



**Xcalibur**

# **Ion Trap Series**

**User Guide**

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Ion Trap series refers to ITQ and PolarisQ instruments. DSQ series refers to all DSQ and DSQ II instruments. Information about the TRACE 1300, TRACE 1310, TRACE GC, and FOCUS GC instruments is included in this document.

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**For Research Use Only. Not for use in diagnostic procedures.**

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## Declaration

Manufacturer: Thermo Fisher Scientific

Thermo Fisher Scientific is the manufacturer of the instrument described in this manual and, as such, is responsible for the instrument safety, reliability and performance only if:

- installation
- re-calibration
- changes and repairs

have been carried out by authorized personnel and if:

- the local installation complies with local law regulations
- the instrument is used according to the instructions provided and if its operation is only entrusted to qualified trained personnel

Thermo Fisher Scientific is not liable for any damages derived from the non-compliance with the aforementioned recommendations.

## 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 in the next section or sections by product name.

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.

### EMC Directive 89/336/EEC

EMC compliance has been evaluated by Professional Testing.

- Polaris Q, ITQ, and Ion Trap Series standards: EMC EN 61326-1:2006. Safety IEC 61010-1:2001, IEC 61010-2-081:2001
- 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
- ISQ standards: EMC EN 61326-1:2006. Safety IEC 61010-1:2001
- TSQ 8000 standards: EMC EN 61326-1:2006. Safety IEC 61010-1:2001

### Low Voltage Safety Compliance

This device complies with Low Voltage Directive 2006/95/EC and harmonized standard EN 61010-1:2001.

## FCC Compliance Statement

THIS DEVICE COMPLIES WITH PART 15 OF THE FCC RULES. OPERATION IS SUBJECT TO THE FOLLOWING TWO CONDITIONS: (1) THIS DEVICE MAY NOT CAUSE HARMFUL INTERFERENCE, AND (2) THIS DEVICE MUST ACCEPT ANY INTERFERENCE RECEIVED, INCLUDING INTERFERENCE THAT MAY CAUSE UNDESIRE OPERATION.



**CAUTION** 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](http://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](http://www.thermo.com/WEEERoHS).

## Conformité DEEE

Ce produit doit être conforme à la directive européenne (2002/96/EC) des Déchets d'Équipements Électriques et Électroniques (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](http://www.thermo.com/WEEERoHS).



## Preface

This guide contains instructions for using your instrument and is designed to increase your understanding and knowledge of the Ion Trap Series.

### Contents

- [About Your System](#)
- [Power Ratings](#)
- [Related Documentation](#)
- [System Requirements](#)
- [Safety and Special Notices](#)
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## 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  $\pm$ 10%, 50/60 Hz, 10 A max

### *Gas Chromatograph (GC)*

- 120 V ac +6/-10%, 50/60 Hz, 16 A max
- 230 V ac  $\pm$ 10%, 50/60 Hz, 16 A max

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

## Related Documentation

Thermo Scientific provides the following documents for the Ion Trap Series mass spectrometer. These documents are also available on a “Print-By-Request” basis.

*Ion Trap Series Preinstallation Requirements Guide* PN 120425-00PI

*Ion Trap Series User Guide* PN 120425-USER

*Ion Trap Series Hardware Manual* PN 120425-00HW

*Instrument Help* is available from within the software.

### ❖ **To view product manuals**

Go to **Start > All Programs > Thermo Foundation 2.0 > Manuals > Ion Trap Series**.

### ❖ **To open Help**

- From the Ion Trap Series window, choose **Help > Ion Trap Series Help**.
- If available for a specific window or dialog box, click **Help** or press the F1 key for information about setting parameters.

For more information, visit [www.thermo.com](http://www.thermo.com).

## System Requirements

Your Ion Trap Series data system must meet these minimum requirements.

System	Requirements
Hardware	<ul style="list-style-type: none"><li>• 2.4 GHz processor with 4 GB RAM</li><li>• DVD/CD-ROM drive</li><li>• Resolution display 1280 × 1024 (XGA)</li><li>• 250 GB hard drive</li><li>• NTFS format</li></ul>
Software	<ul style="list-style-type: none"><li>• Microsoft™ Windows™ 7 SP1 Operating System (32-bit)</li><li>• Microsoft Office™ 2010</li><li>• Thermo Foundation 2.0 or higher (Thermo Scientific software)</li><li>• Xcalibur™ 2.2 or higher</li><li>• TraceFinder™ 2.0 SP1 or higher*</li></ul>

\*Your system will function without TraceFinder, but earlier versions of TraceFinder will not work with the Thermo Scientific software required for this instrument.

## Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

Safety and special notices include the following:



**CAUTION** Highlights hazards to humans, property, or the environment. Each CAUTION notice is accompanied by an appropriate CAUTION symbol.

**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** Highlights information of general interest.

**Tip** Highlights 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. A **WARNING** is intended to prevent improper actions that *could* cause personal injury. A **CAUTION** is 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 alerts you to the presence of 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 *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 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 component *may* occur. This damage may not be covered under the standard warranty.



**LIFTING HAZARD:** This symbol indicates that a physical injury *could* or *may* occur if two or more people do not lift an object.



**MATERIAL AND EYE HAZARD:** This symbol indicates that eye damage *could* or *may* occur.



**RADIOACTIVE HAZARD:** This symbol indicates that exposure to radioactive material *could* or *may* occur.



**READ MANUAL:** This symbol alerts you to carefully read your instrument's documentation to ensure your safety and the instrument's operational ability. Failing to carefully read the documentation *could* or *may* put you at risk for a physical injury.



**TOXIC SUBSTANCES HAZARD:** This symbol indicates that exposure to a toxic substance could occur and that exposure *could* or *may* cause personal injury or death.



This is the general warning symbol that the ISO 3864-2 standard uses to prevent personal injury. This symbol precedes the **WARNING** safety alert word. In the vocabulary of ANSI Z535 signs, 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 you to an imminent or potential hazard that *could cause personal injury*.

## Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

### ❖ To contact Technical Support

Phone	800-532-4752
Fax	561-688-8736
E-mail	<a href="mailto:us.techsupport.analyze@thermofisher.com">us.techsupport.analyze@thermofisher.com</a>
Knowledge base	<a href="http://www.thermokb.com">www.thermokb.com</a>

### ❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
E-mail	<a href="mailto:us.customer-support.analyze@thermofisher.com">us.customer-support.analyze@thermofisher.com</a>
Web site	<a href="http://www.thermo.com/ms">www.thermo.com/ms</a>

### ❖ To get local contact information for sales or service

Go to [www.thermoscientific.com/wps/portal/ts/contactus](http://www.thermoscientific.com/wps/portal/ts/contactus).

