ II.

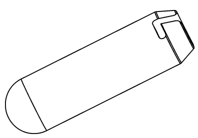
4. Inspect the DSQ II.

a. Remove all the covers (front, top, and left side) from the DSQ II, as described in the *DSQ II Hardware Manual*.

b. Remove the shipping foam that secures the vacuum manifold cover. Store the foam with the DSQ II accessories in case the instrument needs to be moved in the future.

5. Use the sales order to verify the configuration of the DSQ II.

a. Look for any parts that might have come loose during shipping.



Ion Volume Removal Tool

b. Verify that the ion volume is fully inserted. You can use the ion volume tool to push on the ion volume. At room temperature, the ion volume does not fit tightly in the ion source so that it does not seize when the source heats to 300 °C. Adjust the ball valve to a stable position so it can be removed at a 300 °C source temperature.

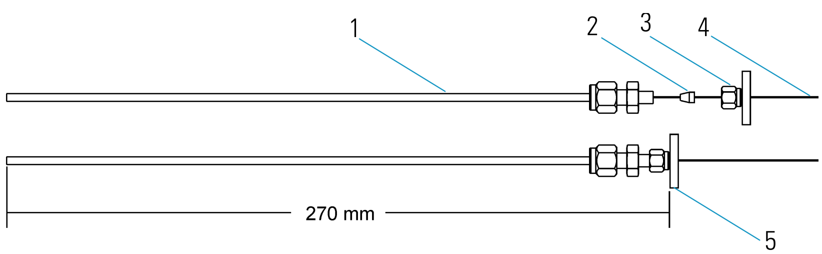
6. Connect the GC column to the DSQ II transfer line, as shown in Figure 9.

a. Lower the oven temperature to 30 °C and allow it to cool before continuing.

WARNING - BURN HAZARD. The oven and transfer line may be hot. Allow them to cool to room temperature before touching them. Do not touch the hot injector.

b. Unwind about one turn of the column from the end of the column outlet.

Figure 9. Using the Column Measuring Tool



1	Column Measuring Tool	4	Column
2	Transfer Line Ferrule	5	Septum
3	Transfer Line Nut		

Note Wear clean, lint- and powder-free gloves when you handle the column and transfer line ferrule.

c. Wipe about 300 mm (12-in.) of the column with a tissue soaked in methanol.

d. Insert the column through the septum, transfer line nut, and ferrule. Wipe the column again with a tissue soaked in methanol. Sliding a septum on the column before the transfer line nut will help you measure the proper distance between the nut and the end of the column. If you want to remove it later, cut the septum from the center to the edge.

e. Screw the transfer line nut onto the column measuring tool.

f. Push the column past the end of the column measuring tool, then use the scoring wafer to score and break the end of the column. Use a magnifying glass to check for an even, flat cut. Repeat if necessary.

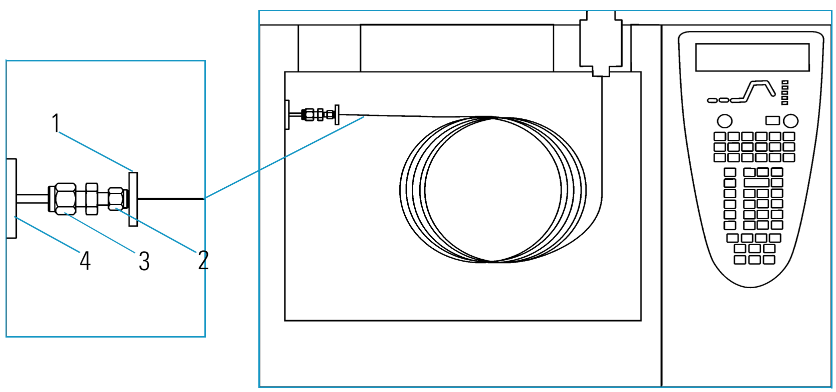
g. Pull the column back so that it is flush with the end of the column measuring tool.

h. Tighten the transfer line nut.

i. Slide the septum up to the back of the transfer line nut.

j. Remove the column, transfer line nut and ferrule from the column measuring tool.

Figure 10. Transfer Line (View of the Front of DSQ II)



1	Septum	3	Transfer Line Union
2	Transfer Line Nut	4	Transfer Line

k. Insert the column into the transfer line, but be careful not to move the septum. For proper operation, the column must extend approximately 1 mm past the end of the transfer line.

l. Tighten the transfer line nut and transfer line union.

7. Condition the transfer line ferrule. Graphite/vespel ferrules like the transfer line ferrule require conditioning to ensure a leak-tight seal.

   a. Raise the oven temperature to 275 °C.

   b. Wait 10 minutes.

c. Lower the oven temperature to 30 °C and allow it to cool before continuing.

WARNING - BURN HAZARD. The oven may be hot. Allow it to cool to room temperature before opening it. Do not touch the hot injector.

d. Re-tighten the transfer line nut and transfer line union.

8. Set up the GC.

a. Make sure the column does not have any sharp bends and that it does not touch any metal objects or walls inside the oven.

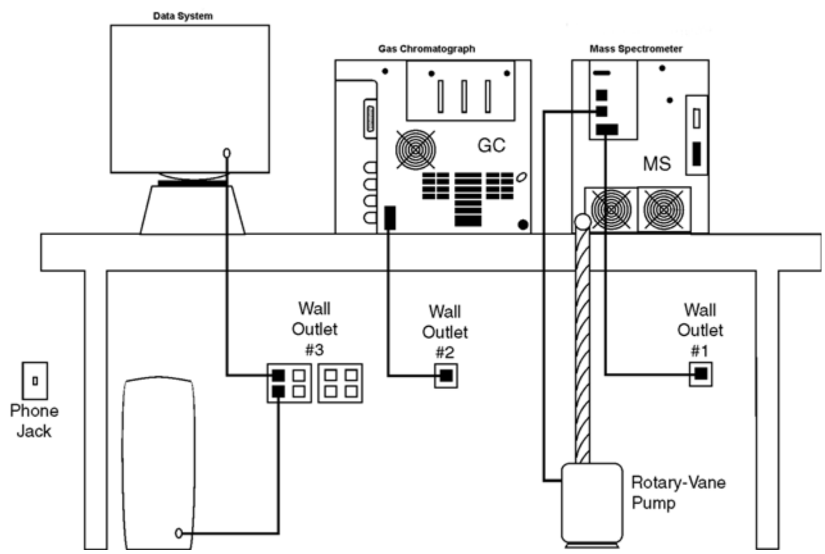
b. Raise the oven temperature to 40 °C.

c. Turn on vacuum compensation, which is under the right or left Carrier menu.

9. Reattach the DSQ II left, top, and front covers.

10. Connect the DSQ II power cord into wall outlet #1 or power conditioner, if installed.

Figure 11. Power Connections



11. Double-check all vacuum, gas, and electrical connections.

Starting the System

To start the system:

1. Power-on the DSQ II by setting the main circuit breaker to ON (I).
2. Power-on the rotary-vane pump.
    a. Allow the fore pressure to reach the proper operating pressure.
    b. Allow the fore pressure monitor circuit to power-on the turbomolecular pump.

CAUTION - INSTRUMENT DAMAGE. If you power-on the DSQ II without column flow, air is drawn through the column and may damage it. This large air leak into the DSQ II also means you must clean the ion source.

3. Set the transfer line to 250 °C.
4. Open the *Xcalibur* application to establish communication and initialize each instrument configured for use.
    a. Wait about 60 seconds for the DSQ II to initialize.
5. When *Xcalibur* displays a "There is not sufficient vacuum" message, click the **Ignore** button and continue monitoring instrument status.
    a. If you see any other error messages, check that all instruments are connected and powered on. Refer to the *Troubleshooting* section of the *DSQ II Hardware Manual* for assistance.
6. Click the DSQ II Tune icon  on the computer desktop to open the *DSQ II Tune* software.

Confirming Readbacks

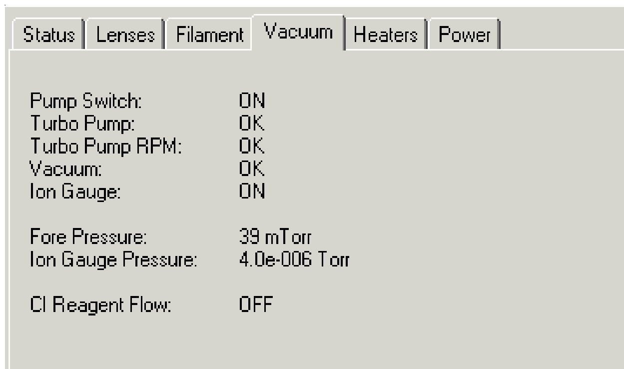
Once the GC/MS system has been initialized, check the DSQ II Instrument Status tabs to confirm the operation of the vacuum and heater readbacks before running diagnostics.

CAUTION - INSTRUMENT DAMAGE. Pay particular attention to the vacuum readbacks because an improper vacuum will damage the filament during an Ionization/Lens test.

1. In *DSQ II Tune*, select **Tune | Show Status View** and click the Vacuum tab to confirm the fore pressure, turbo pump status, and ion gauge status.

   a. Verify that the fore pressure is less than 300 mTorr.

   Figure 12. Vacuum Tab Readbacks

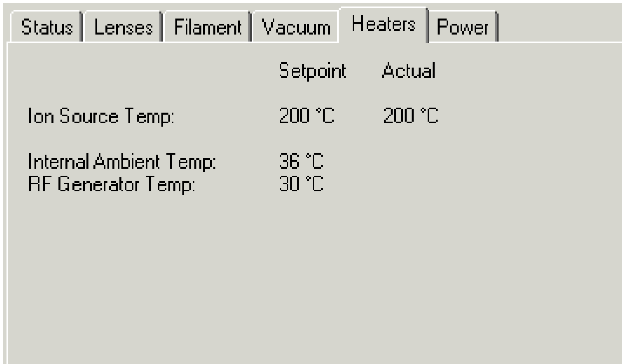
CAUTION - INSTRUMENT DAMAGE. If the fore pressure does not change to less than 300 mTorr within five minutes, there is a large leak that needs to be fixed immediately to prevent damage to the instrument. See the *DSQ II Hardware Manual* for information about troubleshooting a large leak.

   b. Check the Vacuum tab to make sure the turbomolecular pump is powered on. Within five minutes after powering on the pump, its readback should be *OK*, which indicates it has reached operating speed.

   c. Wait until the ion gauge pressure is less than 1 x 10 -4 Torr. If the system is not equipped with an ion gauge, wait at least 15 minutes.

Click the Heaters tab to confirm the ion source temperature is set to 200 °C. To set the temperature, select **Instrument | Set Temperature...** to open the Temperature Setting window, enter **200** in the field and click **OK**.

Figure 13. Confirming the Ion Source Temperature



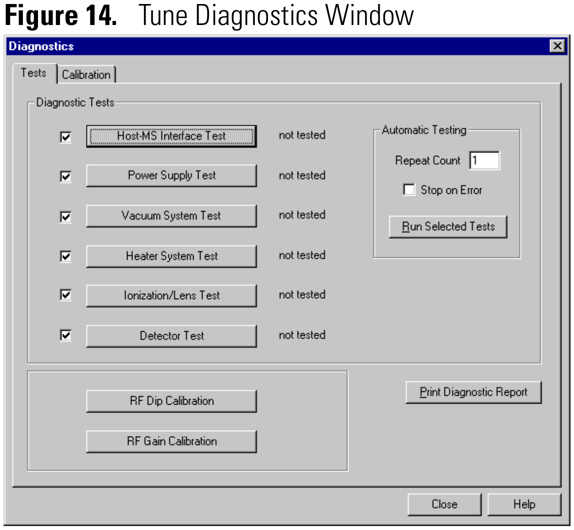
Running Diagnostics

After confirming that the heaters and vacuum readbacks are valid, run *Xcalibur* diagnostics to test other internal components for functionality.

CAUTION - INSTRUMENT DAMAGE. Pay particular attention to the vacuum readbacks because an improper vacuum will damage the filament during an Ionization/Lens test.

1. In *DSQ II Tune*, select **Diagnostics | Run Tests**.

Figure 14. Tune Diagnostics Window



2. Run each individual test in the Diagnostic Tests area so that you can closely monitor each test's readbacks and note any failures. If a diagnostic fails, view the help topic for that diagnostic. However, do not run the RF dip and RF gain calibrations tests until the next procedure.

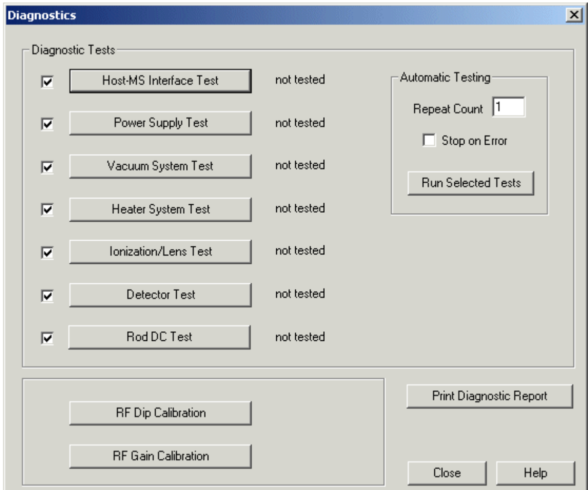
Checking the RF Dip Calibration

Once you have run all the Xcalibur diagnostic tests and they have all passed, you can check the RF dip calibration.

Note Run this test only after the heaters and vacuum have stabilized.

1. In *DSQ II Tune*, select **Diagnostics | Run Tests**.

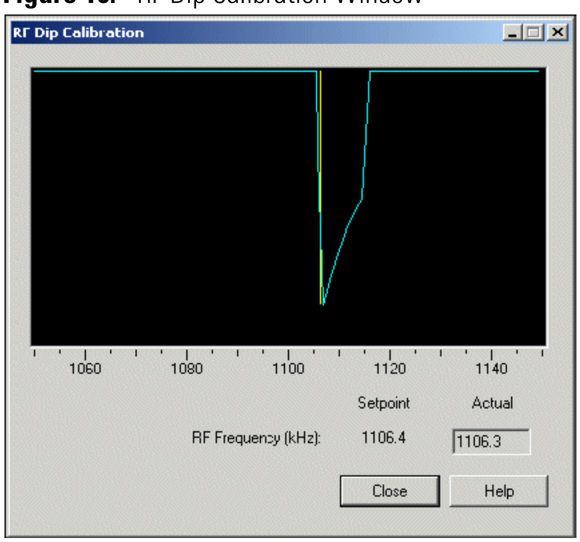
Figure 15. Tune Diagnostics Window



Note The RF frequency is set correctly if the setpoint and actual readings are within 2.0 kHz.

2. Click the **RF Dip Calibration** button to open the RF Dip Calibration window.

Figure 16. RF Dip Calibration Window



a. Allow the display to stabilize for approximately 15 seconds.

b. Verify that the setpoint and actual are within 0.2 kHz. If they are not, see "Adjusting the RF Dip Calibration" on page 80.

> **Note** If the Rod DC Test Fails after the RF Dip Calibration and RF Gain Calibration pass.

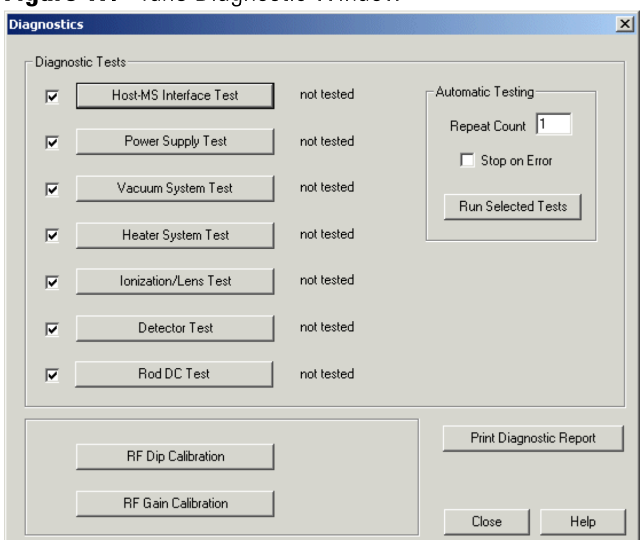
3. Click **Close** to return to the Diagnostics window.

Checking the RF Gain Calibration

After you see a successful RF dip calibration, you can check the RF gain calibration.

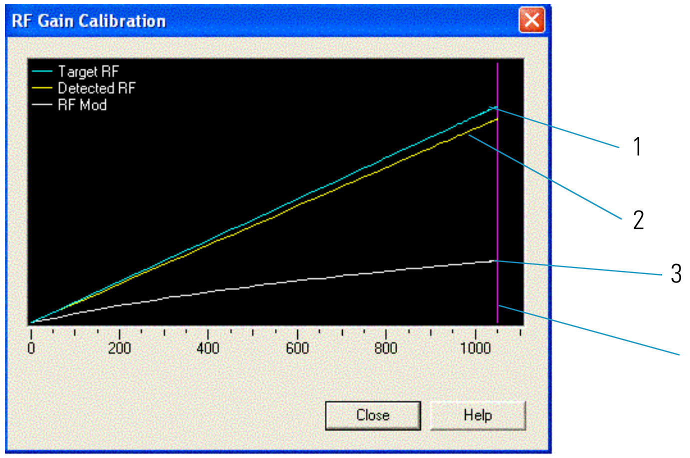
1. In *DSQ II Tune*, select **Diagnostics | Run Tests**.

Figure 17. Tune Diagnostic Window



2. Click the **RF Gain Calibration** button to open the RF Gain Calibration window and run an RF Gain Calibration test.

Figure 18. RF Gain Calibration Window



1	Target RF (blue line)	3	RF Modulation (white line)
2	Detected RF (yellow line)	4	*m/z* 1050 (red/purple vertical line)

This window plots the following values versus *m/z*:

- Target RF (see line 1) ramp is linear and corresponds to the ramp used to scan the quadrupole to produce a mass spectrum.
- Detected RF (see line 2) measures the actual RF applied to the quadrupole. It must be a linear ramp all the way to the *m/z* 1050 line (see line 4).
- RF Modulation (see line 3) measures the power output of the RF generator. It is usually slightly curved.

a. Allow the display to stabilize for approximately 15 seconds.

b. Verify that the Detected RF is linear to the *m/z* 1050.

If the detected RF is not linear to the *m/z* 1050, the mass calibration may be incorrect. At this point, check the mass calibration by viewing the calibration gas spectrum (see Step 5. Check the calibration gas spectrum., on page 29.)

If the masses are not within 2 *m/z* of the theoretical *m/z*, wait until the automatic tune calibration is finished to pass the RF gain calibration diagnostic.

If the detected RF shows noise or spikes, shut down the instrument and check for dust or fibers on the quadrupole and prefilter, or check for loose connections between the RF coil, low pass filter, and quadrupoles.