### ❖ To suggest changes to documentation or to Help

- Fill out a reader survey online at [www.surveymonkey.com/s/PQM6P62](http://www.surveymonkey.com/s/PQM6P62).
- Send an e-mail message to the Technical Publications Editor at [techpubsaustin@thermofisher.com](mailto:techpubsaustin@thermofisher.com).

# Getting Started

This chapter provides an introduction to the software used on your Ion Trap Series mass spectrometer. You will also learn how to configure your instrument.





## Contents

- [Using Desktop Shortcuts](#)
- [Configuring Instruments](#)

## Using Desktop Shortcuts

After the instrument is connected, it's a good idea to get acquainted with how your software is organized on the desktop. You can access all the programs from the Windows start menu. There are also desktop shortcuts to help you quickly access commonly used functions.

**Note** You might find it helpful to copy this page and keep it out to use as a quick reference template.

Desktop Shortcuts	What it Does...
 Instrument Configuration	Launches the Instrument Configuration program. Use this program to set up your instruments and connect or remove them from the data system.
 Tune	Launches the ITQ Tune Window. Use the Tune window to customize your instrument's tuning parameters.
 Xcalibur	Launches the Xcalibur Roadmap.
 XReports	Launches the XReport Application. Use this to custom design your reports. Files created here are templates for your reports. Templates are saved as *.xrt files and (by default) stored in the Xcalibur\templates folder.

**Desktop Shortcuts**    **What it Does...**

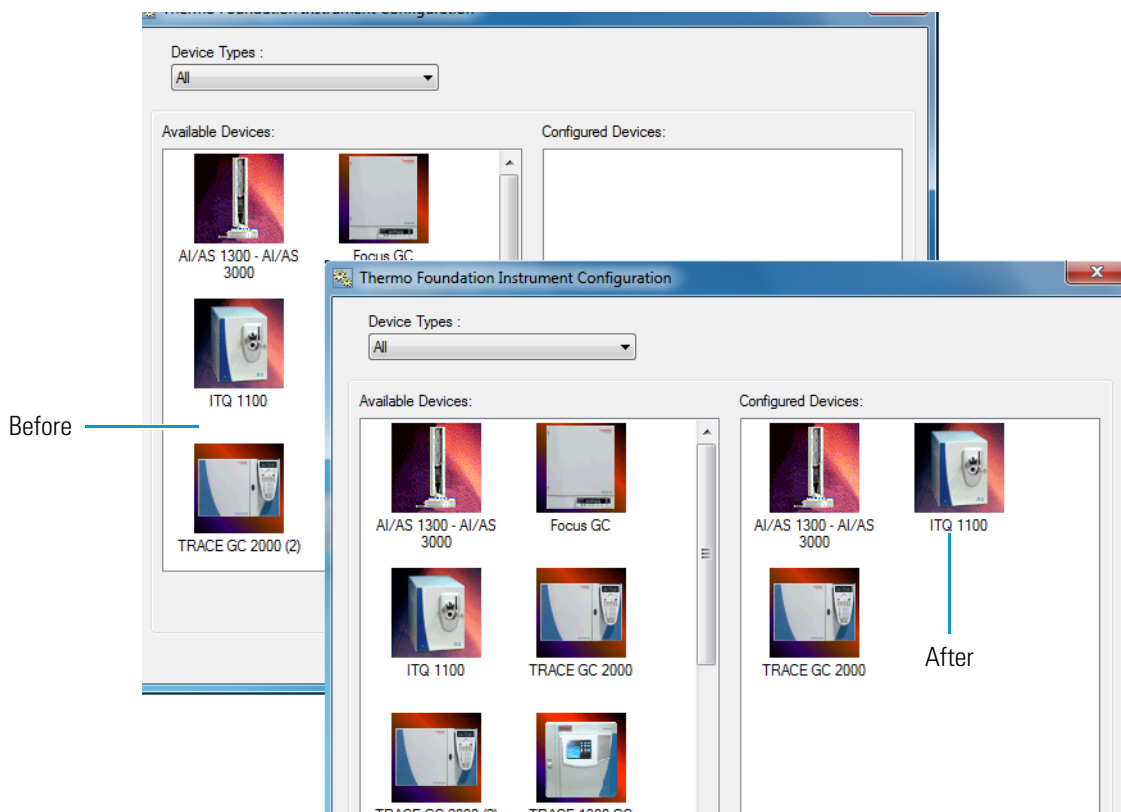


Launches the XReport Application. Use this to custom design your reports. Files created here are templates for your reports. Templates are saved as \*.xrt files and (by default) stored in the Xcalibur\templates folder.

## Configuring Instruments

1. Click the Instrument Configuration shortcut from the Windows desktop or browse to Instrument Configuration through the Windows™ start menu. It will be in the Thermo Foundation program group.
2. Configure the mass spectrometer (MS).

**Figure 1.** Instrument Configuration Windows<sup>1</sup>



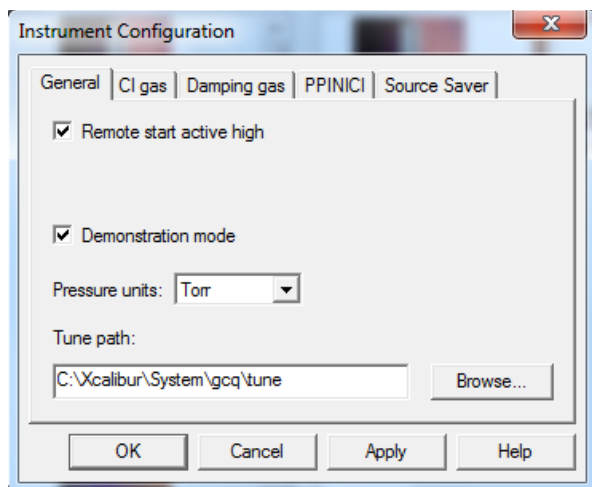
- a. Select the ITQ image located in the list of Available Devices column and click **Add** to move it to the list of Configured Devices.
- b. Select the ITQ image in the Configured Devices column and click **Configure** to display the Instrument Configuration screen.

<sup>1</sup>Your system may not be equipped with the devices shown here. You should only configure devices that are part of your system.



- c. Use the tabs on the Instrument Configuration window to select options to display on the Instrument setup and Tune windows.
3. Configure General options.