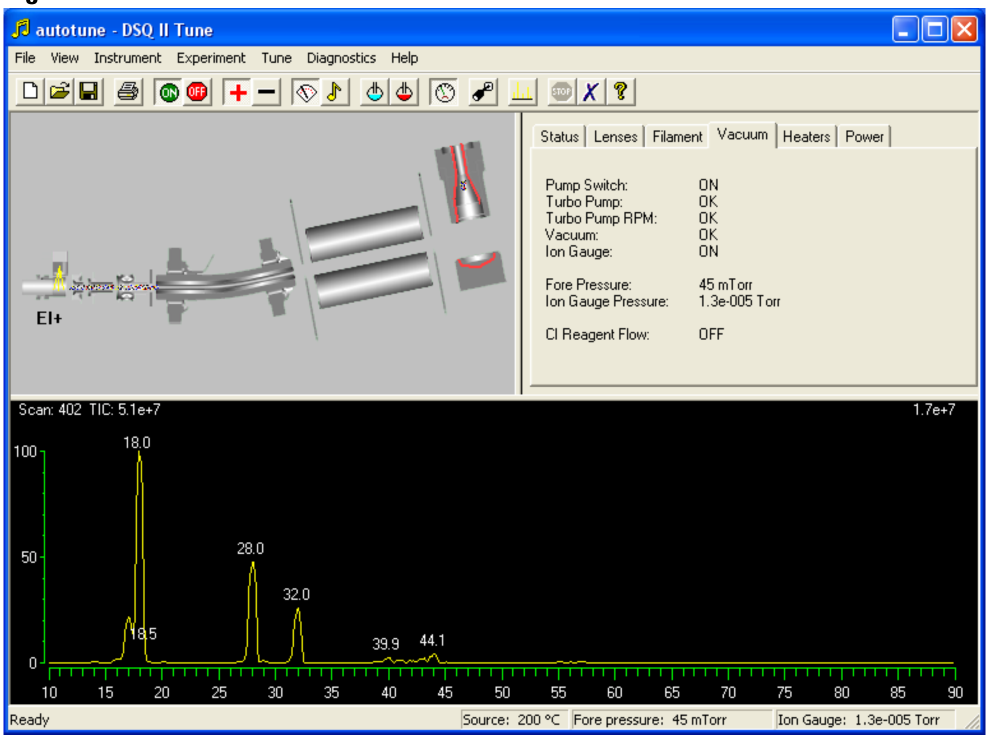
3. Click **Close** to return to the Diagnostics window.
4. Click **Close** to return to the Tune window.

Checking the Air/Water Spectrum

After successfully completing the RF Gain Calibration test, you should check the air/water spectrum for leaks.

1. In *DSQ II Tune*, click the Vacuum tab.

Figure 19. Tune Vacuum Tab



a. Verify that the fore pressure is less than 50 mTorr.

   For some instruments that have been exposed to high humidity while vented for an extended period of time, this may take several hours. It is common for an instrument shipped with the 200/200 L/s pumping option to have a foreline pressure of > 50 mTorr because the large surface of this turbomolecular pump needs time to outgas.

b. If the system has an ion gauge, verify that the ion gauge pressure is less than 7 x 10-5 Torr.

c. If the pressure is too high, there is a leak that must be fixed immediately. Refer to the *DSQ II Hardware Manual* for troubleshooting instructions.

2. Make sure the calibration gas has been off for at least five minutes because the calibration gas flow module introduces air into the instrument, which invalidates the reading. Also, multiple successive tunes will make air appear higher.

3. Check the air/water spectrum.

   a. Open the *autotune.DSQtune* file by selecting **File | Open | autotune.DSQtune**.

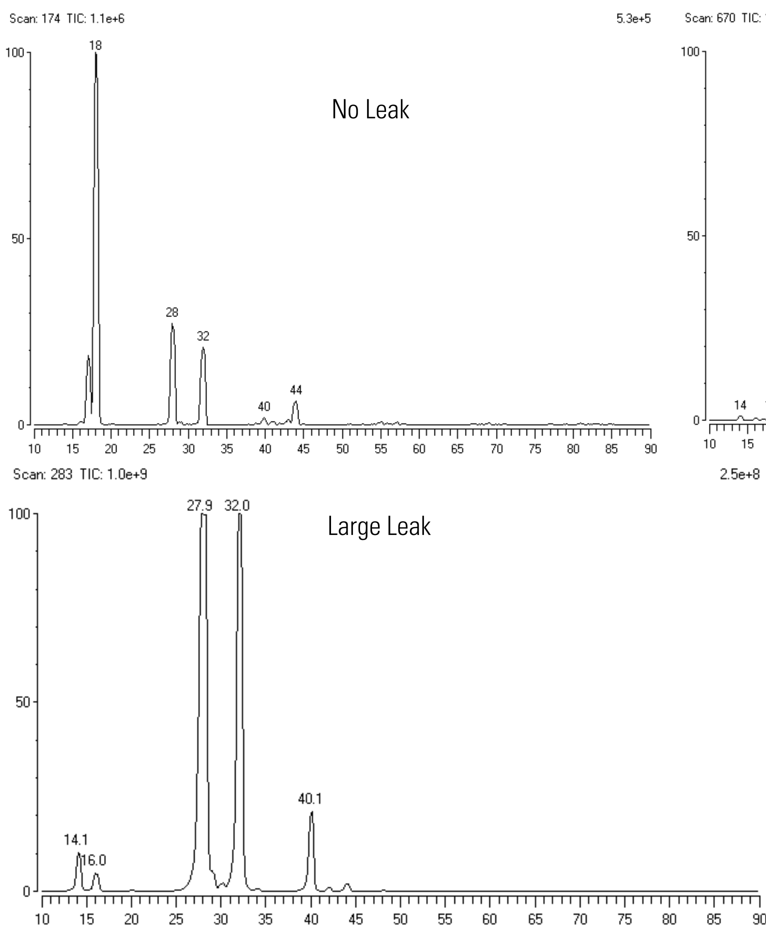
   b. Select **Experiment | Full Scan** and scan from *m/z* 10 to 90.

   c. Select **Instrument | Fil/Mult/Dyn On** to power-on the instrument.

   d. Compare the Air/Water Spectrum with those in Figure 20 to determine whether or not you have a leak. Usually, if *m/z* 28 is larger than *m/z* 18, there is a leak. See "Checking for Leaks" on page 28 for more information.

> **Note** The spectrums displayed in Figure 20 were acquired with a 250 L/s turbomolecular pump system. Relative abundance of air/water ions can vary depending on the pump option and the amount of air in the helium supply. Nitrogen is typically the most abundant contaminant in any helium supply.

Figure 20. Air/Water Spectrum Comparisons



CAUTION INSTRUMENT DAMAGE. Do not operate the system if you get a 10% air/leak reading on the report output. It could damage the filament and create a high voltage arch.

Checking for Leaks

You should check for leaks when the Air/Water spectrum indicates *m/z* 28 ion is larger than *m/z* 18. To check for leaks, you will need:

- Dusting spray containing tetrafluoroethane (Falcon® Dust-Off®, MicroCare® MicroBlast™, or equivalent)
- Leak detector (Thermo Scientific GLD Pro PN 66002-001 or equivalent)

1. Check for external leaks.

   a. Use the leak detector to check all carrier and CI reagent gas fittings for leaks. Also check the capillary column connection to the injector. Even a small leak in a gas line can allow air to enter.

   b. Use the leak detector to check the septum for a leak. Replace if necessary.

2. Check for vacuum leaks.

   a. Scan from *m/z* 50 to 100 by selecting **Experiment | Full Scan** in *DSQ II Tune*.

   b. Spray the dusting spray near the suspected leak while monitoring for an increase in *m/z* 69 and 83. Common leaks occur at the transfer line capillary column connection and the vacuum manifold cover.

Checking the Initial Tune

After a successful air/water test, you should check the initial tune of the system.

1. Open *DSQ II Tune*.

2. Make sure the DSQ II is powered on by selecting **Instrument | System On**.

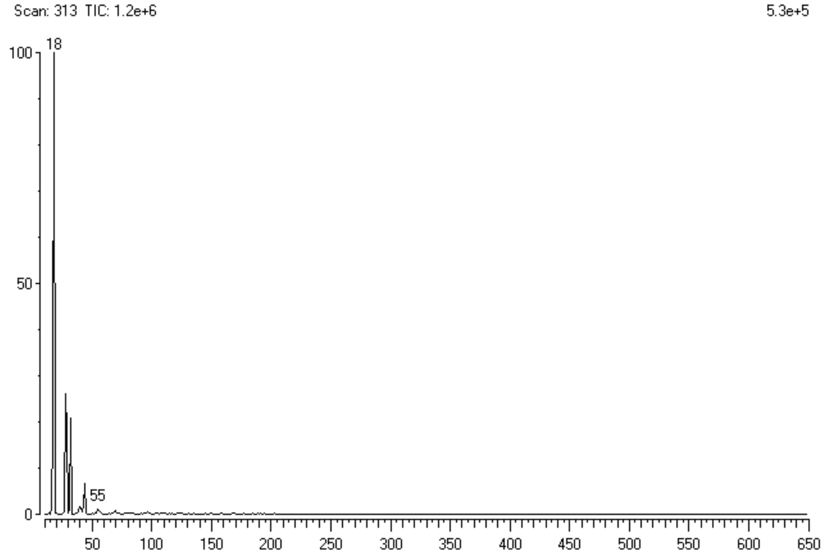
3. Make sure the filament is on by selecting **Instrument | Fil/Mult/Dyn On**.

4. Check the background spectrum.

   a. Select **Experiment | Full Scan** and scan from *m/z* 10 to 650.

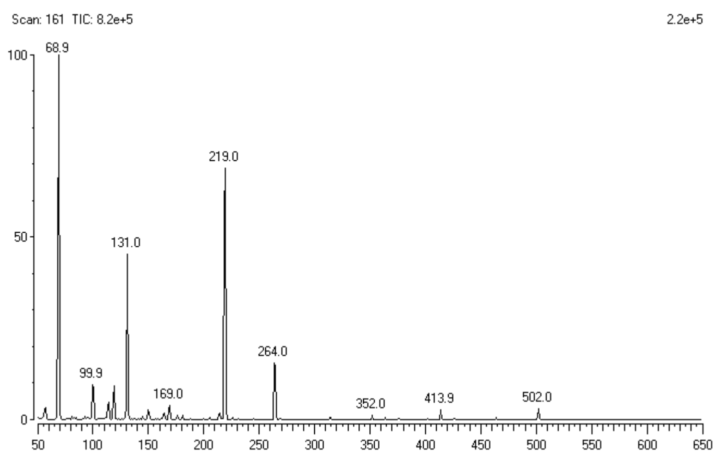
   b. Verify that the background spectrum is similar to the spectrum shown in Figure 21. The background may be higher the first day after being pumped down.

Figure 21. Background Spectrum (*m/z* 10 - 650)



5. Check the calibration gas spectrum.
   a. Select **Experiment | Full Scan** and scan from *m/z* 50 to 650.
   b. Select **Instrument | Calibration Gas | EI/NICI** to turn on the EI calibration gas.
   c. Verify that all peaks are present (*m/z* 69, 131, 219, 264, 414, and 502), as shown in Figure 22.

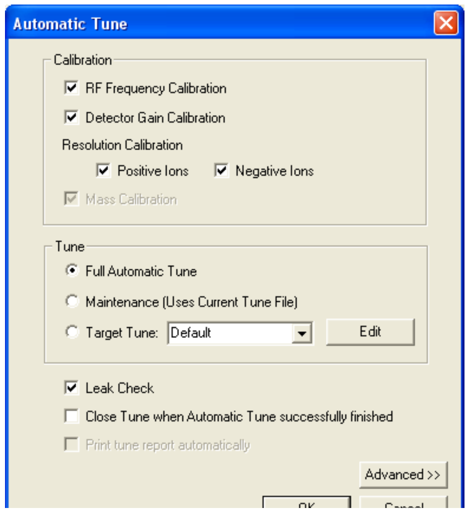
Figure 22. Calibration Gas Spectrum (*m/z* 50 - 650)



6. If the ions' masses are within ±12.5% or ±20 *m/z* units (whichever is smaller), run a full automatic tune to calibrate the instrument.
   a. Select **Tune | Automatic Tune** to open the Automatic Tune window.
   b. Select the options shown in Figure 23. However, only select **Resolution Calibration** for negative ions if the instrument will be used for negative chemical ionization.

This calibration may require that the DSQ II gain to be increased from 1 x 10^5 to 3 x 10^5 in order to pass. Only increase the DSQ II gain if the calibration fails on the first attempt. The tune report will display *m/z* -452 when this calibration has been run. It is normal for this ion to display poor resolution. The resolution for negative ions can be tuned once the instrument is switched to negative chemical ionization mode.

Figure 23. Full Automatic Tune



7. Select **Instrument | Fil/Mult/Dyn Off** to turn off the filament.

Stabilizing the System

Once the initial tune looks good, allow the system to bake-out, the vacuum to stabilize, and the gas lines to purge before performing the installation qualification tests on Day Two.

1. Replace any covers that were removed.
2. If the system has the CI option, set the CI reagent gas flow to 2.5 mL/min.
3. Perform a GC column evaluation.
4. Perform a GC leak check.
   a. Set the GC oven temperature to 100 °C greater than the temperature used to perform a column evaluation.
   b. Run the automated leak check on the GC.
   c. If the report indicates a leak, use a leak detector to fix leaks at all the GC fittings. Repeat this step until no leaks are found.

CAUTION - INSTRUMENT DAMAGE. Do not raise the oven temperature until you are sure the system is free of leaks. The column will be destroyed if it is exposed to oxygen at temperatures above 150 °C.

5. Set the GC to ramp from 40 °C to 250 °C at a rate of 5 °C/min. Allow the temperature to stay at 250 °C for 30 minutes and then return it to 40 °C.
6. Set the ion source temperature to 300 °C.
7. Allow the CI reagent gas flow to purge.
8. Allow the ion source and oven to bake out overnight.

Running EI Qualification Tests

The DSQ II ships with the instrument methods pre-loaded onto the computer so you can run your own qualification tests. You can find these files in *C:\Xcalibur\Examples\Methods* and they are organized according to the configuration of your GC. The sequence and specific methods that were used for factory specification testing are in *C:\Xcalibur\Methods*.

To run EI qualification tests, you will need:

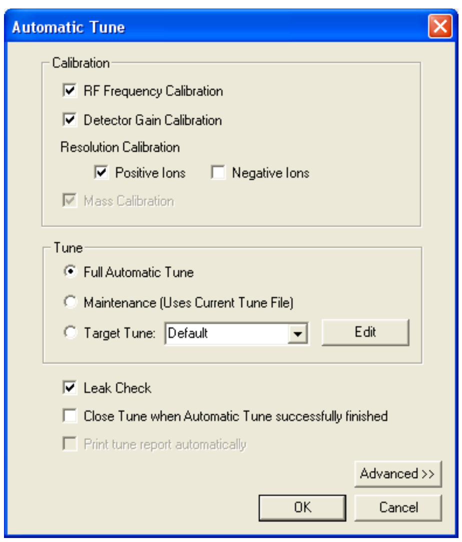
- Syringe, 10 µL, 70 mm needle
- DSQ Test Mix, PN 120150-TEST, Octafluoronaphthalene (OFN) and Benzophenone (BZ)

1. In Xcalibur, click the Instrument Setup icon and select the appropriate *EI.meth* file.
2. Install the CEI ion volume.
3. Set the ion source temperature to 200 °C.
4. Set the emission to 50 µa.
5. Set the GC oven temperature to 40 °C.
6. Set the GC column flow to 2 mL/min.
7. Turn off the CI reagent gas.
8. Wait at least 30 minutes after temperatures stabilize on the system.
9. Check the air/water spectrum.
    a. Open *DSQ II Tune* and select **Experiment | Full Scan**.
    b. Scan from *m/z* 10 to 90 by entering these numbers as the First and Last Mass.
    c. Power-on the DSQ II by selecting **Instrument | Fil/Mult/Dyn On**.
    d. Compare the air/water spectrum with the spectrum shown in Figure 20 to determine whether or not you have a leak. Usually, if *m/z* 28 is larger than *m/z* 18, there is a leak. See "Checking for Leaks" on page 28 for information.
    e. Archive the air/water spectrum.

> **Note** When archiving data, include the DSQ II serial number and sales order number.

10. Check the background spectrum.
    a. In *DSQ II Tune*, select **Experiment | Full Scan**.
    b. Scan from *m/z* 10 to 650 by entering these numbers as the First and Last Mass.
    c. Verify that the background spectrum is similar to the spectrum shown in Figure 21.
    d. Archive the background spectrum.
11. Check the calibration gas spectrum.
    a. In *DSQ II Tune*, select **Experiment | Full Scan**.
    b. Scan from *m/z* 50 to 650 by entering these numbers as the First and Last Mass.
    c. Turn on the EI calibration gas.
    d. Verify that all peaks are present (*m/z* 69, 131, 219, 264, 414, and 502), as shown in Figure 22.
12. Run a full automatic tune.
    a. In *DSQ II Tune*, select **Tune | Automatic Tune**.
    b. Check the options shown in Figure 24 and click **OK**.

Figure 24. Full Automatic Tune



    c. When finished, archive the Tune report.
    d. Power-off the DSQ II by selecting **Instrument | Fil/Mult/Dyn Off.**.
    e. Save the tune file for the EI Qualification Test as *EI.DSQtune*.
    f. Click **OK** to return to the Tune window.
13. Inject 1 µL of a 1 pg/µL solution of Octafluoronaphthalene (OFN) using the *EI.meth* file selected in Step 1 as the instrument method. Actual injection volume in a split/splitless injector will be 1µL plus needle volume.

14. Review the results.

    a. Look at the background subtracted spectrum in *Xcalibur's Qual Browser*.

    b. Archive the chromatogram and spectrum.

    c. Open the Signal-to-Noise Calculator. The minimum signal to noise ratio should be 450:1.

    d. Archive the signal to noise result.

15. Repeat the Octafluoronaphthalene (OFN) injection.

    If the DSQ II does not pass after several injections, check for leaks, especially at the transfer line union.

    Tip For troubleshooting, compare the factory test raw files to your files. Look for any discrepancies in your methods or instrument readbacks by selecting **View | Report | Status log**, **Tune Method**, and **Instrument Method** in Qual Browser.

Running CI Qualification Tests

If your DSQ II has the CI (chemical ionization) optional upgrade, you must run PCI qualification tests with methane as the reagent gas. To run CI qualification tests, you will need:

- CI ion volume
- I/R tool and guide bar
- Syringe, 10 µL, 70 mm needle
- Test mix, Octafluoronaphthalene (OFN) and Benzophenone (BZ)

1. Load the appropriate CI method.

    a. Open the *Xalibur* application.