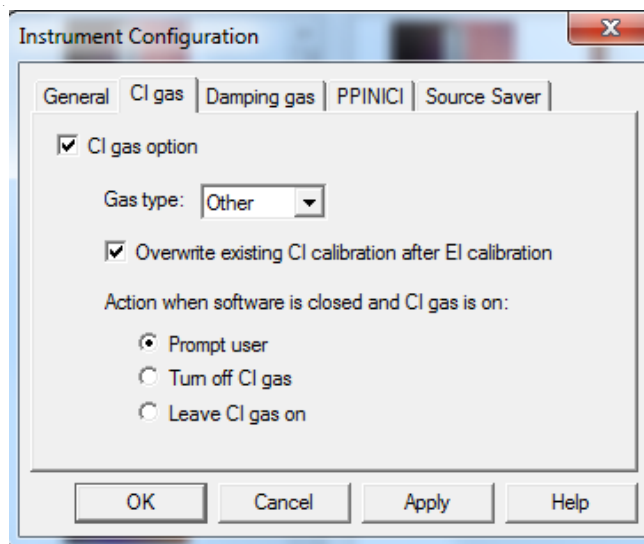
**Figure 2.** Instrument Configuration: General



- a. Select the General tab.
- b. The default setting for Remote Start Active High is unchecked. Select this option to start the GC with an active high signal instead of active low.
- c. Demonstration Mode. Check this option to start the instrument in demonstration mode. This mode is useful if no instrument is connected, but you would like to demonstrate the software. But don't select this to run your first sample.
- d. Specify the Pressure Units to display in the Tune window and the Status tab.
- e. Specify the Tune Path for Xcalibur to automatically retrieve stored tune files. Use the Browse button to quickly navigate to the folder storing your tune files. The factory default is **Xcalibur | System | GCQ | Tune**.

4. [Option Upgrade] Configure CI Gas options.

**Figure 3.** Instrument Configuration: CI Gas



- a. Click the CI Gas tab. Select the CI Gas option only if the CI option is installed.
- b. CI Gas option: Select to activate all the gas options on this tab.
- c. CI Gas Type: Select a gas type.

Select this option to activate chemical ionization gas controls. Options include: Ammonia, CO<sub>2</sub>, Isobutane, Methane, and Other. Other refers to any gas type not listed in this list. When Other is selected, the flow module is set to a pressure of 0.3–7.4 psig against a fixed flow restriction. If a specific gas is selected, the CI flow module outputs a calibrated flow for that gas in mL/min.

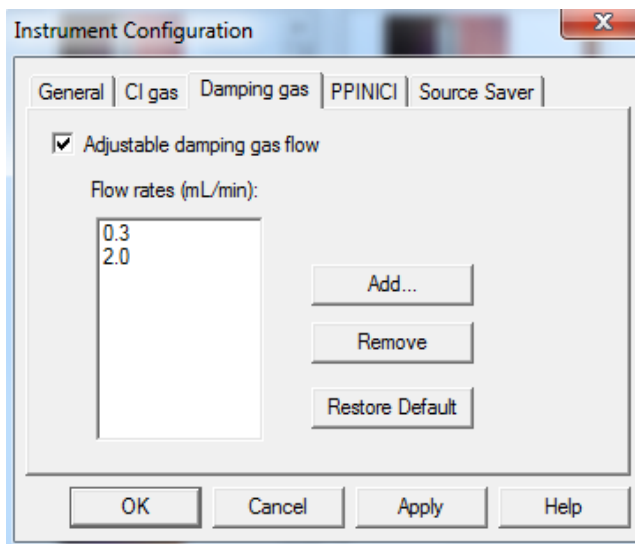
- d. Action when Software is closed and CI Gas is on: When Xcalibur software is closed, these options determine what happens if the CI gas is on. You can choose to turn it off, leave it on, or receive a prompt at the time the software is closed asking if you want to turn the CI gas off.

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. [Option Upgrade] Configure Damping Gas options. Options included on this tab display adjustable damping gas options.

**Note** If the variable damping gas option is present, you must check the Adjustable Damping Gas Flow and have at least the default value 0.3 configured. Failure to configure the installed variable damping gas option will result in unknown damping gas flow rates.

**Figure 4.** Instrument Configuration: Damping Gas



- a. Select the Damping Gas tab.
- b. Select Adjustable Damping Gas to allow the computer to control the damping gas pressure in the ion trap.

By increasing the damping gas flow rate, the damping gas pressure increases proportionally. The default flow is 0.3 mL/min, which corresponds to a pressure of approximately 0.13 Pa (1 mTorr) inside the ion trap. Increasing this flow may increase sensitivity, but at the expense of resolution. You can configure the instrument for up to six damping gas flow rates (0.3 mL/min is always one of them). You can also configure your methods to use one of these flows in Instrument setup. Before using a flow rate, Automatic Tune must be run in the Tune window for that flow.

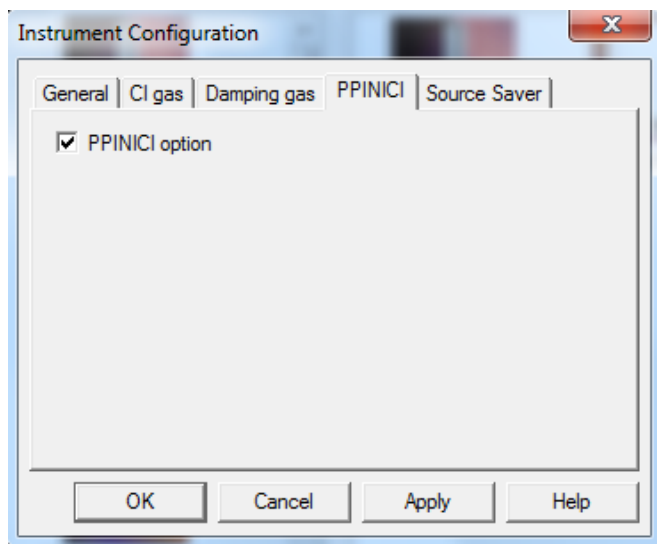
- c. Items listed in the Flow Rates (mL/min) box indicate the default damping gas flow rates. Use the Add or Remove buttons to enter up to six quantities of desired damping gas flow rates. Select the Restore Default button to restore the factory default gas flow rates.

Flow rates listed here display in the Instrument setup window and in the Tune window. Add or delete from the list of available flows between 0.3 and 5.0 mL/min. However, you cannot remove the default damping gas flow rate of 0.3 mL/min.

Once the desired number of damping gas flow rates have been selected, it will be necessary to retune the ion trap, so tune parameters can be stored for each of the selected flow rates.

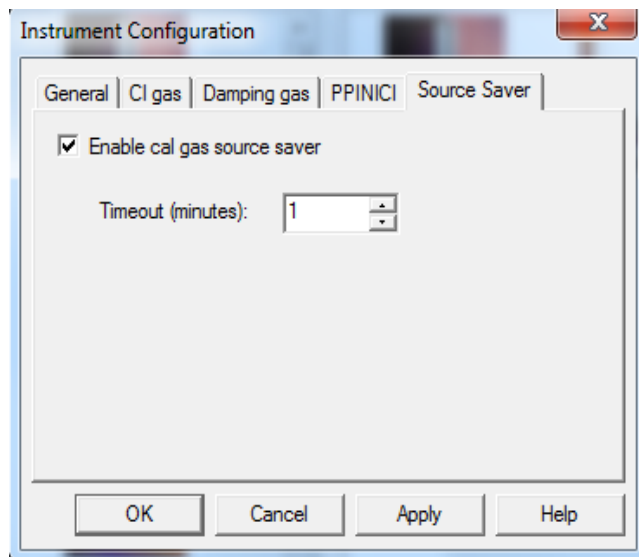
6. [Optional] Configure PPINICI options.

**Figure 5.** Instrument Configuration: PPINICI



- a. Select the PPINICI tab.
  - b. Check the PPINICI option, if you have the PPINICI option installed on your mass spectrometer.
7. Configure Source Saver options.

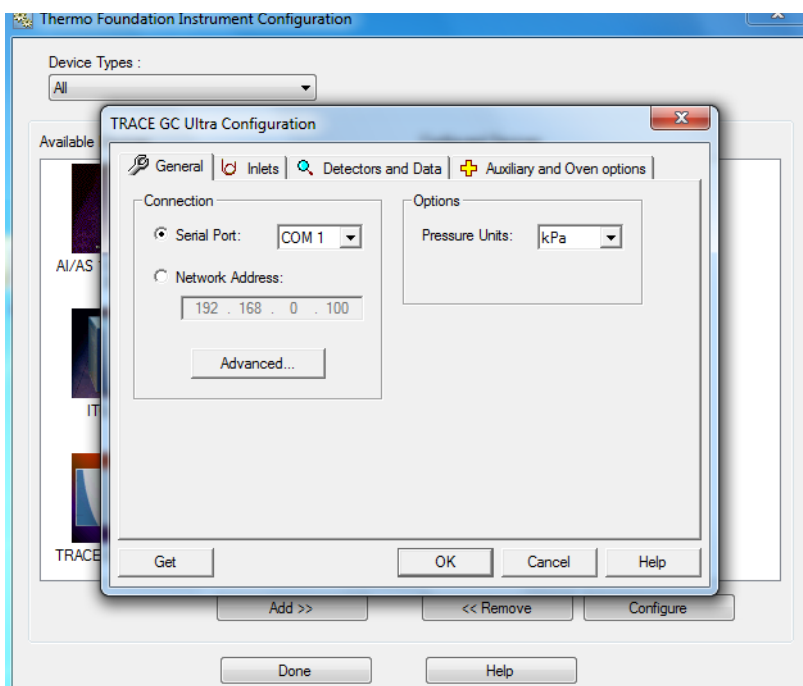
**Figure 6.** Instrument Configuration: Source Saver



- a. Select the Source Saver tab.

- b. Enable Cal Gas Source Saver: Check this option to enable the instrument to turn off the filament and cal gas if left unattended with the cal gas on. If the cal gas is not on, source saver will not turn off the filament.
  - c. Timeout (minutes): Enter the time in minutes that the instrument must wait after the last user action in tune before turning off the filament and cal gas.
  - d. Press the **OK** button to return to the Instrument Configuration window.
8. Configure the gas chromatograph (GC).

**Figure 7.** Instrument Configuration: GC



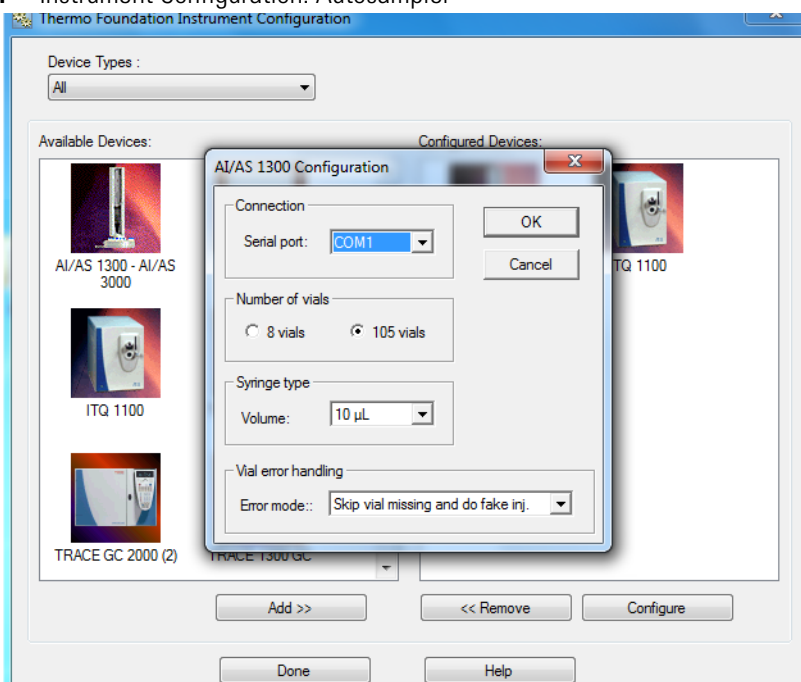
- a. Select the GC image from the Available Devices column and click **Add** to add the GC to the Configured Devices column.
  - b. Select the GC image from the Configured Devices column and click **Configure** to display the Instrument Configuration screen.
  - c. Refer to the GC user manuals to determine the best settings for your GC.
9. Make these selections on the General tab:
- a. Serial Port = COM 1. This is typically the port to which the GC is attached. Your system may be different.
  - b. Set the preferred pressure units.
  - c. Click the Get button to retrieve the GC configuration through the serial port to Xcalibur.
10. Verify the settings on the Inlet tab match the GC configuration.
11. Verify the settings on the Detectors and Data tab match the GC configuration.

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

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

13. [Optional] Configure the autosampler (AS).

**Figure 8.** Instrument Configuration: Autosampler



- a. Select the autosampler image from the Available Devices column and click **Add** to add the GC to the Configured Devices column.
  - b. Select the autosampler image from the Configured Devices column and click **Configure** to display the Instrument Configuration screen.
14. Enter autosampler parameters in the autosampler Configuration window.

**Note** The AI/AS 3000 can be connected to a COM port on the computer or through the GC. The TriPlus RSH can only be connected via LAN on the computer. See the autosampler user documentation if you want to connect to a network.