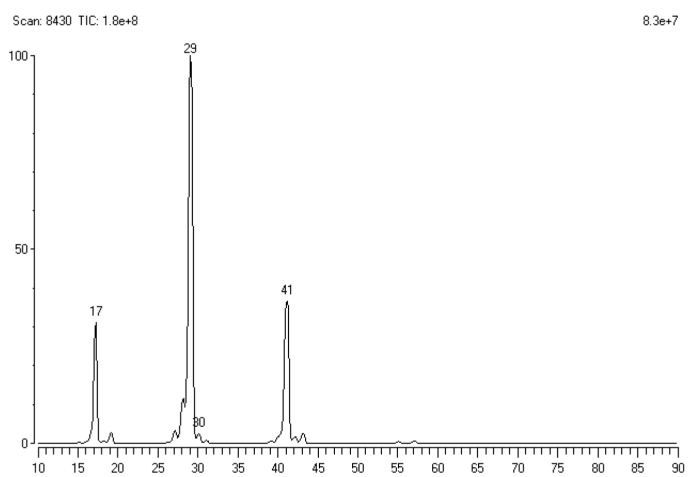
    b. Click the Instrument Setup icon on the *Xcalibur* Home Page.

    c. Select **File | Open** to open the appropriate factory instrument method.

    d. Navigate to C:*Xcalibur**Examples**Methods*. Method files are organized according to the configuration of your GC, so you can choose the *PCI.meth* file for positive ion CI. The specific methods used for factory tests are in C:*Xcalibur* \ *Methods*.

2. Prepare the DSQ II for CI mode.
   a. Use the I/R tool to install a clean CI ion volume.
   b. Open the *DSQ II Tune* application and select **Instrument | CI Reagent Gas** to open the CI Reagent Gas Flow window.
   c. Check the Reagent Gas On checkbox.
   d. Enter 2.5 mL/min in the Reagent Gas Flow field or use the slider to set the flow.
   e. Click **Apply** and **OK** to return to the Tune window. The Automatic Tune window has now changed from EI to CI mode.
   f. Wait at least 30 minutes for the ion volume to heat up and bake out.
3. Check the reagent gas spectrum.
   a. In *DSQ II Tune*, select **Experiment | Full Scan**.
   b. Scan from *m/z* 10 to 90 by entering these numbers as the First and Last Mass.
   c. Verify that the reagent gas spectrum is similar to the spectrum in Figure 25.

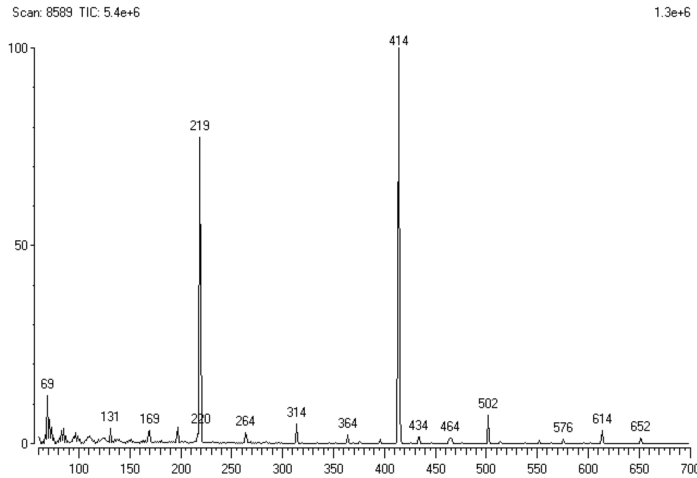
   Figure 25. Positive Ion CI Spectrum (2.5 mL/min Methane)

   d. The presence of the 41 ion with at least 20% intensity indicates proper source conditions for optimum CI results.
   e. If *m/z* 29 and 41 are not similar in ratio to Figure 25, verify that the ion volume is inserted correctly (adjust it with the I/R tool) or that the filament is properly aligned with the electron lens hole (shut down the instrument and use a needle to bend the filament wire to the center of the electron lens hole.)
   f. Archive the reagent gas spectrum.
4. Check the calibration gas spectrum.
   a. In *DSQ II Tune*, select **Experiment | Full Scan**.
   b. Scan from *m/z* 60 to 700 by entering these numbers as the First and Last Mass.
   c. Select **Instrument | Calibration | PICI** to turn on the PICI calibration gas.

d. Verify that the calibration gas spectrum is similar to the spectrum in Figure 26.

Figure 26. Positive Ion Calibration Gas CI Spectrum (2.5 mL/min Methane)



If the spectra are not similar, verify that the ion volume is inserted correctly (adjust it with the I/R tool) or that the filament is properly aligned with the electron lens hole (shut down the instrument and use a needle to bend the filament wire to the center of the electron lens hole.)

e. For optimum CI results, the reagent gas supply regulator and CI reagent gas control module must be purged with reagent gas long enough (optimal time is at least 4 hours) to ensure that any trace of air and moisture is gone.

5. Tune the system for PCI operation.

   a. Select **File | Open | Tune** and select the *autotune.dsqtune* file.

   b. Change lens 2 to approximately 2 V closer to 0 V.

   c. Change the electron energy to 120 eV.

   d. Change the emission current to 50 µA.

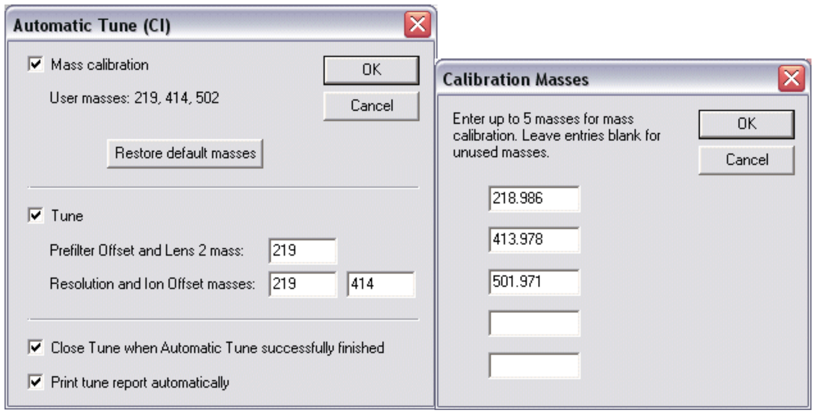
   e. Save this Tune file as *PICIautotune.DSQtune*.

6. Begin PICI tests.

   a. In *DSQ II Tune*, select **Tune | Automatic Tune**.

   b. Select the options shown in Figure 27.

   Figure 27. CI Automatic Tune - PICI Tests

   c. Click the **Calibration Masses** button to open the Calibration Masses window.

   d. Enter the masses 218.986, 413.978, and 501.97 for the mass calibration.

   e. Click **OK** to return to the Tune window.

   f. Save the PICI Autotune file as *PCI.DSQtune* for the installation qualification test.

   g. Archive the calibration gas spectrum.

   h. Close the Tune window.

7. Perform a PICI installation qualification test.

   a. Open *Xcalibur* and click the Sequence Setup icon to open the preset method *PCI.meth* file.

   b. Inject 1 µL of a 10 pg/µL test mix using the preset instrument method *PCI.meth* file. For heated injections, actual volume will be 1 plus needle volume.

   c. Open *Qual Browser* to review the results by looking at the background subtracted spectrum.

   d. Archive the chromatogram and spectrum.

   e. Run the Signal-to-Noise Calculator and open the file to run a test. The signal-to-noise ratio must be greater than 50:1.

8. Begin Negative NCI Installation Qualification tests.

   a. Open *DSQ II Tune* and select **File | Open** to open the *autotune.DSQtune* file.

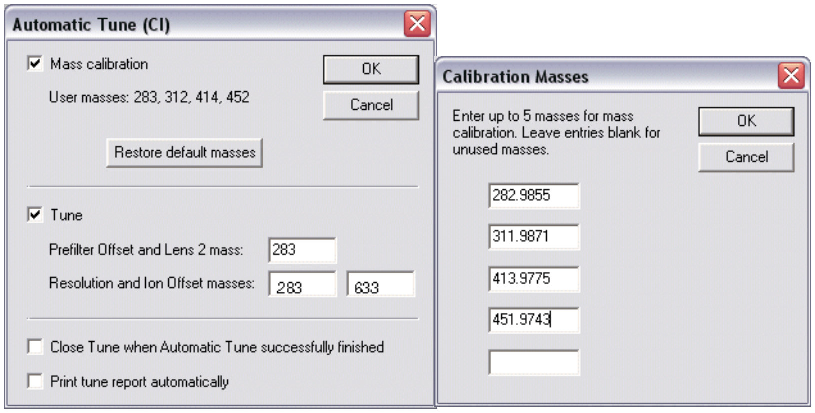
   b. Click the negative-ion  button to change to negative ion mode.

   c. Select **Instrument | CI Reagent Gas** to open the CI Reagent Gas window.

   d. Check the **CI Reagent Gas On** checkbox to turn on the CI reagent gas.

e. Select **Tune | Automatic Tune** to open the Automatic Tune (CI) window and enter the Prefilter settings shown in Figure 28.

Figure 28. Automatic Tuning - Negative CI Tests



f. Click the **Change Masses** button to enter the *m/z* values 282.9855, 311.9871, 413.9775, 451.9743 in the Calibration Masses window.

g. Save the NICI Autotune file as *NCI.DSQtune* for the Installation Qualification test.

h. Close the Tune window.

9. Perform the NCI installation qualification test.

a. In *Xcalibur*, click the Sequence Setup icon and open the preset method *NCI.meth* file.

b. Inject 1 µL of a 1 pg/µL solution of Octafluoronaphthalene (OFN) using the preset instrument method *NCI.meth* file. In a heated injector, the actual volume injected will 1 µL plus needle volume.

c. Go to *Qual Browser* to review the results by looking at the background subtracted spectrum.

d. Archive the chromatogram and spectrum.

10. Run the Signal-to-Noise Calculator and open the file to run a test. The signal-to-noise ratio must be greater than 5000:1.

11. Archive the signal to noise ratio.

12. Repeat the Octafluoronaphthalene (OFN) injection.

Installing Optional Upgrades

Once you have finished installing and testing the DSQ II system, you can install any optional upgrades. Upgrade options may include:

- Autosampler(s): With a GC, connect the AI/AS 3000 Series or TriPlus serial cable, either through the GC or directly through the PC through the appropriate port (serial or LAN), to the GC. Refer to the autosampler documentation for more information.
- Direct Sample Probe (DIP or DEP). Refer to the appropriate probe documentation for more information.

Providing Basic Training

Now that the system is running to factory specifications, show the customer how to use the Xcalibur software.

1. Demonstrate instrument configuration.
   a. Start Instrument Configuration from the desktop.
   b. Show how to add, configure, and delete components.
2. Demonstrate the Roadmap View in the *Xcalibur* Home Page.
   a. Start the *Xcalibur* Home Page from the desktop.
   b. Show how to use the Roadmap View.
   c. Show how to view the instrument status.
3. Demonstrate instrument setup.
   a. Start Instrument Setup from the *Xcalibur* Home Page.
   b. Show how to set up a GC method.
   c. Show how to set up a DSQ II method.
   d. Show how to set up an autosampler method (if applicable).
4. Demonstrate the *Tune* window.
   a. Start *DSQ II Tune* from Instrument Setup.
   b. Show how to open tune files.
   c. Show how to look at an air/water spectrum.
   d. Show how to look at a calibration gas spectrum.
   e. Show how to run an automatic tune.
   f. Show how to run diagnostics.

5. Demonstrate the Sequence View on the *Xcalibur* Home Page.
   a. Set up a new sequence.
   b. Run a sample.
6. Demonstrate *Qual Browser*.
   a. Open a *.raw* file.
   b. Add a cell to view a spectrum.
   c. Explain how to use push-pins.
   d. Explain background subtraction.
   e. Demonstrate how to change the chromatogram range and mass.
7. Remind the customer to go to "Configuring the Xcalibur Software" on page 41 to reinforce all that you have demonstrated today.

2

Configuring the Xcalibur Software

This chapter describes how to configure the *Xcalibur* software for use with a DSQ II system.

Contents

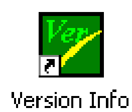
To remain current with the *Xcalibur* software, visit our website (http://www.thermo.com) for the latest releases on application notes, new manuals, software and firmware updates, and information on new features.

Using Desktop Shortcuts

After the DSQ II is connected, you should get acquainted with how your software is organized on the desktop. *Xcalibur* desktop shortcuts can help you quickly get where you want to go.

Note You might find it helpful to copy this page and keep it out to use as a quick reference template while you're getting used to *Xcalibur*.

Desktop Shortcut	What it Does...
	Launches the *DSQ II Tune* software. When running *Xcalibur*, you can also use the Q shortcut located in your Windows task bar.
	Launches the *Signal to Noise Test* software. Use this program to calculate signal to noise specific ranges within *.raw* files.

Desktop Shortcut	What it Does...
	Launches the PDF file containing the signal-to-noise instructions. Use this document for help in using the signal-to-noise test.
	Launches existing tune reports that are stored in the C:*Xcalibur\system\DSQ\Reports* folder.
	Select this shortcut to view installed applications and configured instruments.
	Launches the *Xcalibur* Home Page.
	Launches the *XReport* software. Use this program to customize your reports. These files become templates for your reports. Templates are saved as *.xrt* files and (by default) stored in the C:*Xcalibur\templates* folder.

Configuring Instruments for Use

To configure an instrument for use in *Xcalibur*:

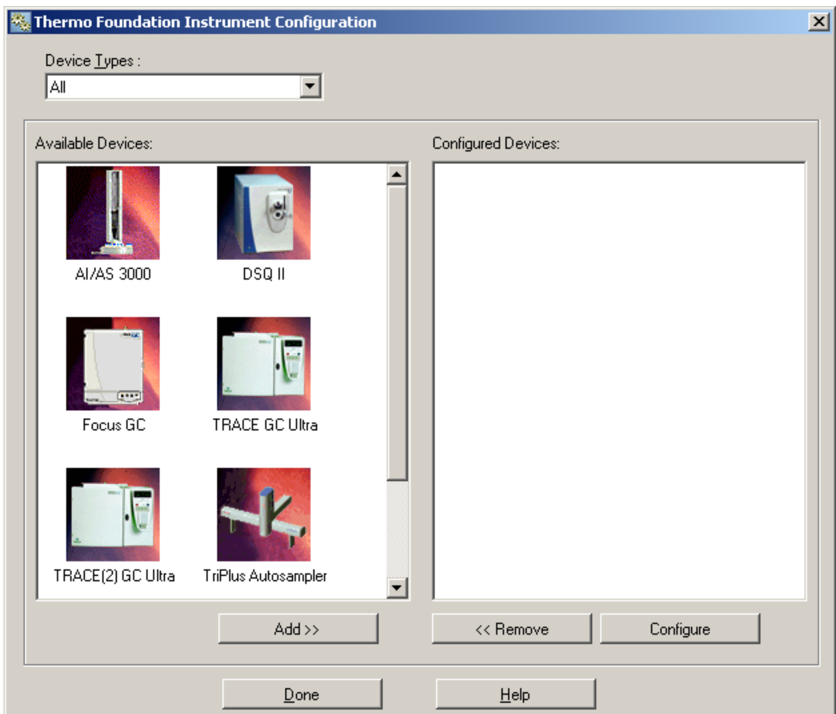
1. Select **Start | All Programs | Thermo Foundation 1.0 | Instrument Configuration** to open the Instrument Configuration utility. *Foundation* will display a message that it is unloading the instrument drivers.

   Note Click the **Help** button to access the online help for more detailed instructions.

2. Configure the DSQ II.

   a. Double-click the DSQ II icon in the Available Devices pane and move it to the Configured Devices pane.

   Figure 29. DSQ II Instrument Configuration

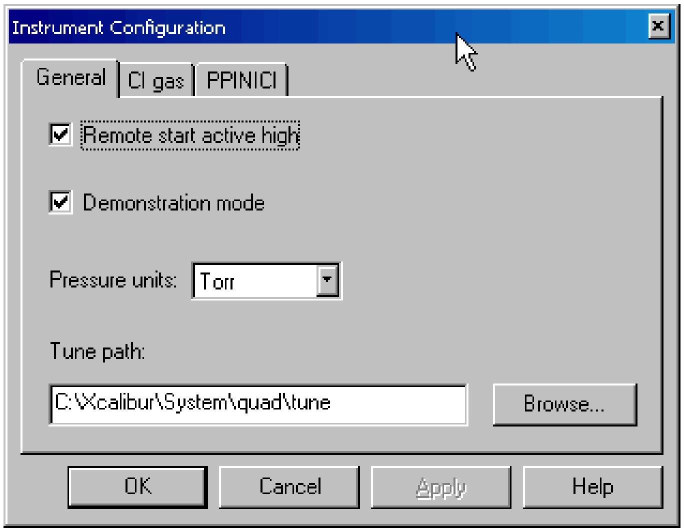
   

   b. Double-click the DSQ II icon in the Configured Devices pane or click the **Configure** button to open the Instrument Configuration window.

   c. Use the tabs in the Instrument Configuration window to select options to display on the Instrument Setup and Tune windows.

3. Configure the General tab.

Figure 30. Instrument Configuration: General Tab

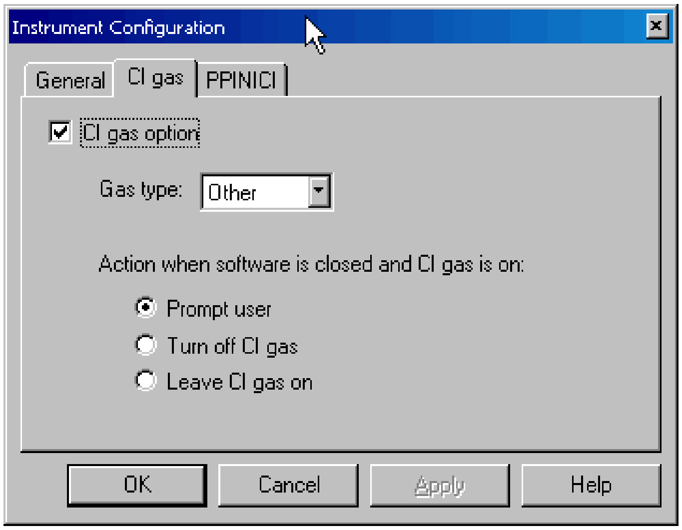


a. Click the General tab.

- The default setting for Remote Start Active High is unchecked. This setting starts the GC with an active high signal instead of an active low signal.
- Demonstration Mode is used to start the instrument in demonstration mode. This mode is useful if no instrument is connected, but you would like to demonstrate the software. Do not select this option when running samples.
- Specify the Pressure Units to display in the Tune window and Status tab.
- Specify the Tune Path for *Xcalibur* to automatically retrieve stored tune files. Use the **Browse** button to quickly navigate to the folder containing your tune files. The factory default is *C:\Xcalibur\System\DSQ\Tune*.

4. Configure the CI Gas tab if you have the CI option installed. Otherwise, continue to the next step.

Figure 31. Instrument Configuration: CI Gas Tab

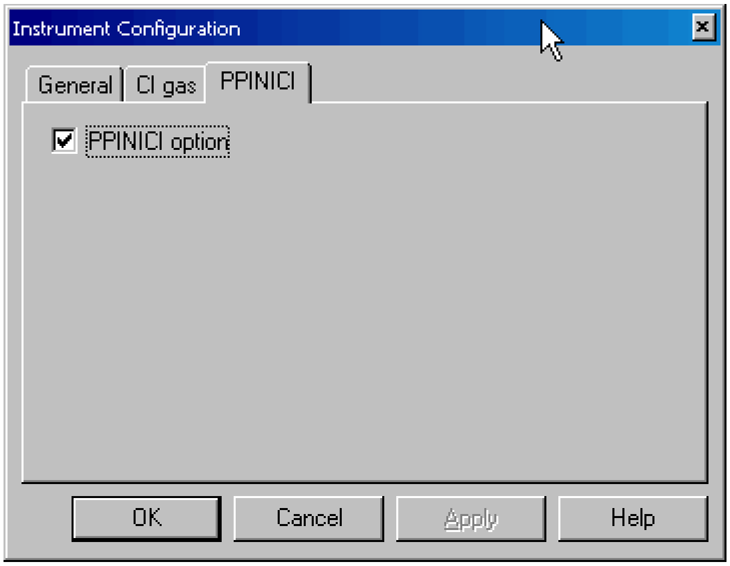


a. Click the CI gas tab.