15. Set up the GC handshaking parameters by referring to the GC operation manuals for configuration instructions.

16. Check that all instruments are communicating with Xcalibur.

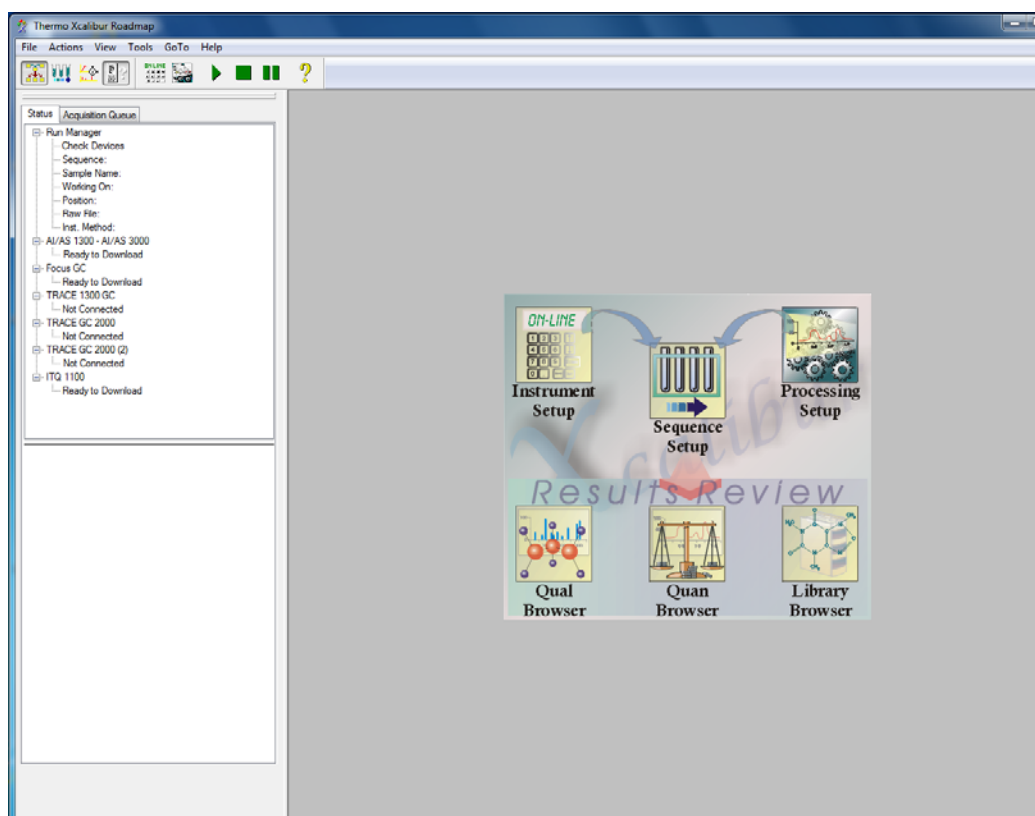


a. Click the Xcalibur shortcut to display the Xcalibur Roadmap.

**Note** The MS may take up to one minute to initialize.

b. Verify that the ITQ is listed in instrument Status as Ready to Download.

**Figure 9.** Xcalibur Roadmap



c. All instruments configured should report Ready to Download. If not, consult the troubleshooting section of the instrument’s manual.

d. Go to “[Running Your First Sample](#)” on [page 11](#) to begin running a sample.





## Running Your First Sample

After your instruments are configured for use they are ready to run samples. In just three easy steps, you'll be running your first sample using the test compound that comes with your instrument.

### Contents

- [Calibrating and Tuning the Instrument](#)
- [Setting Up Methods](#)
- [Running Methods](#)
- [Analyzing Data: Compounds with a Known Retention Time](#)
- [Analyzing Data: Compounds with a Known Ion Pattern](#)
- [Analyzing Data: Peak Height and Area](#)
- [Analyzing Data: Signal-to-Noise Ratio](#)

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

- Compounds with Known Retention Times
- Compound with Known Ion Patterns
- Peak Height and Area
- Signal-to-Noise Ratios

**Note** These instructions are written assuming you are using a TRACE GC Ultra and an AI/AS 3000. If you are using a different GC or autosampler, refer to that product's user documentation for setup instructions.

## Calibrating and Tuning the Instrument

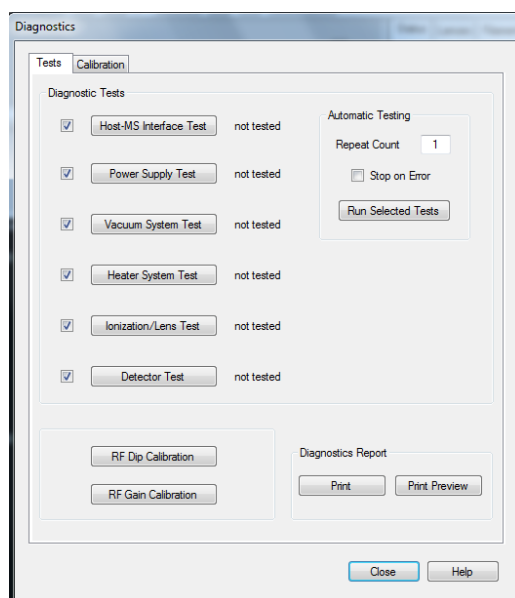
Before you run a sample, you should calibrate and tune the instrument using the *Tune* application.

1. Open the *Tune* application using one of these methods.

**Note** Select online help for Tune window information.

- Select the **Tune** button on the instrument's method editor
  - Select the *Tune* shortcut on the desktop
2. Check the instrument's basic operation by selecting **Diagnostics | Run Tests** to display the Diagnostic window.

**Figure 10.** Diagnostics Window



- a. Make sure all tests are selected.
  - b. Click the **Run selected Tests** button to run each test.
  - c. Click the **Print Diagnostics Report** button to print the results from all the tests you ran.
  - d. Click the **Close** button to close the Diagnostic window.
3. Check the last Tune report.
    - a. Select **Tune | View Tune Report** to view the last tune report and determine when the instrument was last calibrated.
    - b. Click the **Print** button and retain a hard copy for future reference, if desired.

- c. Close the Tune report and return to the Tune window.

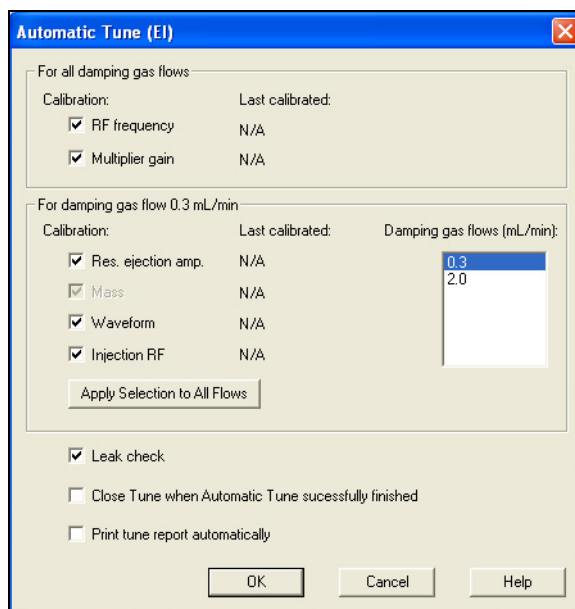
**Note** How often you tune your instrument is determined by the number and type of samples you run. See the “Automatic Tune Flow Chart” on page 66 for information.