- Check the **CI Gas** checkbox to activate CI gas options.
- Select a Gas Type from the pull-down menu to activate chemical ionization gas controls. Options include: Ammonia, CO2, Isobutane, Methane, and Other. When Other is selected, the flow module is set to a pressure of 0.3–7.4 psig against a fixed flow restrictor. If a specific gas is selected, the CI flow module outputs a calibrated flow for that gas in mL/min.
- Choose an action to occur when the software is closed and CI gas is on. When *Xcalibur* is closed, these options determine what happens if CI gas is on. You can choose to turn it off, leave it on, or receive a prompt at the time the software is closed asking if you want to turn the CI gas off. If you choose to leave the CI gas on, it remains on until you restart the software. However, as soon as you restart the software, the CI gas is turned off.

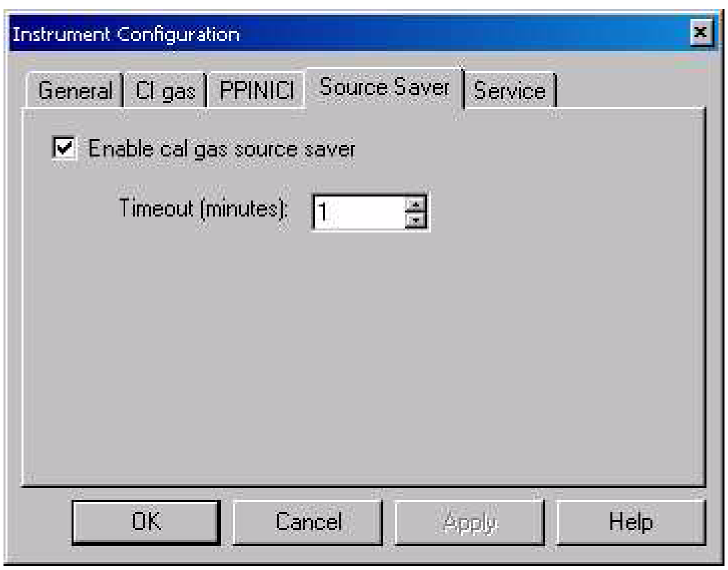
5. Click the PPINICI tab and check the PPINICI checkbox if you have the PPINICI option installed on your DSQ II.

Figure 32. Instrument Configuration: PPINICI Tab



6. Configure the Source Saver tab.

Figure 33. Instrument Configuration: Source Saver Tab

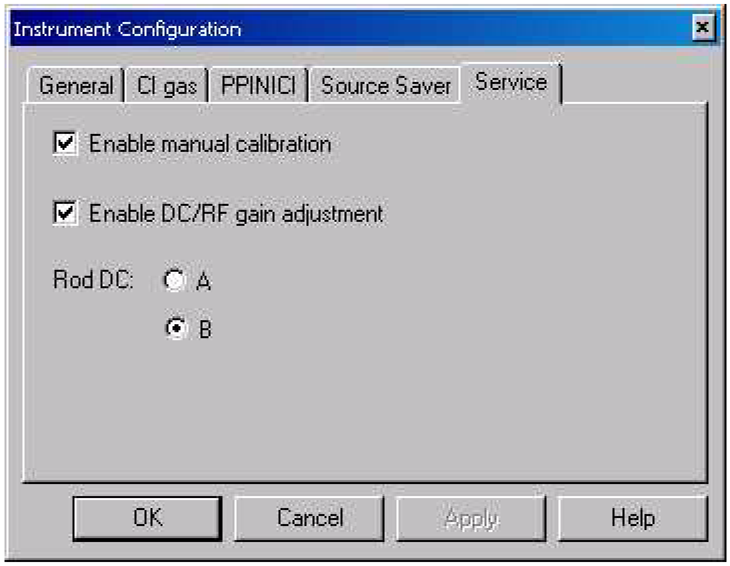


a. Click the Source Saver tab.

- Check the Enable Cal Gas Source Saver checkbox to enable the instrument to turn off the filament and calibration gas if left unattended with the calibration gas on. If the calibration gas is not on, source saver will not turn off the filament.
- Enter a time in the Timeout field that the instrument must wait after the last user action in Tune before turning off the filament and calibration gas.

7. [Field Service Engineers Only] Configure the Service tab.

Figure 34. Instrument Configuration: Service Tab



a. Click the Service tab.

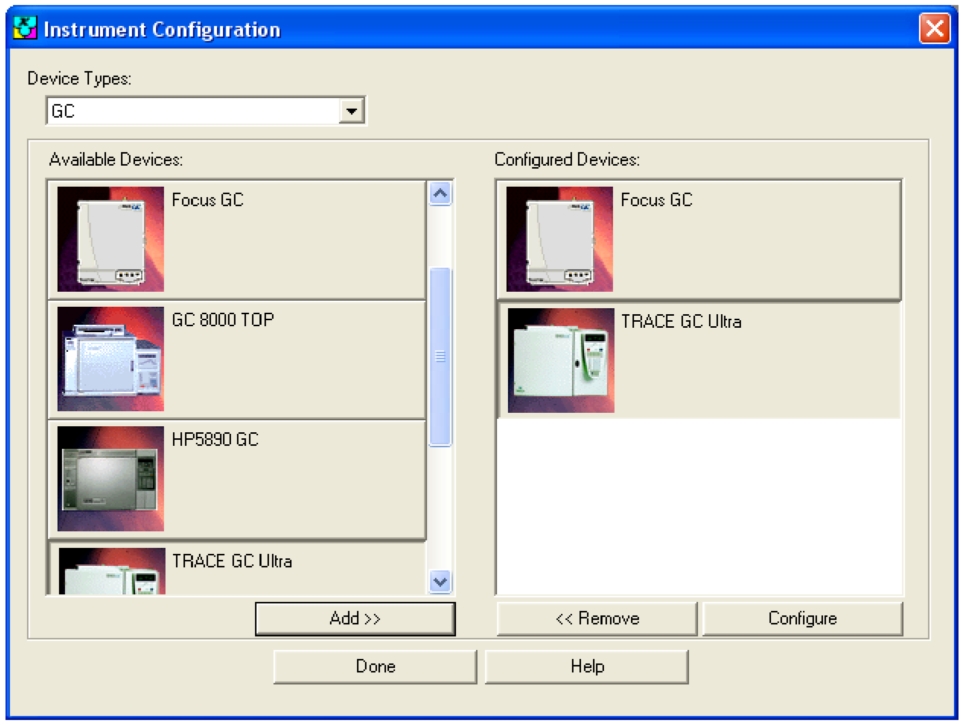
CAUTION - INSTRUMENT DAMAGE. Do not adjust these settings. Only factory-trained Field Service Engineers are qualified to set the options in the Instrument Configuration Service tab. Altering the default values may result in poor instrument performance.

- Check the **Enable Manual Calibration** checkbox to display the Manual Calibration menu item in *DSQ II Tune*. This allows the Field Service Engineer to manually calibrate the coarse mass calibration and resolution for troubleshooting. We do not recommend using manual calibration values for normal operation because the calibration will not be correct. This selection should be left unchecked for normal customer operations.
- Check the **Enable DC/RF Gain Adjustment** checkbox to display the DC/RF Gain menu item in *DSQ II Tune*. This selection should be left unchecked for normal customer operations.
- Select A or B in the Rod DC field. This should be set in the factory and never changed unless the DC Driver PCB, RF subsystem, or quadrupole mass filter is changed. If changed, calibrations for both positive and negative ions must be performed. The terms A and B refer to the selection of which DC polarity is applied to each quadrupole rod pair for each ion polarity.

8. Configure the GC.

a. Move the appropriate GC icon from the Available Devices pane to the Configured Devices pane.

Figure 35. GC Instrument Configuration



b. Select the appropriate GC icon in the Configured Devices pane and click the **Configure** button to open the GC Configuration window.

c. Make these selections on the General tab:

- Serial Port = COM
- Set the preferred pressure units.
- Click the **Get** button to retrieve the GC configuration through the serial port to *Xcalibur*.

d. Verify the settings on the Inlet tab match the GC configuration.

e. Verify the settings on the Detectors and Data tab match the GC configuration.

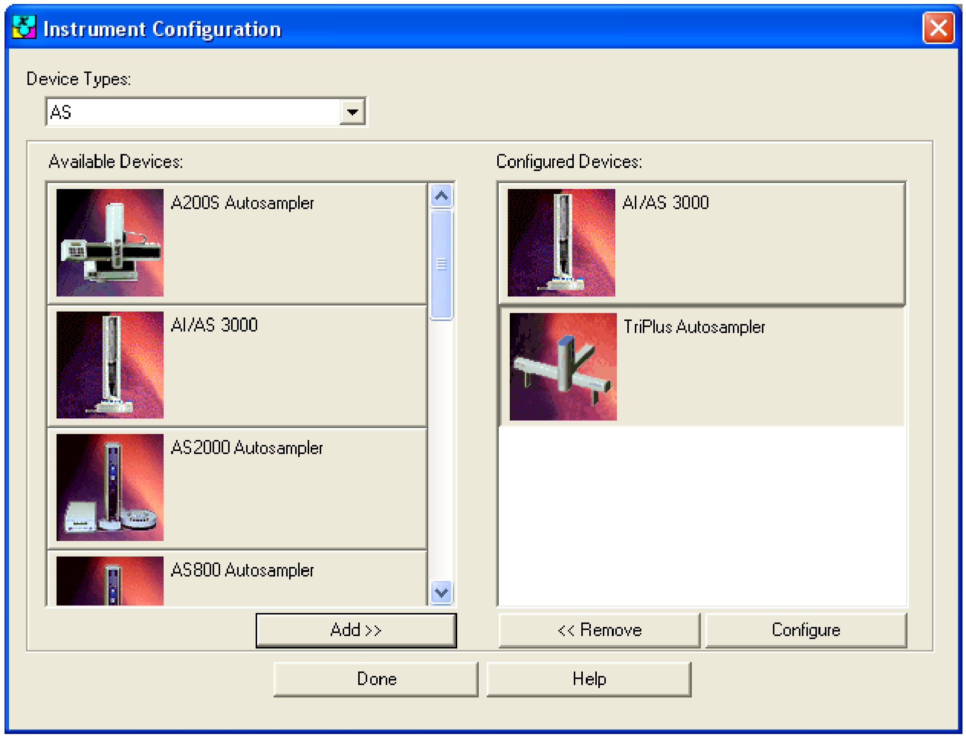
f. Verify the settings on the Auxiliary and Oven Options tab match the GC configuration and Aux 1 Present has the MS Transfer Line selected.

g. Click **OK** if no problems are detected and return to the Instrument Configuration window.

9. Configure the autosampler.

a. Move the automsampler icon from the Available Devices pane to the Configured Devices pane.

Figure 36. Autosampler Instrument Configuration



b. Double-click the autosampler icon in the Configured Devices pane and click the **Configure** button to open the AS Configuration window.

c. Enter the autosampler parameters in the AS Configuration window. The autosampler is usually connected to a COM port on the computer (with a FOCUS GC) or through the GC (with a TRACE GC Ultra and an AI/AS 3000 Series or TriPlus.) A 10 µL syringe is standard.

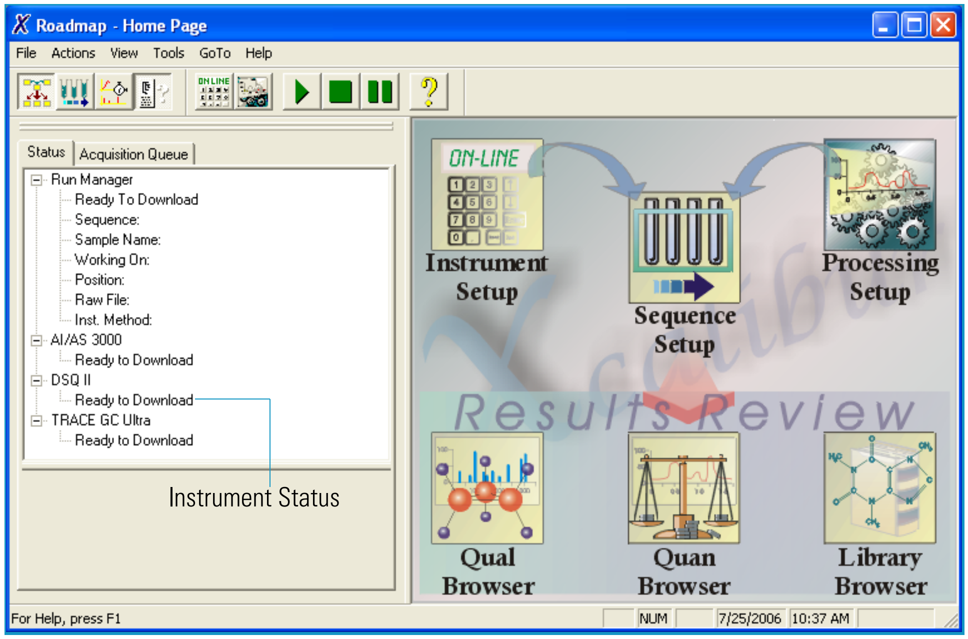
d. Set up the GC handshaking parameters by referring to the GC documentation for configuration instructions.

Table 2. GC Handshaking Parameters

Remote Start In	High to Low
Inhibit Ready In	When High
End of Run Out	High to Low
Start of Run Out	High to Low
GC Ready Out	When Low
Prep Run Out	When Low

e. Click the Xcalibur icon on the computer desktop.

Figure 37. Xcalibur Home Page



f. Verify that the DSQ II, GC and autosampler are communicating with *Xcalibur*.

g. Check the Instrument Status in the Status tab of Info View. All instruments should report *Ready to Download*. If not, consult the troubleshooting section of the instrument's documentation.

Note The DSQ II may take up to one minute to initialize.

Running Your Samples

This chapter describes how to run your test compound.

Contents

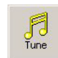
After running your method, you will learn how to analyze your data from four perspectives:

- Compounds with known retention times
- Compounds with a know ion pattern
- Peak height and area
- Signal to noise ratios

Note These instructions are written for a TRACE GC Ultra and AI/AS 3000 II autosampler. A system with a FOCUS GC or TriPlus autosampler may require different operating commands. However, making the necessary modifications and/or omissions will still help you accomplish each step.

Calibrating and Tuning the DSQ II

To tune the DSQ II:

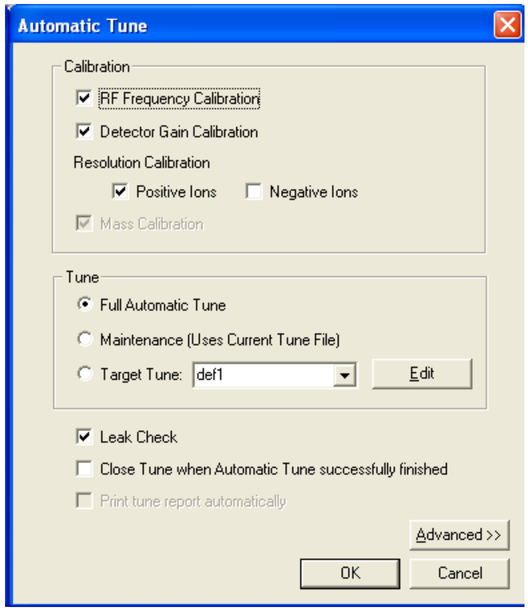
1. Open the *DSQ II Tune* software.
   - Click the **Tune** button 

     from within *Xcalibur* or double-click the DSQ II Tune icon 

     on the computer desktop.
2. Verify the basic operation of the DSQ II.
   a. Select **Diagnostics | Run Test**.
   b. In the Diagnostics window, select each test and click the **Run Selected Test** button.
   c. Click the **Print Diagnostics Report** button to print the results of the tests, if desired.
   d. Close the Diagnostics window.
3. Select **Tune | View Tune Report** to view the last Tune report and determine when the DSQ II was last calibrated. Click the **Print** button if you want a printed copy. All Tune reports are stored in C:*Xcalibur**System**DSQ**reports*. A drop-down menu on the top of the Tune Report View window allows you to display stored Tune reports for review.
4. Close the Tune report.
5. [Optional] Perform a full automatic tune if you have just performed maintenance or if your standard operating procedure requires it. It is not necessary to calibrate and tune the instrument more than once a week. However, the number and type of samples you run determine how often you must tune your instrument.

a. Select **Tune | Automatic Tune** to open the Automatic Tune window.

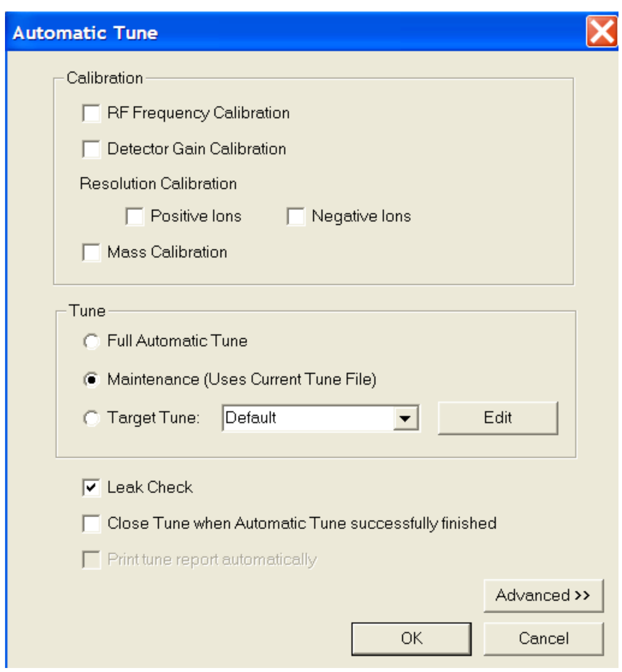
Figure 38. Full Automatic Tune Window



6. Perform a maintenance tune to evaluate the current status of your DSQ II.

   To determine whether a full automatic tune is needed, run maintenance tune on a regular basis. Maintenance tune uses the calibration and lens parameters from the currently loaded tune file. It checks mass calibration and resolution first and, if these are okay, it generates a new Tune report based on the currently loaded tune file. It is good practice to run the leak check with a maintenance tune to monitor for air leaks.

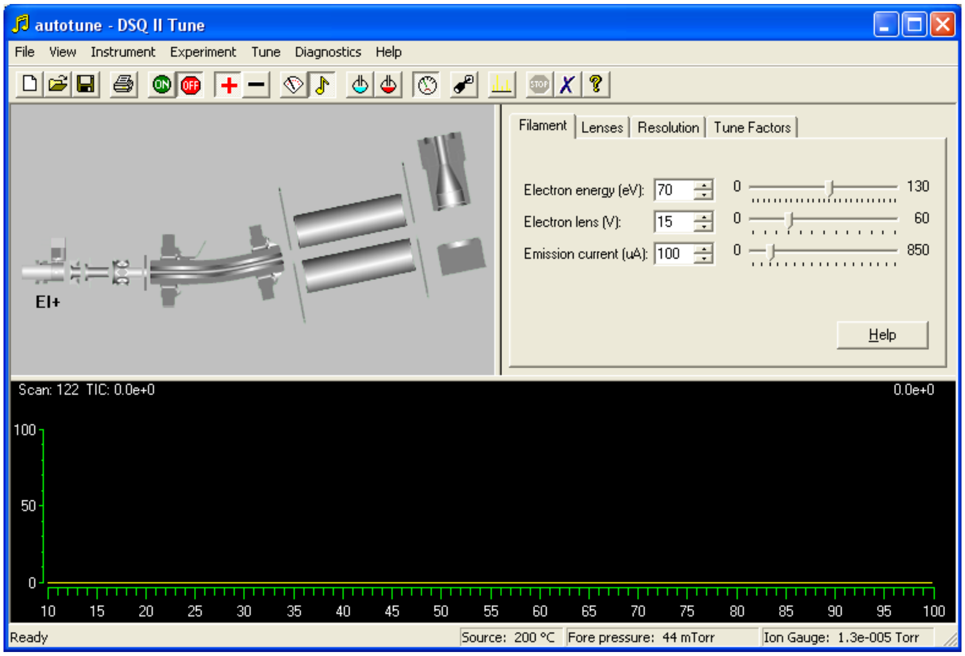
Figure 39. Performing a Maintenance Tune



7. [Optional] Perform a manual tune if needed for other applications. The tuning parameters generated during an automatic tune work well for most applications, but you may find the manual tune options suitable for other applications.

   a. Select **Tune | Show Manual Tune View** to manually set the tune parameters in the tabs shown in Figure 40.

   Figure 40. Manual Tune Tabs



   b. Select **File | Exit** to close the Tune window.

Setting Up Methods

After your DSQ II is calibrated and tuned, you can up the instrument methods using *Xcalibur's* Instrument Setup. Instrument methods are created and modified in the Instrument Setup window and saved as *.meth* files, which are stored in the *C:\Xcalibur\Methods* folder. In this example, you will enter the method parameters for the DSQ II, TRACE GC Ultra and autosampler.

1. Load an instrument method.

   a. Open *Xcalibur*.

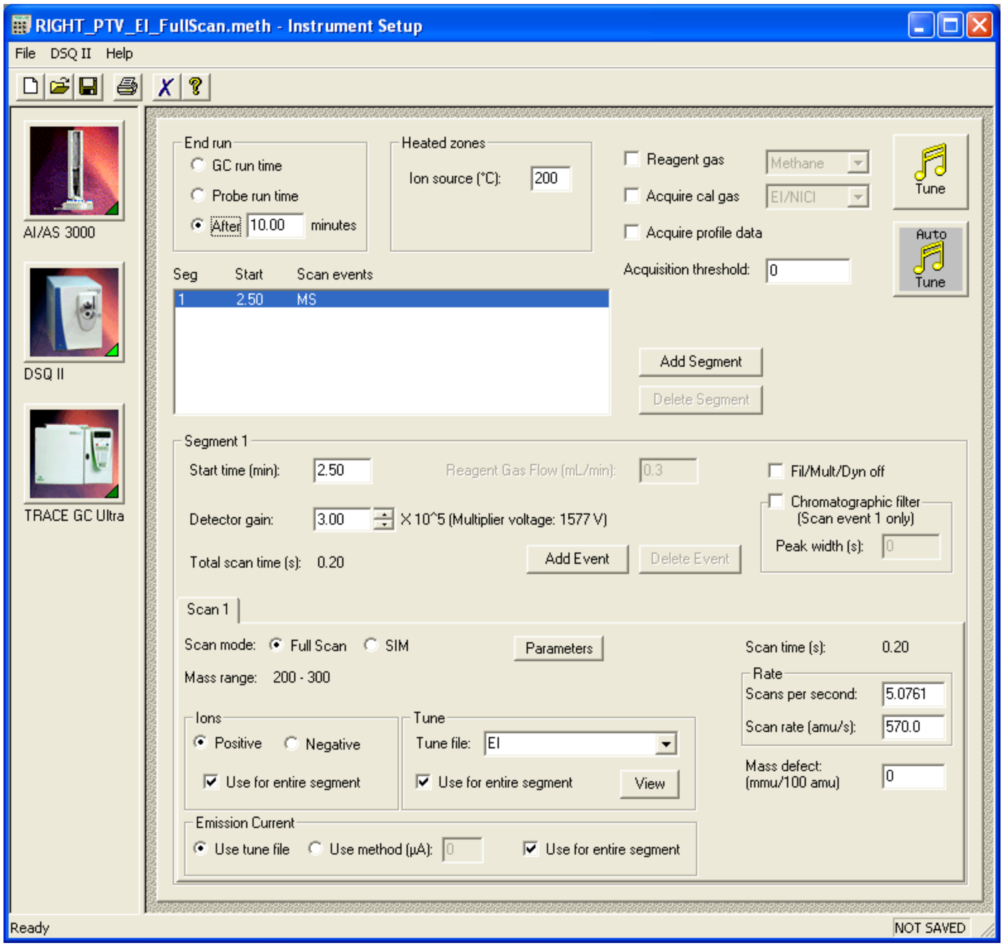
   b. Click the Instrument Setup icon on the *Xcalibur* Home Page.

   c. Select **File | Open** and navigate to C:*Xcalibur\Methods*.

   d. Select the *EI_FullScan.meth* file. This full scan method file was used to validate that your instrument met factory specifications. This file was saved for you to acquire a test sample. You can also navigate to *C:\Xcalibur\Examples\Methods* and select the folder matching your GC instrument configuration.

2. Review the DSQ II method parameters by clicking the DSQ II icon in the Instrument Setup window.

Figure 41. Right_PTV_EI_FullScan.meth Parameters

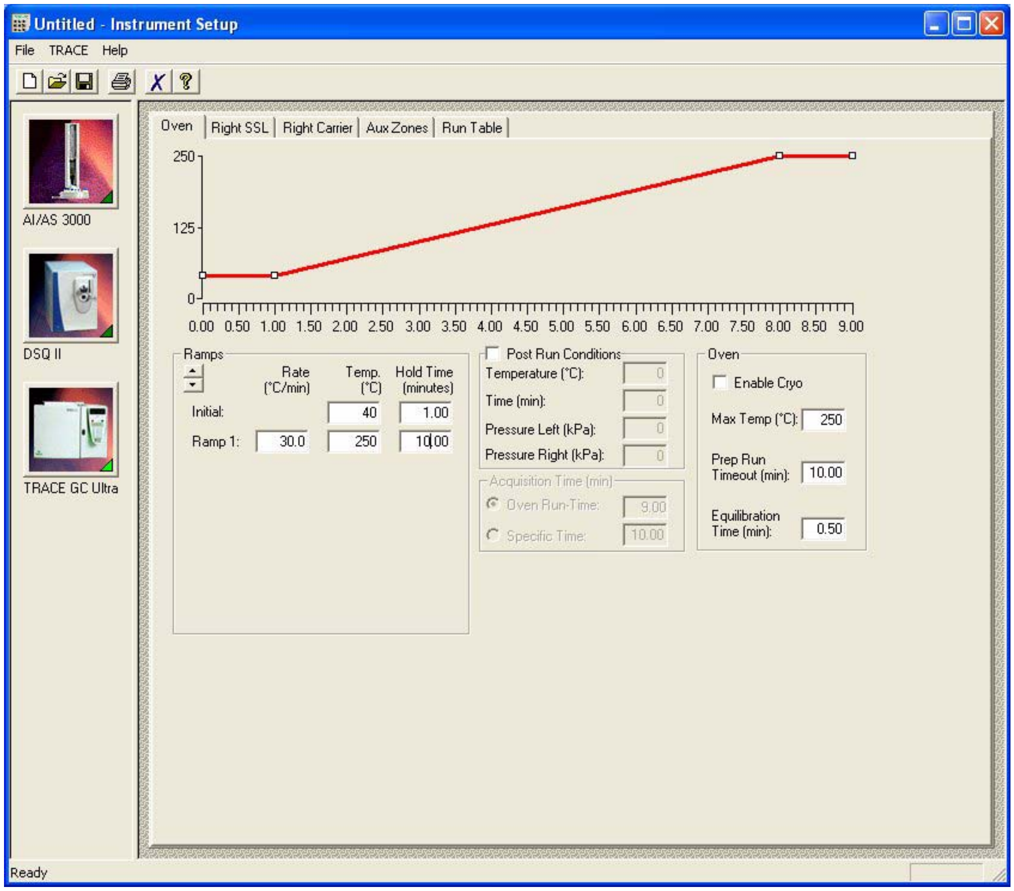


Note To open the method above, go to *C:\Xcalibur\Examples\Methods\TRACE Right PTV Methods\RIGHT_PTV_EI_Fullscan.meth*.

This method acquires *m/z* 200–300. It starts 2.5 min after the GC injection to allow the solvent to elute from the GC column. It uses the Tune file named EI and sets the source temperature at 200 °C. The Detector Gain is set to 3.00 x10^5. Set the scan rate to 570.0 amu/s.

3. Review the TRACE GC Ultra method parameters by clicking the TRACE GC Ultra icon in the Instrument Setup window.

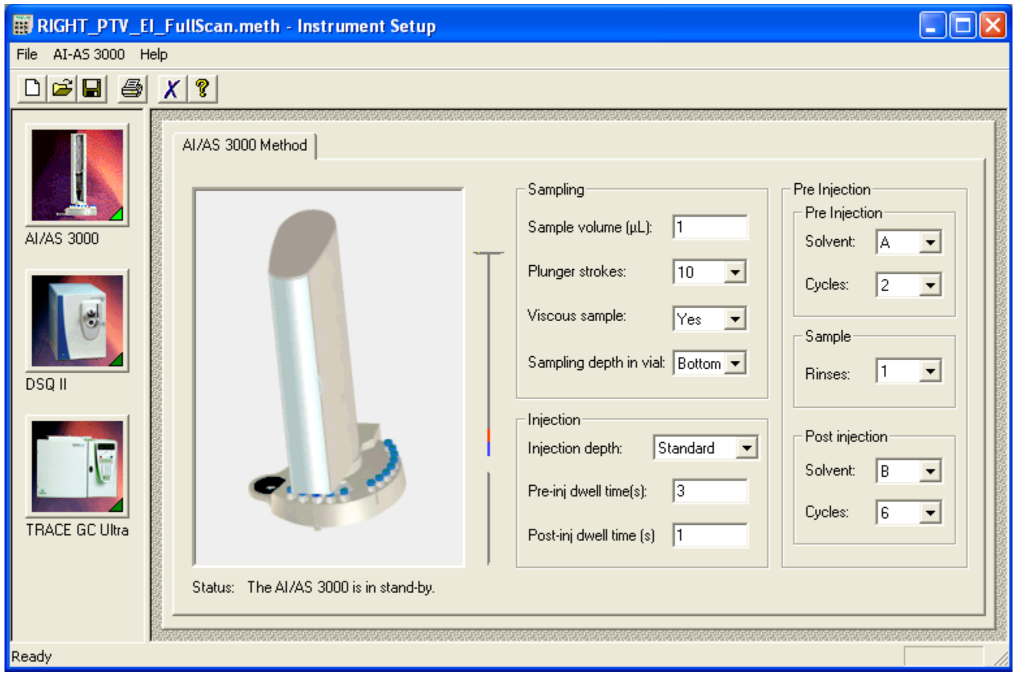
Figure 42. TRACE GC Ultra Method Parameters



This method holds the GC at 40 °C for 1 minute, ramps it at 30 °C/min to 250 °C, and holds it there for 10 minutes. On the Right SSL tab, the injector is 220 °C in splitless mode. The column flow is 1.0 mL/min and the transfer line temperature is 250 °C.

4. [Optional] Review the autosampler method parameters by selecting the autosampler icon in the Instrument Setup window.

Figure 43. AI/AS 3000 Method Parameters



a. If you are using an AI/AS 3000 Series, you can enter the parameters shown in Figure 43. For other autosamplers, there are several basic settings common for all autosamplers for sampling/injection and washes. All other parameters can be left at their default values.

- Sample volume - 1 µL is the sample volume that will be injected.
- Plunger strokes - 10. Also called pull-ups or bubble elimination strokes. This is the number of times the plunger is pulled up and down while in the sample vial. The plunger volume should be set larger than the sample volume.
- Viscous sample - Select **Yes** for slower pull-up speeds.
- Sampling depth in vial - Select **bottom** or **center**. If you select Bottom, the needle inserts to the bottom of the vial before the sample is pulled up into the syringe.

All other parameters are discussed in the *AI/AS 3000 Operating Manual*. If you have a TriPlus autosampler, the instrument parameters are the same and are entered into the appropriate tabs.

b. Fill the autosampler solvent vials A and B with a suitable rinse solvent, such as the solvent used for the samples.

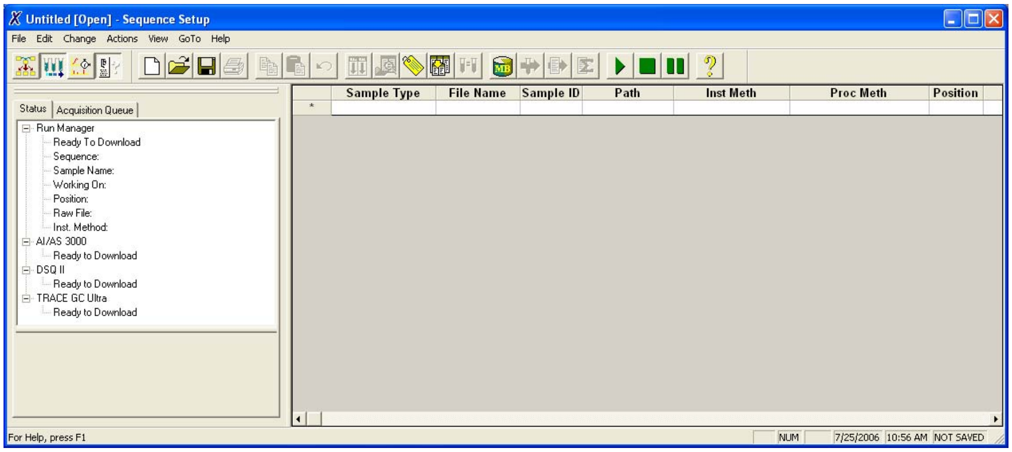
5. Save the instrument method for use in the next step. Method files have the *.meth* extension and are by default saved to the *C:\Xcalibur\Methods* folder. But you can save method files to any folder you prefer.

Running Methods in Sequence Setup

After setting up your methods in Instrument Setup, you can run them in Sequence Setup.

1. Open Xcalibur and click the **Sequence Setup** icon to open the Sequence Setup window.

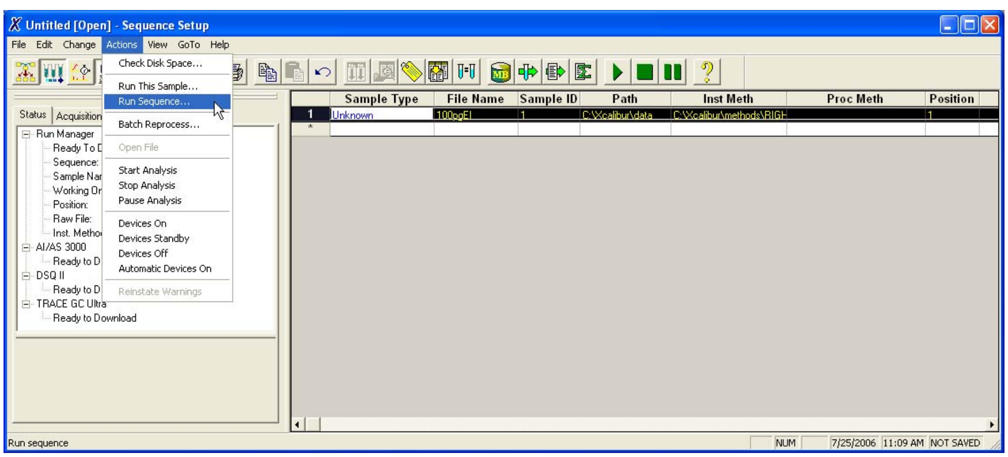
Figure 44. Sequence Setup Window



2. Create a sequence to run in the Sequence Setup window that will record sample details and determine how you want to acquire the data. Sequence Setup works just like a spreadsheet, with each row representing a single sample and each column an item of information required for a sample.

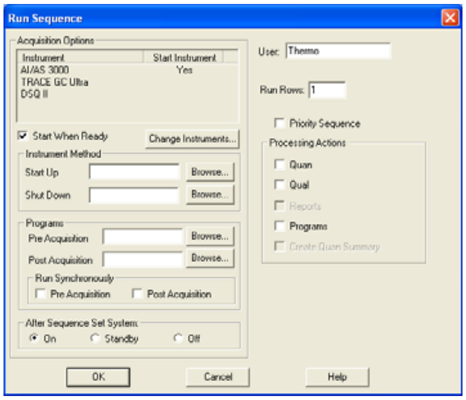
3. Run the sequence by clicking on the sequence number to highlight the row or by clicking * if you did not add any rows.

Figure 45. Running a Sequence



4. Select **Action | Run Sequence** to open the Run Sequence window.

Figure 46. Run Sequence Window



a. Select **Start When Ready.**

b. Click **OK** to return to the Sequence Setup window.

5. Run the sequence by clicking on the row number you want to run.

6. Select **File | Save** to save the sequence and enter a filename, such as *OFN.sld*. *SLD* is the default extension for sequence files.

Note If you run the same row more than once, *Xcalibur* will generate a new filename with date and time appended to the existing filename. This prevents duplication of files.

Changing the Column Arrangement

In the Sequence Setup window of *Xcalibur*, you can select **Change |Column Arrangement** to change the column labels. Some of the column descriptions are shown in Table 3. You can select more columns by selecting **Change | Column Arrangement**. Sample type selections are dependent on the bracket type selected in the sequence wizard.