4. [Optional] Perform a full automatic tune if you have just performed maintenance or it is required by your standard operating procedure.

It should not be 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 display the Automatic Tune window.

**Figure 11.** Automatic Tune Window: Full



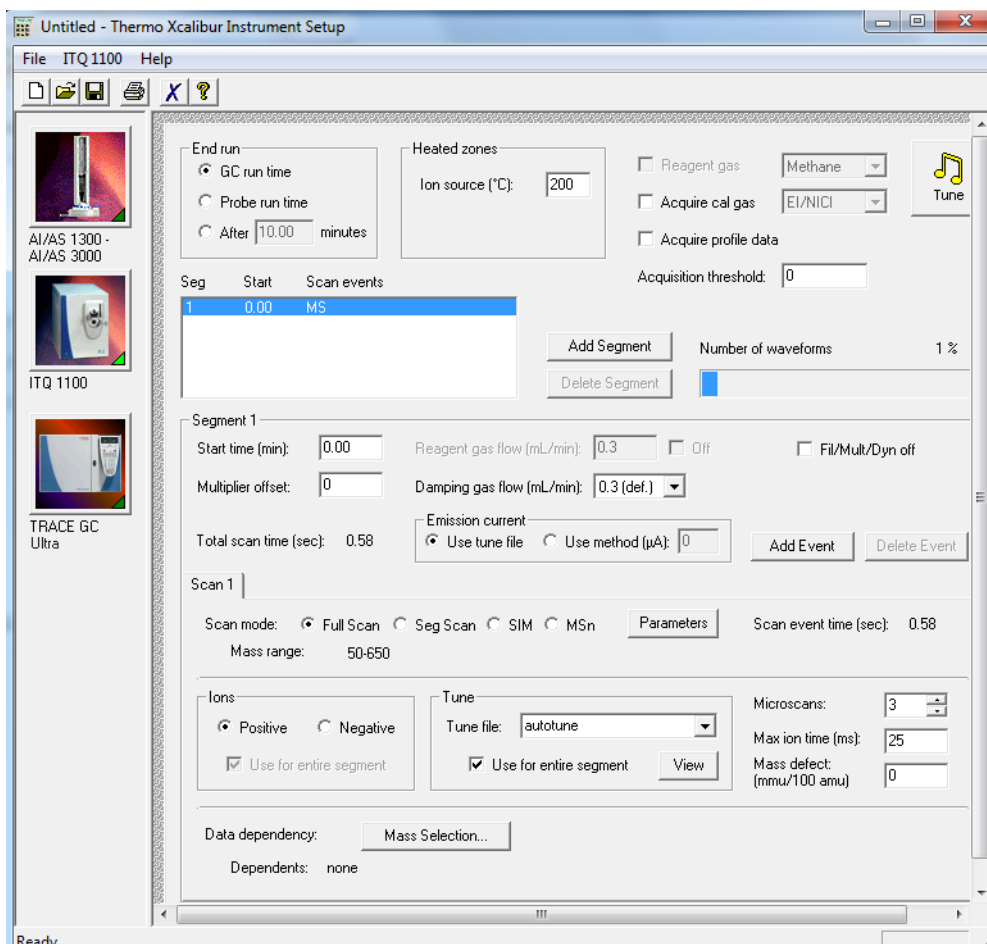
- b. Click **OK** to run the automatic tune and return to the Tune window.
- c. Select **File | Exit** to close the Tune window.

## Setting Up Methods

After your instrument is calibrated and tuned, you're ready to set up the instrument methods using Instrument setup. Instrument methods are created and modified in the Instrument setup window and saved as *\*.meth* files. Method files are stored in the *\Xcalibur\Methods* folder. In this example, you will enter the method parameters for the mass spectrometer, GC, and AS.

1. Load an instrument method.
  - a. Select Instrument Setup from the Xcalibur Roadmap to display the Instrument setup window.
  - b. Select **File | Open** and navigate to *Xcalibur\Methods*. Alternatively, navigate to the folder matching your GC instrument configuration.
  - c. Choose an existing *\*EI\_FullScan.meth*. This is the full scan method file that was used to validate that your instrument met factory specifications and then stored for you to acquire a test sample. The file is stored in *c:\Xcalibur\Methods*.
2. Review the MS method parameters by clicking the MS instrument image from the Instrument Setup window.

Figure 12. Instrument Setup: ITQ Method Editor



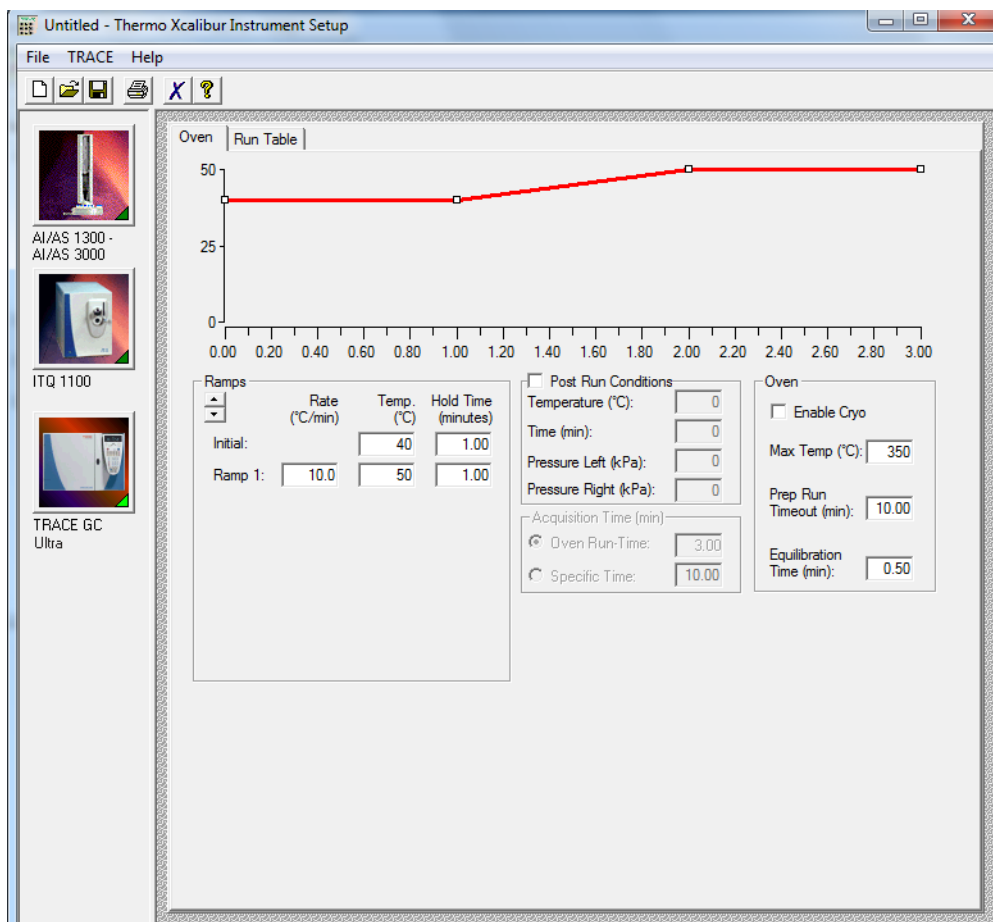
This method acquires  $m/z$  50-300. It starts 4.0 min after the GC injection to allow the solvent to elute from the GC column.

The MS run time ends when the GC run time ends. To select a different MS run time, check the After checkbox and enter the desired MS run time. Usually a shorter MS run time is selected when the GC program is allowing for column bakeout.

**Tip** It is a good idea to set the MS end run time shorter than the GC run time to preserve filament lifetime and reduce ion source contamination caused by ion burns from column bleed.

3. Review the GC method parameters by selecting the GC instrument image from the Instrument setup window.

**Figure 13.** Instrument Setup: TRACE GC Ultra Method Editor



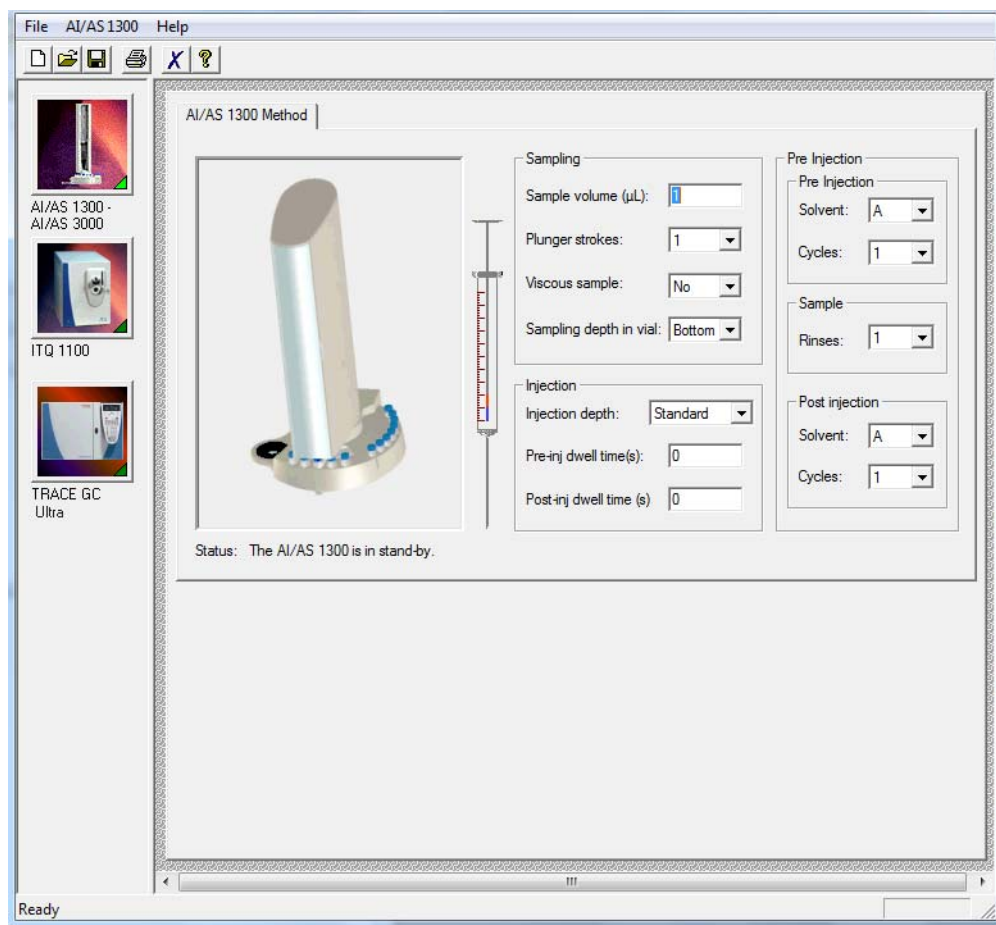
This method holds the GC at 40 °C for 1 min, ramps it at 30 °C/min to 300 °C, and holds the final temperature for ten minutes. The injector is 220 °C operated in splitless mode. The column flow is 1.0 mL/min. The transfer line temperature is 300 °C.

**IMPORTANT** Vacuum Compensation must be on whenever the MS is used as a detector.

If you have a TRACE 1300, TRACE 1310, or Focus GC instead of a TRACE GC Ultra, the instrument parameters are the same and entered into the appropriate fields in your GC user interface. See your GC user documentation for specific information.

4. [Optional] Review the AS method parameters by selecting the AS instrument image.

**Figure 14.** Instrument Setup: AI/AS 3000 Method Editor



- a. If you're using an AI/AS 3000 you can enter the parameters shown in [Figure 14](#). For other autosamplers, there are several basic settings for all autosamplers for sampling/injection and washes. All other parameters can be left at their default values.

- Sample volume: 1 µL. This is the sample volume that will be injected.
- Plunger strokes: 1. This is 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.
- Viscous sample: No. Select Yes to allow for slower pull up speeds.
- Sampling depth in vial: Two selections are available, bottom and center. If you select Bottom the needle inserts to the bottom of the vial before sample is pulled up into the syringe.

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

- b. Fill Solvent vials A and B with a suitable rinse solvent such as Methylene chloride.
5. Save the instrument method for use in the next step.