Table 3. Sequence Setup Columns

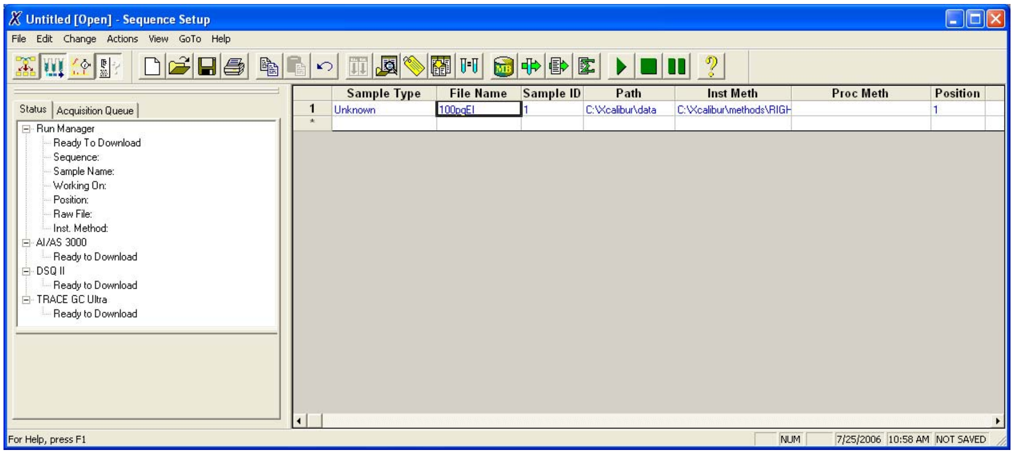
Item	Description
File Name	Name of the file used to save the sample data. *Xcalibur* creates this file with the extension *.raw*.
Inj Vol	Only the TriPlus can use the sequence column for injection volume.
Inst Meth	The path and filename of the instrument method used for acquisition.
Level	Used with standard and QC samples to enter the sample's concentration level.
Path	The path to the raw file that *Xcalibur* creates for the sample data. Double-click on this field to select a directory.
Position	The sample's vial number.
Proc Meth	The path and filename of the processing method used to process the data after acquisition.
Sample ID	An identifier unique to the sample. This field can also be used to import a barcode identifier.
Sample Type	The types of samples are as follows: • Unknown (the normal choice for qualitative analysis; all other types are only normally used for quantitative analysis) • Blank • QC (quality control) • Standard Clear • Standard Update • Start Bracket • End Bracket • Standard Bracket

Adding a Sequence

To add a sequence:

1. Enter information in the first blank row.

Figure 47. Adding a Sequence



Note Press F2 on your keyboard to edit text already in a cell. Press F2 twice to open an Edit dialog box.

2. Click in the File Name field and enter sample information, such as *Data01*.
3. Select a *.meth* file.
   a. Click in the Inst Meth field.
   b. Right-click in the field to view the drop-down menu.
   c. Click **Browse...** to select an existing method file to use for existing sample information.

Inserting Another Row

To insert another row within a list of samples:

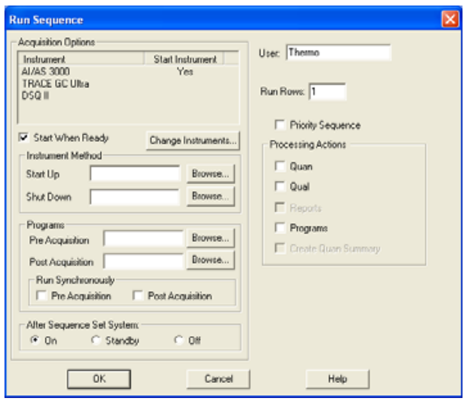
1. Right-click in the row below where you want to insert a new sample.
2. Select **Insert Row** from the menu.
3. In the Insert Row window, select **Yes** to insert a row at the end of this sequence.
4. You can also enter a number in the position cell of an empty row to duplicate the sample information and increment the filename.

Running Automatic Injections

When you instruct *Xcalibur* to make an injection, the autosampler performs an automatic injection. Basically, you set the autosampler that is listed in the In Use field to say *Yes* in the Start Instrument field.

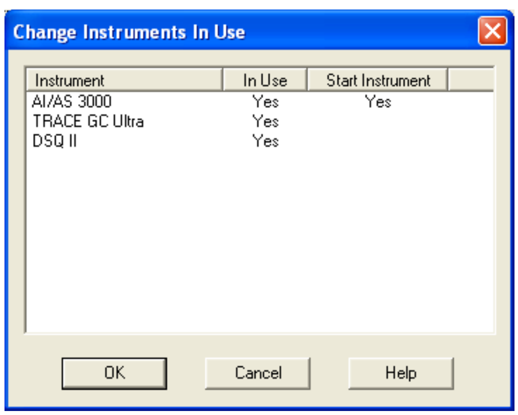
1. Select an *.sld* file to open in the Sequence Setup window.
2. Select **Actions | Run Sequence** to open the Run Sequence window.

Figure 48. Run Sequence Window



3. Click the **Change Instruments** button to open the Change Instruments In Use window.

Figure 49. Change Instruments In Use Window (Automatic Injections)



   a. Configure the Change Instruments In Use window for automatic injections by toggling the In Use field to display *Yes* for each instrument, as shown in Figure 49. However, if *Yes* is not listed, click on the blank field to toggle it on.

   b. Toggle *Yes* to display in the Start Instrument field for the autosampler to make the autosampler start the automatic injection as soon as all devices are ready.

   c. Click **OK** to return to the Run Sequence window.

4. Prepare the injection.

   a. Transfer your sample into an autosampler vial. A sample vial containing 1 pg/µL of Octafluoronaphthalene (OFN) shipped with your instrument.

b. Load the sample vial into position 1 of the autosampler.

5. Start the run by clicking **OK** in the Run Sequence window to return to the Sequence Setup window.

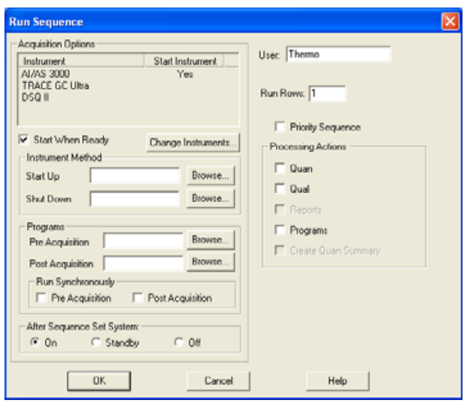
Running Manual Injections

Manual injections are used when you do not have an autosampler to run a method.

When a sample is manually injected by inserting a syringe into the GC/MS, the In Use Entries for all instruments, except the GC and DSQ II, must be a blank space. All instruments used for the sequence submitted for processing must display *Yes* in the In Use column.

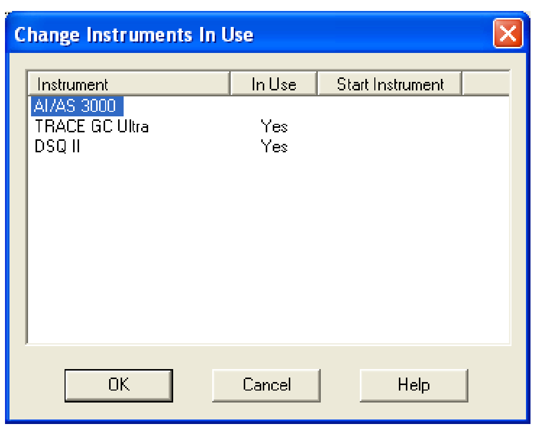
1. Select an *.sld* file to display it in the Sequence Setup window.
2. Select **Actions | Run Sequence** to open the Run Sequence window.

Figure 50. Run Sequence Window



3. Click the **Change Instrument** button to open the Change Instruments window.

Figure 51. Change Instruments In Use Window (Manual Injections)



4. Configure the Change Instruments In Use window for manual injections.

a. Toggle *Yes* to display the DSQ II and TRACE GC Ultra in the In Use fields. If *Yes* is not listed, click on the blank field to toggle it on.

b. Make sure the DSQ II and TRACE GC Ultra Start Instrument fields are empty. The operator making the injection starts the injection.

c. Make sure the autosampler (if listed) does not say *Yes* in both the In Use and Start Instrument fields. This allows you to perform the manual injection.

d. Click **OK** to return to the Run Sequence window.

5. Click **OK** in the Run Sequence window to start the run and return to the Sequence Setup window.

6. Monitor the Status View until the instrument indicates it is *Waiting for Contact Closure*.

7. Prepare the injection.

a. Draw 1 µL of your sample into a syringe. Be sure there are no air bubbles in the syringe. A sample vial containing 1 pg/µL of Octafluoronaphthalene (OFN) shipped with your instrument.

b. Remove the syringe from your sample and pull back the plunger until air is visible inside the syringe.

8. Make the injection and start the TRACE GC Ultra.

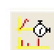
a. Carefully insert the needle into the injector port.

b. Wait three seconds and push the plunger.

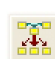
c. Press the Start button on the front of the TRACE GC Ultra.

d. Remove the syringe.

9. Watch the data while the sequence is running. You can choose one of the two views:

a. Click the **Real Time Plot** button  to view the Chromatogram and Spectrum acquisition in real time. The real-time plot starts after the filament delay has timed out. When the run is finished, this window goes blank.

b. Click the Acquisition Queue tab in the Status view for the list of samples you want to run. Green items indicate the sequence is running.

10. Click the **Roadmap** button  to return to the *Xcalibur* Home Page.

11. At this point, you can begin:

- "Analyzing Compounds with a Known Retention Time" on page 65
- "Analyzing Compounds Chromatographically" on page 70
- "Analyzing the Peak Height and Area" on page 72
- "Using the Signal-to-Noise Test" on page 75

Analyzing Compounds with a Known Retention Time

When you are ready to analyze your data, use Xcalibur software components (Qual, Quan, and Library) to view the data file results. With Qual Browser, you can answer the question, "Does this sample contain compound 'X' at a known retention time?" Then you can determine the peak height, area, and signal-to-noise ratio.

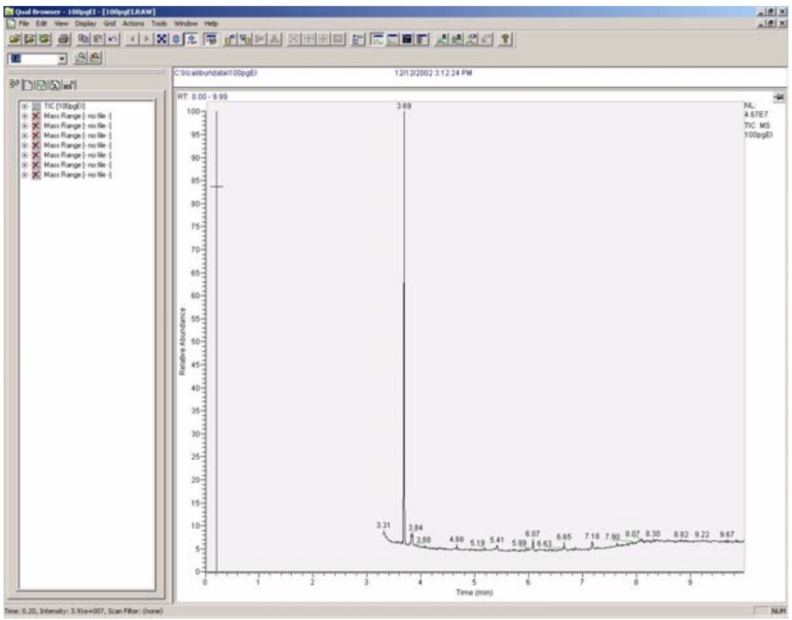
In this example, we used the C:*Xcalibur\Data\100pgEI.raw* file that was acquired in Step 8. Make the injection and start the TRACE GC Ultra., on page 64, which has a retention time of approximately 3.7 min. If you did not acquire this sample, you can use the sample file located in C:*Xcalibur\Data\Factory Test Data\100pgEI.raw*.

1. Open Qual Browser and select the *.raw* file that contains the data for the sample you want to work on.

   a. Open Xcalibur and click the Qual Browser icon.

   b. Select **File | Open** and navigate to C:*Xcalibur\Data\100pgEI.raw* or another *.raw* file.

   Figure 52. Opening the 1pgEI.raw File

   Do not be surprised if the Qual Browser window looks different than Figure 52. The default layout can be changed and saved.

2. Display a chromatogram and a mass spectrum in the same window. If you want to identify the compound that is eluting at approximately 3.69 min, look at the mass spectrum recorded at that time in the chromatogram.

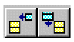
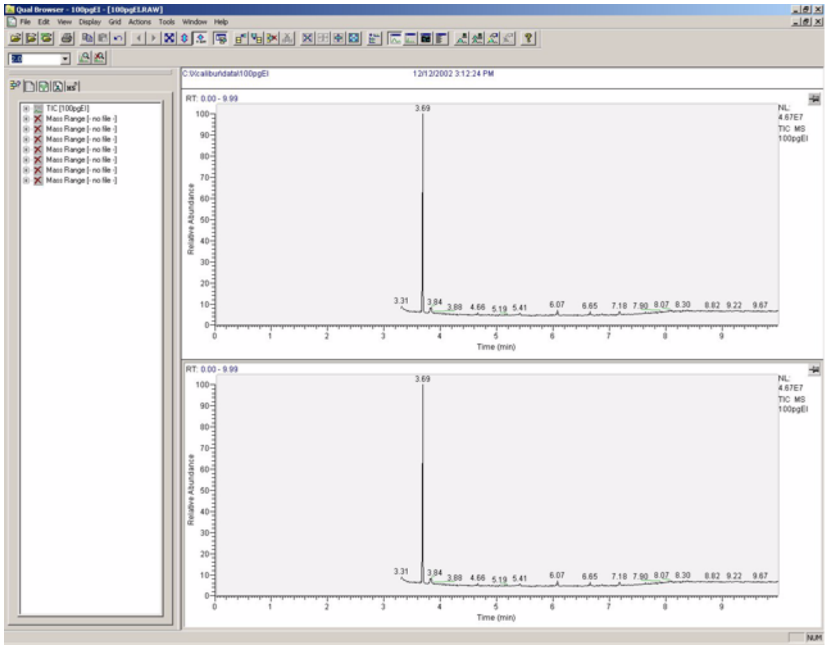
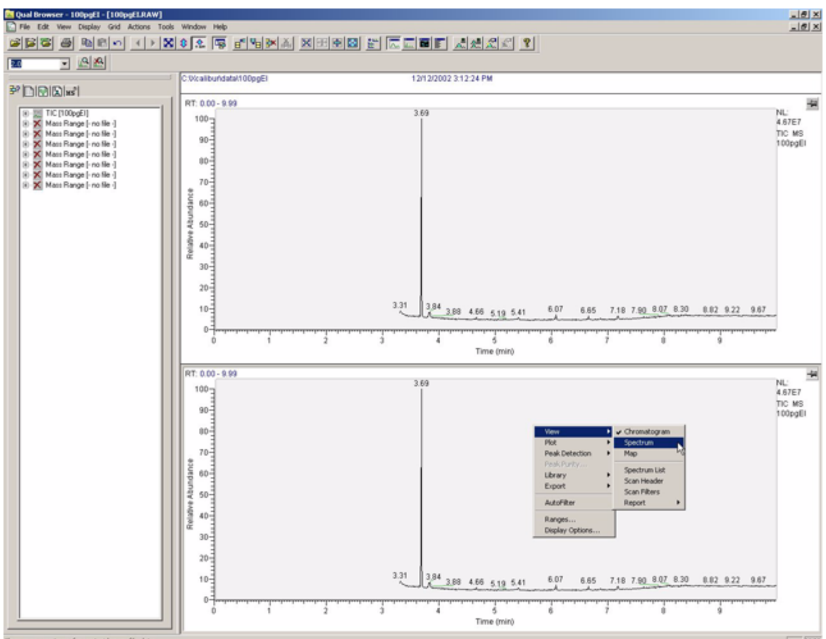
   a. Click the **Insert Cell** button  in the toolbar to display a new cell containing the same information as the existing cell.

Figure 53. Displaying Two Chromatograms



b. Select the lower cell and right-click to display the context-sensitive menu.

Figure 54. Qual Browser Chromatogram Menu



c. Select **View | Spectrum** to change the view from chromatogram to spectrum. The lower cell now displays spectral data.

Notice that the lower cell now displays a graph of Relative Abundance versus *m/z* (a mass spectrum). Initially, you'll see the first mass spectrum.

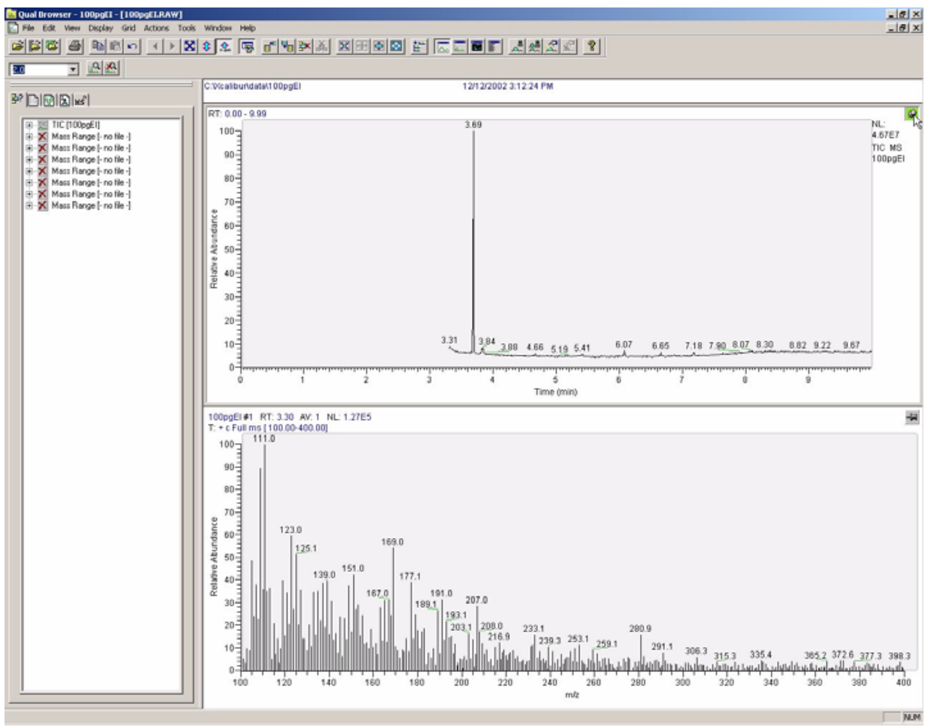
3. Zoom in on a time period. Although the full TIC chromatogram is currently displayed in the upper cell, only the retention time of three or four minutes is of interest. So zoom in on that part of the chromatogram and view it in more detail. You can use the mouse or range functions.

Using the Mouse to View the Retention Time

To use the mouse to view the retention time:

1. Pin the view you are interested in viewing.
   a. Click the pin button  located in the top right corner of the chromatogram cell so it is green (pinned).

Figure 55. Chromatogram Using Mouse Functions



2. Position the cursor at the start time you are interested in at a position close to or on the baseline.

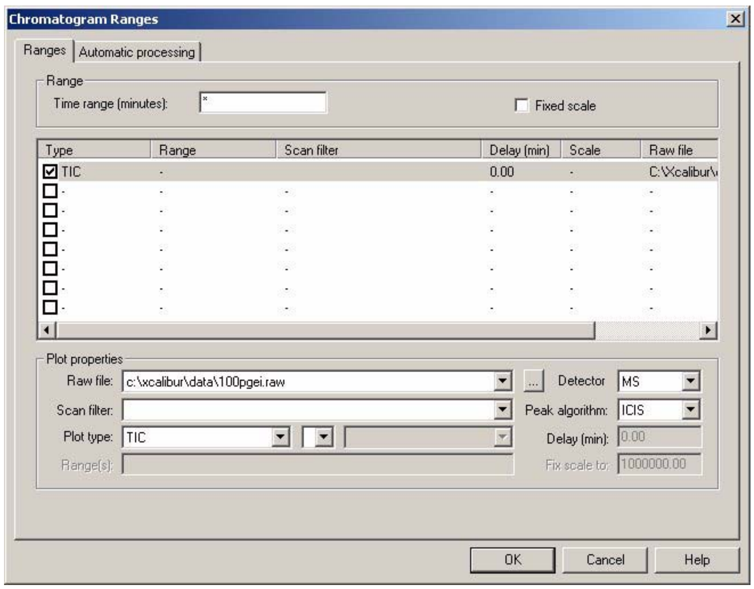
3. Click and drag the cursor parallel to the time axis to the end of the period required. Notice that a line is drawn on the screen as you drag it. As the cell redisplays, notice only that part of the chromatogram within the line you have just drawn.

Using Range Functions to View Peaks, Spectrum and Library Search

To use range function to view the retention time:

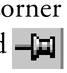
1. Right-click on the chromatogram to display the context-sensitive menu.
2. Select **Ranges** to display the Chromatogram Ranges window.
3. Enter the time range of interest in the Time range field. For example, 3.4 to 4.0 min.

Figure 56. Chromatogram Ranges Window Using Range Functions



- Click **OK** to return to Qual Browser.

4. View the mass spectrum for a specific chromatogram retention time. Currently, a selected chromatogram time period is displayed in one cell and a mass spectrum in another cell. This step describes how to select a particular retention time on the chromatogram and view the corresponding mass spectrum.

   a. Locate the pin button shown in the top right corner of the mass spectrum cell and click on it. The button changes from unpinned  to pinned .

   b. Move the cursor over the chromatogram until it is positioned at the retention time you are interested in and click on it to view the mass spectrum for the retention time.

5. Subtract the background contamination from the spectrum. Peaks eluting from a GC column can contain low levels of contamination due to material bleeding from the matrix of the column. This material will have its own mass spectrum that will be superimposed on that of the sample compound. The mass spectrum of a chromatogram peak can be made up of mass peaks resulting from the sample compound plus mass peaks resulting from background contamination.To obtain a mass spectrum for the compound alone (that can be used in a library search), subtract the mass spectrum of the background contamination.

a. Make sure that the mass spectrum cell is pinned.

b. Select **Actions | Subtract Spectra | 2 Ranges**. You can choose between subtracting the background from either one side of the peak you are interested in or from both sides. To get the best results, you want to subtract from both sides, so choose two ranges.

c. Move the cursor into the chromatogram cell and position it slightly to one side of the peak you are interested in.

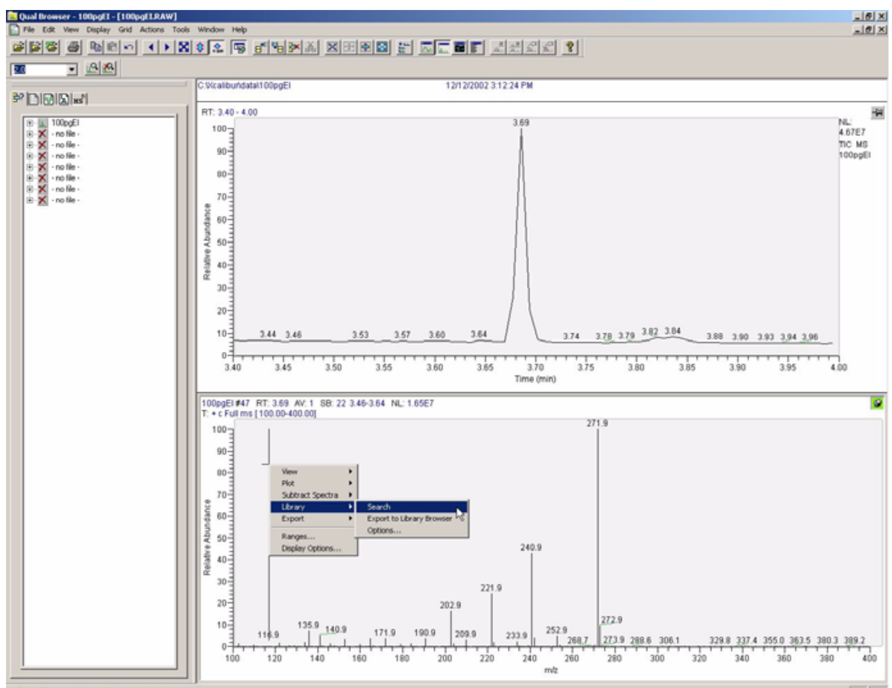
d. Click and drag the cursor away from the peak, making sure to stop before reaching the next discernible peak on the chromatogram. Notice a line is drawn on the screen.

e. Repeat to mark the opposite side of the peak. In general, after background subtraction, most of the larger mass peaks in the mass spectrum will be unchanged; these are "true" peaks, due to the sample compound. Common contamination peaks are typically at *m/z* 207, and 281. Removing such contamination peaks will help you to obtain a more accurate result from a library search.

6. Use the spectrum to perform a library search. When you have a clean mass spectrum, you can use it to search the NIST library to determine the nature of the compound.

   a. Right-click in the mass spectrum cell and choose **Library | Search**.

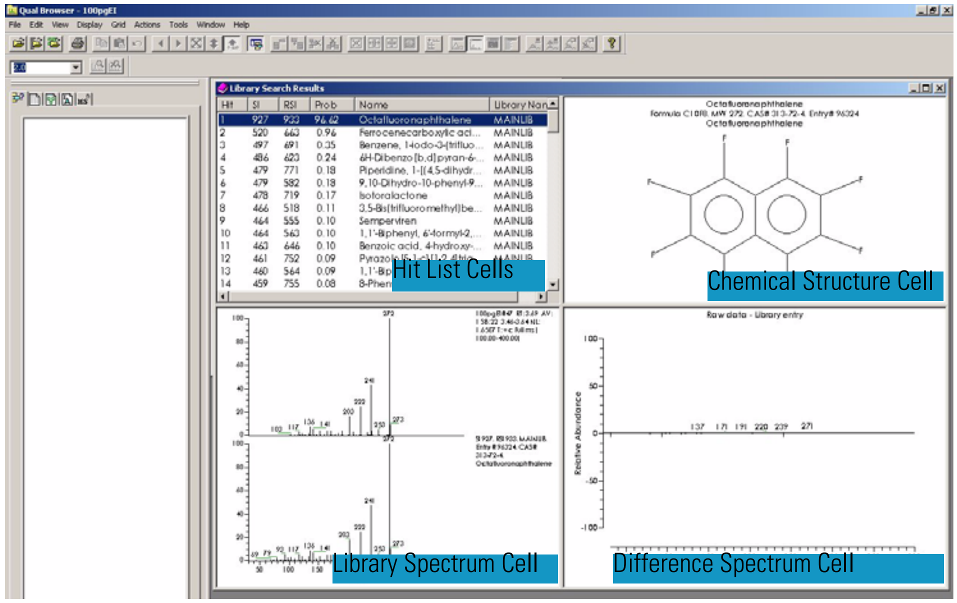
Figure 57. Library Search Menu



   b. If you have the optional NIST library installed, look for the results in the hit list cell for the most likely compounds in decreasing order of match probability.

   If Octafluoronaphthalene (OFN) is not one of the top hits, you may not have the optional NIST library. Check for library availability for search by selecting the **Library Options** pull-down menu.

Figure 58. Library Search Results Window



For each compound in the hit list, Xcalibur displays a chemical structure, a library spectrum to compare with your spectrum, and a difference spectrum that is the library spectrum subtracted from your spectrum.

Analyzing Compounds Chromatographically

Using Qual Browser, you can answer the question, “Does this sample contain compound “x”? X being the Octafluoronaphthalene (OFN) file you acquired in Section “Running Methods in Sequence Setup” on page 58. Then you can determine the peak height, area, and signal-to-noise ratio.

In this example, we used the C:*Xcalibur\Data\100pgEI.raw* file you acquired in Step 8. Make the injection and start the TRACE GC Ultra., on page 64, which has a retention time of approximately 3.7 minutes.

In this example, we will assume you have some knowledge of the mass spectrum of compound 'X' and you know the characteristic ions present in its mass spectrum. For the purposes of this example, *m/z* 272 represents an ion, perhaps the molecular ion of the compound, and this ion represents a “marker” for the compound.

1. Open *Qual Browser.*

   a. Set up the cells so you only have one chromatogram cell. You can delete other cells by pinning them and clicking the **Delete Grid Row** button on the toolbar or by selecting **Grid | Delete | Row** from the menu.

   b. Reset the time range to the full range by clicking the **Zoom Reset** button on the toolbar.

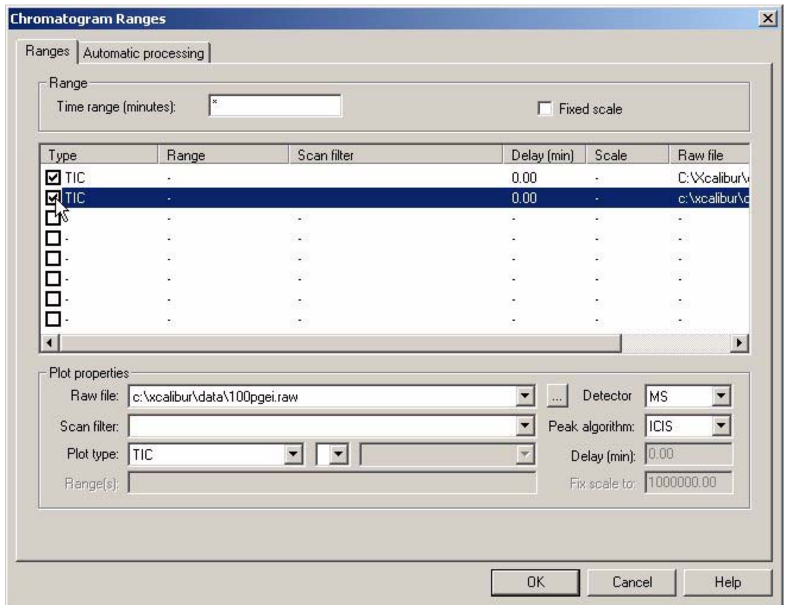
2. Add a mass range chromatogram.

a. Select the chromatogram cell and then right-click to view the menu.

b. Select **Ranges** from the menu to open the Chromatogram Ranges window.

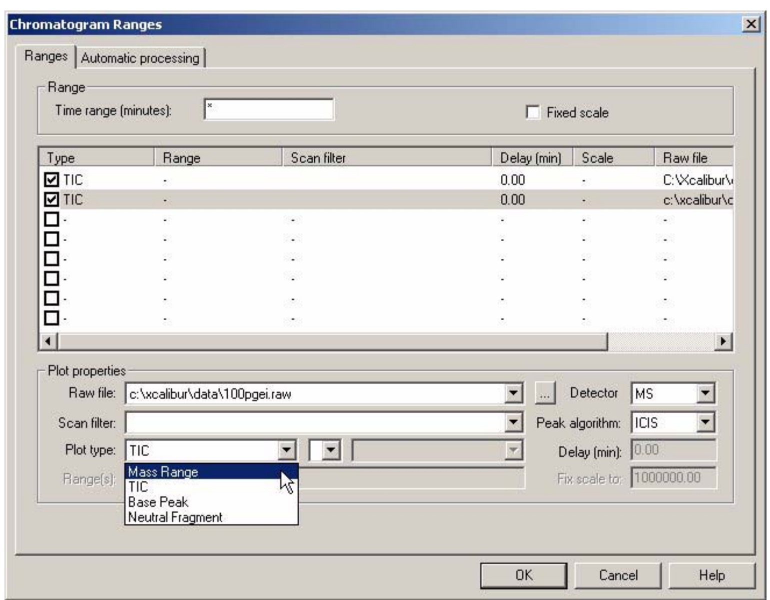
c. Add another plot by selecting the checkbox in the Type column.

Figure 59. Qual Browser—Chromatogram 1



d. Select **Mass Range** in the Plot Type field.

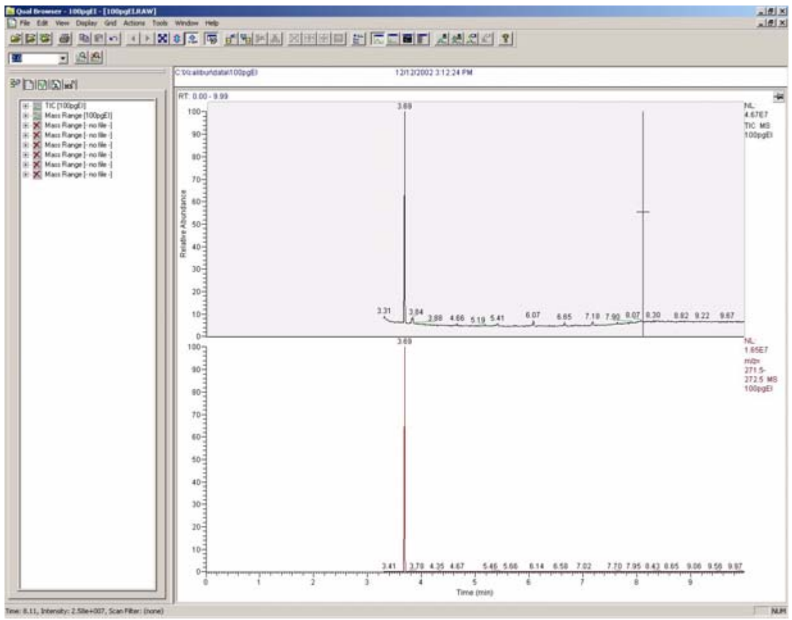
Figure 60. Qual Browser—Chromatogram 2



e. Enter *272* as the mass range in the Range(s) field.

f. Click **OK** to return to *Qual Browser* where the chromatogram cell now shows a mass TIC and a chromatogram for the selected mass *m/z* 272.

Figure 61. Displaying a TIC and Mass Range Chromatogram



The result in this example shows that the peak at retention time 3.69 minutes is of particular interest because it includes *m/z* 272, the molecular ion from Octafluoronaphthalene (OFN).

3. View the mass spectrum. Having identified a particular retention time, you can investigate the peak further by looking at the mass spectrum. Follow the same procedure you did in the previous section for adding a spectrum cell.

Analyzing the Peak Height and Area

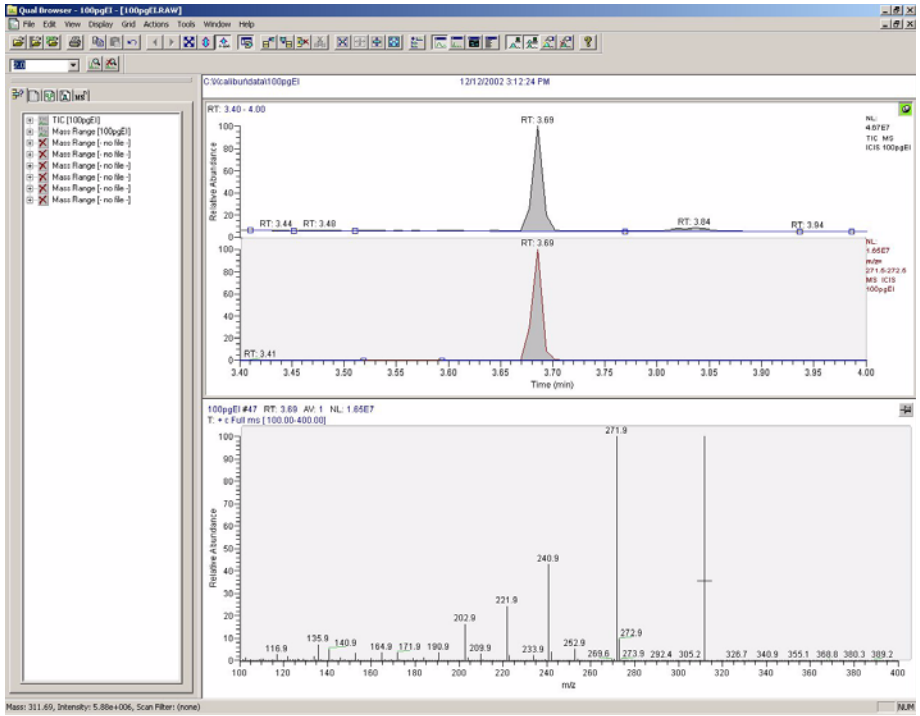
Using *Qual Browser*, you can analyze the data's peak height and area. In a chromatogram, the area of an isolated peak is directly proportional to the amount of material present; for peaks that overlap, height may give a more accurate determination. Determining the area and/or height of a peak is therefore an important feature of quantitation.

1. Open Qual Browser and browse to a *.raw* file you stored in the Sequence Setup window.

2. Zoom in on the part of the chromatogram that is of particular interest (3.4 – 4.0 min.)

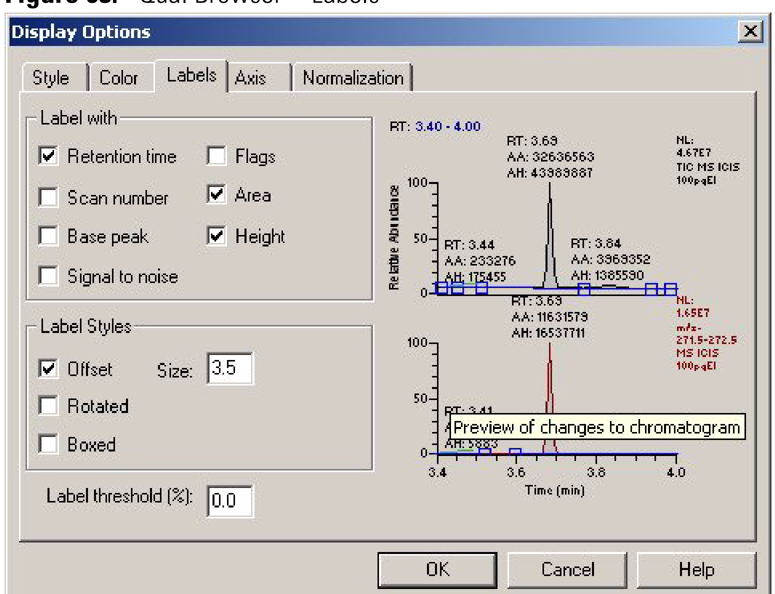
   a. Right-click on the chromatogram and choose **Peak Detection | Toggle Detection in All Plots** from the menu. Individual peaks are shown shaded and the extent of each peak shown by blocks on the baseline.

Figure 62. Qual Browser—Peak Detection



b. Right-click on the chromatogram and select **Display Options** to open the Display Options window.

Figure 63. Qual Browser—Labels



c. Click the Labels tab.

d. Select the Area and Height checkboxes.

e. Click **OK** to return to the chromatogram.

Using Qual Browser to Determine the Signal-to-Noise Ratio

To use *Qual Browser* to determine the signal-to-noise ratio:

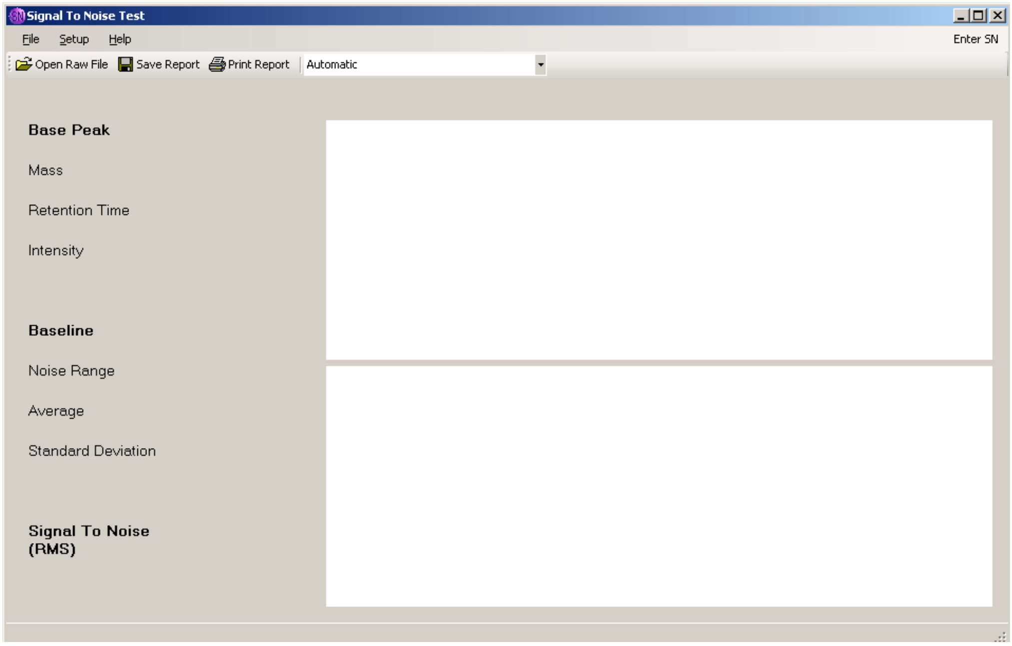
1. Open the *.raw* file in *Qual Browser* and display the signal-to-noise label on the chromatogram.
   a. Right-click on the chromatogram to access the drop-down menu.
   b. Select **Display Options** from the menu to open the Display Options window. If you do not see the Info Bar window, select **View** and check the Info Bar checkbox or click the button on the toolbar.
   c. Click the **Labels** tab.
   d. Check the **Signal-to-Noise** checkbox.
   e. Click **OK** to return to the chromatogram.
2. Choose the baseline noise range.
3. Click the Peak Detection Settings tab in the Info bar.
4. Pin the chromatogram cell by clicking the top right corner. Click on the chromatogram plot on which you want to measure the signal-to-noise. It will turn gray.
5. Check the **Manual Noise Region** checkbox in the Info bar.
6. Enter a noise range near the peak, such as 4.0–4.5 min. Avoid choosing a region with a peak in it.
7. Click **Apply** to display the RMS (root mean square) signal-to-noise calculation.
8. Look for a red line in the chromatogram to view the chosen noise range.
9. If you want to see the effect of smoothing on the signal-to-noise, right-click to display the drop-down menu.
   a. Select **Ranges**.
   b. Click the Automatic Processing tab.
   c. Check the **Smoothing** checkbox.
   d. Select **Boxcar** in the Type field.
   e. Enter three points in the Points field. If you select **Boxcar** in the Type field and enter three points in the Points field, this improves the signal-to-noise ratio. Entering a higher value of points reduces the signal-to-noise ratio.

Using the Signal-to-Noise Test

To use the *Signal-to-Noise Test* to determine whether the installation qualification specifications have been met:

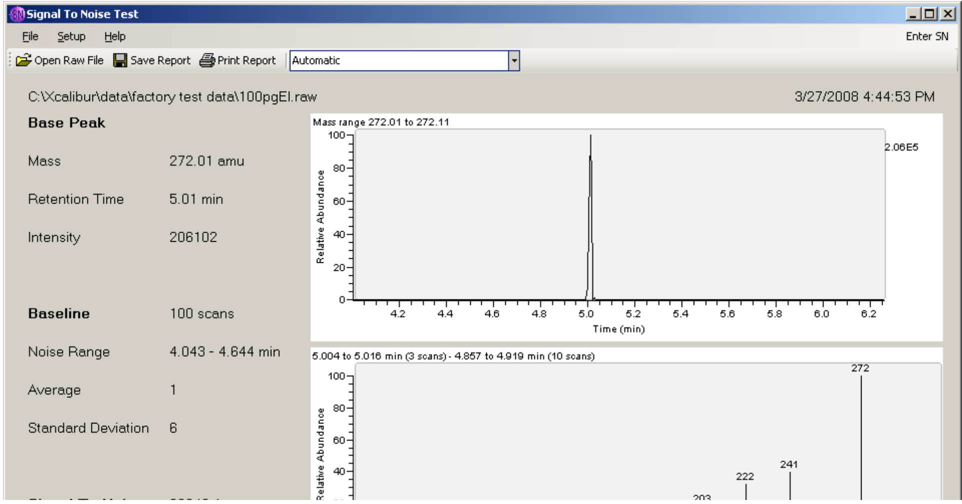
1. Double-click the Signal-to-Noise Test icon on the computer desktop. To add the Signal-to-Noise Test to the *Xcalibur* Tools menu, select **Tools | Add Tools** and specify the program location as *C:\Program Files\Thermo\Signal to Noise Test 1.1\Signal To NoiseTest.exe*.

   Figure 64. Signal-to-Noise Test Window

   a. Select **File | Open Raw File** and open *100pgEI.raw* or another data file. Xcalibur begins processing the file upon opening.

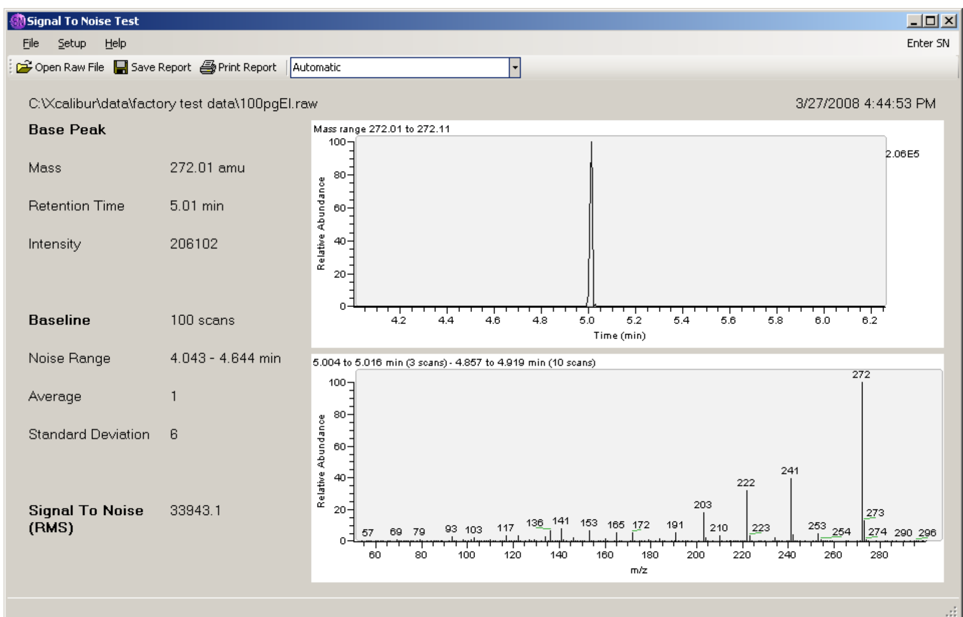
Figure 65. Processing the Raw File



The automatic processing method looks for all the standard test compounds mass ranges and retention times. If you would like to find the signal-to-noise ratio for a different compound, select the custom option from the list.

b. Select **Custom** from the list. In custom mode, you can select the mass and the retention time to use.

Figure 66. Selecting Custom Mode



c. Press the F5 button on your keyboard to refresh the screen after selecting your custom parameters.

2. Reprocess the file by selecting **Setup | Reprocess**.

Additional Help

This section contains additional instructions for swagelok fittings and specialized situations.

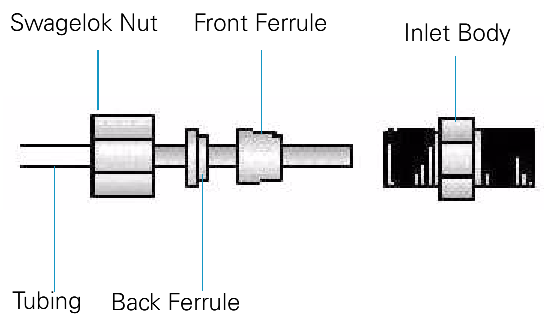
Contents

Assembling Swagelok Fittings

Building Swagelok compression fittings and connecting tees and crossings are essential to a leak-free system. A Swagelok fitting is a compression fitting that has four components—Swagelok nut, a back ferrule, a front ferrule, and an inlet body. The assembly is completed when the Swagelok and ferrule assembly is affixed to tubing. Two ferrules merge when the nut is tightened, forming a safe and leak-free seal between the tubing and the inlet body. To assemble a Swagelok fitting, you will need an open-ended wrench set (5/16-in., 7/16-in., 9/16-in.,1/2-in.).

1. Place a Swagelok nut on the end of the tubing. The threads on the nut should face the open end of the tubing, as shown in Figure 67.

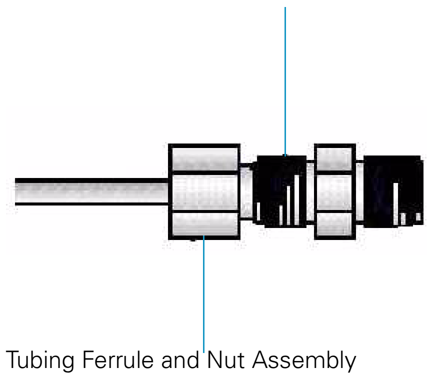
Figure 67. Swagelok Ferrule and Nut



Note Do **not** put tape on the threads of a Swagelok fitting.

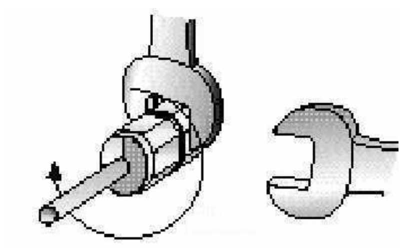
2. Place a Swagelok back ferrule over the tubing with the smaller side facing the open end of the tubing.
3. Place a Swagelok front ferrule over the tubing with the smaller side facing the open end of the tubing.
4. Push the ferrules down into the Swagelok nut.
5. Insert the tubing into the Swagelok inlet as far as it will go, as shown in Figure 68.

Figure 68. Swagelok and Inlet Connection



6. Slide the nut over the inlet and tighten until finger-tight.
7. Pull the tubing out from the nut very slightly (1/16-in.)
8. While holding the inlet tight with a backup wrench, tighten the nut 3/4-turn past finger-tight as shown in Figure 69.You can make a mark on the nut before you tighten it. This helps ensure that you have turned the nut a 3/4-turn.

Figure 69. Tightening Swagelok Fittings



Using a Swagelok Tee or Cross to Fix Leaks

To use a single gas source for more than one inlet or detector module, you must use a Swagelok tee or cross to properly split the gas flow. You will need a ruler or measuring tape, Swagelok fitting and plugs, and a tubing cutter.

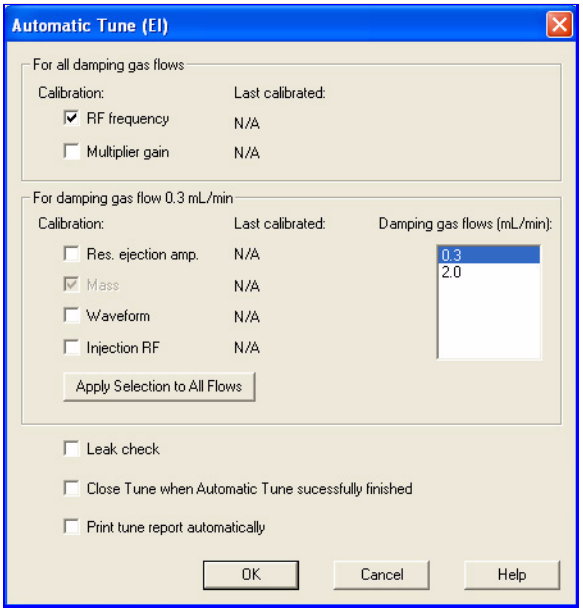
1. Cut the tubing with a tubing cutter where the tee or cross will go.
2. Connect the tubing to the tee or cross with a Swagelok fitting, as described in "Assembling Swagelok Fittings" on page 78.
3. Measure the distance from the tee or cross to the inlets or detectors and cut the tubing in the appropriate lengths.
4. Connect the tubing to the tee or cross ends with Swagelok fittings.
5. Install Swagelok plugs instead of an inlet body on any open ends located on a tee or cross that are not connected with tubing.

Adjusting the RF Dip Calibration

You can adjust the RF Dip Calibration readback, but make sure you run this calibration **after** the heaters and vacuum have stabilized.

1. Make sure the heaters and vacuum status readbacks have stabilized.
2. Open *DSQ II Tune* and adjust the RF dip calibration.
   a. Double-click the Tune icon on the computer desktop.
   b. Select **Tune | Automatic Tune** to open the Automatic Tune window.

Figure 70. Adjusting the EI Mode RF Frequency



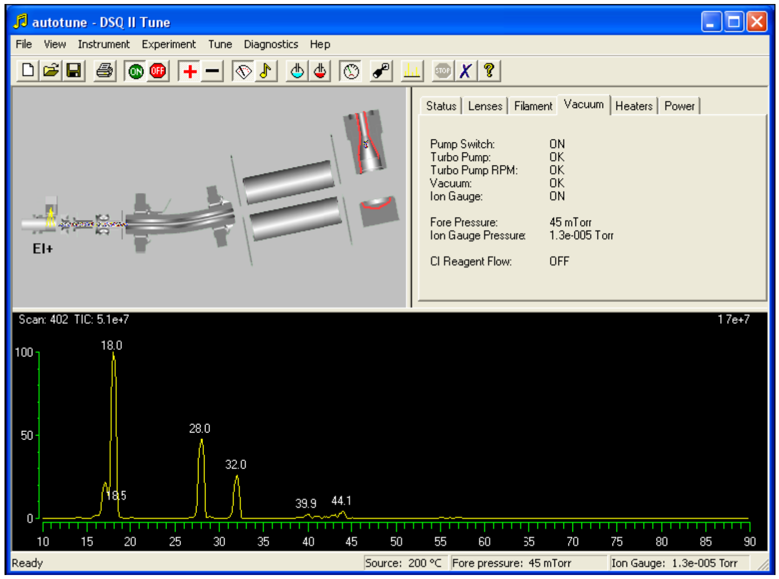
   c. Select the RF Frequency checkbox.
   d. Uncheck all other options.
   e. Click **OK** to adjust the RF Dip Calibration automatically.

Baking Out the Source

You can bake out the source to reduce background noise. This is especially useful after a system has been cleaned.

1. After startup, open *Tune* and set the source temperature to 300 °C.
2. Allow the source temperature to equilibrate and the fore pressure to decrease to less than 100 mTorr.
3. View the air/water spectra and verify water is the maximum peak, which is typically *m/z* 18.

Figure 71. Air/Water Spectra



If the air/water spectra are typical for a system with no leaks, note the fore pressure for future reference.

4. Increase the DSQ II source temperature and transfer line to 300 °C. As the source temperature rises, the pressure will begin to increase.

5. Allow the source to remain at 300 °C until the fore pressure begins to decrease to a pressure equal to or below the fore pressure noted in the previous step.

6. Once the operating temperature has been reached, wait one hour while the system stabilizes.

7. Perform a tune and continue.

Reviewing Cursor Actions in Browsers

Before you begin using the browsers, let's review some of the cursor actions and effects within the chromatogram and spectrum cells:

- A click picks a point on the cell
- A line dragged parallel to any axis picks a range
- A line dragged in any diagonal direction selects an area

The effect of these actions depends on one of these cell states:

- Inactive
- Active and unpinned— Each cell has a pin button in its top right corner. Only one of the cells can be active at any one time. The active cell is highlighted with a gray border.

- Active and pinned — Pinning fixes the active status of a cell.

In the browser, you can perform the following cursor actions:

- Unpin an active cell by clicking once on the pin button.
- Make a cell active by clicking anywhere in the cell.

  Xcalibur highlights the cell with a gray border. Click on its pin button if you want to fix it as the active cell. Cursor actions in an active cell cause the cell to be scaled according to the dimensions of the dragged line or area (see Table 4).

Table 4. Cursor Actions In Active and Unpinned Cells

Cursor Action	Effect
Drag parallel to X-axis	Rescale graph showing selected X range only, same Y range
Drag parallel to Y-axis	Rescale graph showing selected Y range only, same X range
Dragged area	Rescale graph showing both the selected X and Y ranges

The same actions in the unpinned or inactive cell have a very different effect. In this case, the cursor actions affect the active, pinned cell (see Table 5).

Table 5. Cursor Actions in an Inactive or Unpinned Cell

Pinned cell	Cursor action	Effect
Spectrum	Click in a chromatogram cell	The spectrum cell displays the mass spectrum at that retention time.
Spectrum	Drag across a time range in a chromatogram cell	The spectrum cell displays the averaged mass spectrum from that retention time range.
Chromatogram	Click in a spectrum cell	The chromatogram cell displays the mass chromatogram of the selected mass. If the Plot Type is TIC or Base Peak, it is changed to Mass Range.
Chromatogram	Drag across an *m/z* range in a spectrum cell	The chromatogram cell displays the mass range chromatogram of the selected mass range. If the Plot Type is TIC or Base Peak, it is changed to Mass Range.

Important points to note are:

- The cursor action is always applied to the pinned cell
- Within an active cell, cursor actions rescale the plot.

Reinstalling the Data System

You can reinstall the data system if you have installed a new computer or hard drive.

1. Follow the instructions on the *Xcalibur* CD that came with your instrument. You may either have a single CD or a series of discs, depending on which version of *Xcalibur* shipped with your instrument.

   a. Insert the *Xcalibur* CD into your computer. This should automatically display the Xcalibur Setup window. If it does not, use Windows to run the *XInstall.exe* from the CD.

   b. Click the **Installation Help** button to open the *Instructions.doc* file and print it. Follow the instructions to install the data system software.

   Note Click the **Read Me** button located on the Setup window to read important information about the software.

2. Install any optional upgrade software. You should now install any optional software like libraries. Follow the instructions provided with these options.

3. Configure the instruments, as described in "Configuring Instruments for Use" on page 43.

Index

D

E

F

G

H

I

K

L

M

N

O

P

Q

R

S

T

U

V

W

X

Z