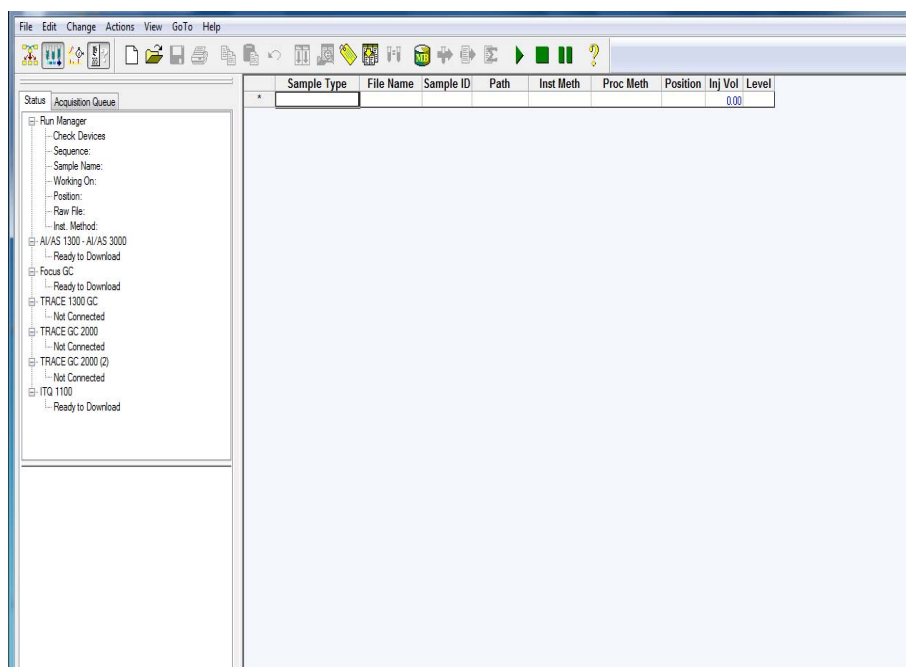
Method files have the *\*.meth* extension and are by default saved to the *Xcalibur/Methods* folder. However, you can save method files to any folder you prefer.

## Running Methods

After setting up the methods in Instrument Setup, you're ready to run the method in Sequence Setup.

1. Create a sequence to run in the Sequence Setup window to record sample details and determine how you want to acquire the data.
  - a. In Xcalibur, click the Sequence Setup icon.

**Figure 15.** Sequence Setup Window



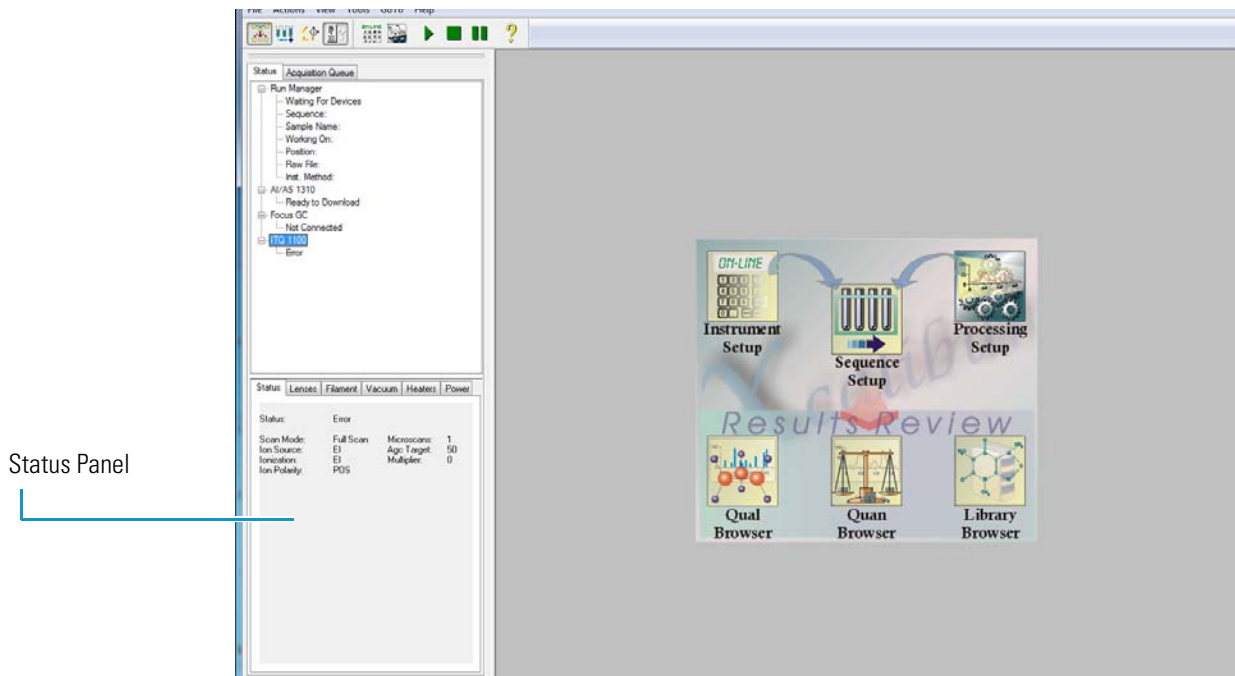
Sequence setup works just like a spreadsheet, with each row representing a single sample and each column an item of information required for a sample.

2. Change the Column Arrangement, as described in [“To change the column arrangement”](#) on [page 20](#).
3. Insert information in the first sequence row, which is described in [“To add a sequence”](#) on [page 21](#).
4. Select **File | Save** to save the sequence and enter an appropriate name, such as *Specification.sld*.



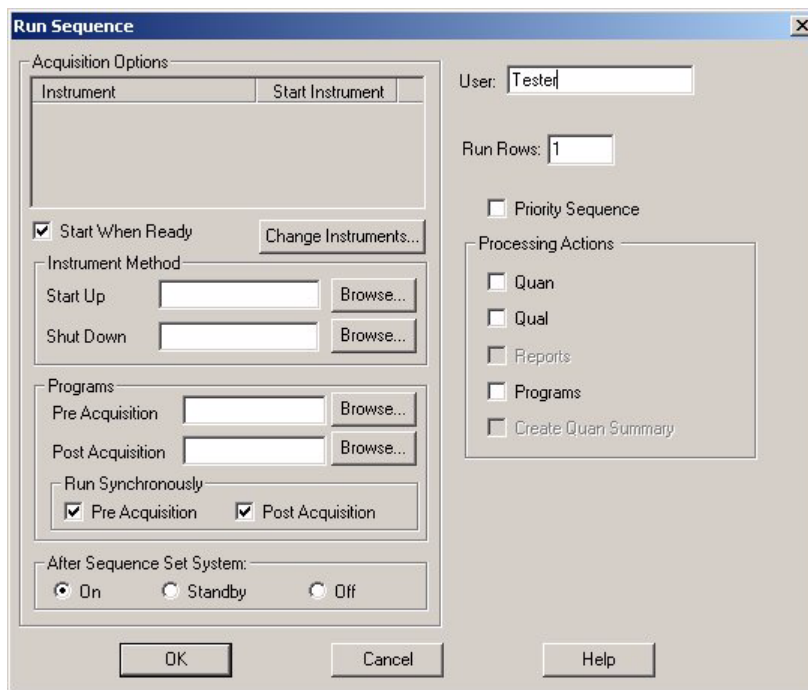
- Run the sequence by clicking on the sequence number (this highlights the row) or \* (if you did not add any rows).

**Figure 16.** Sequence Setup: Running a Sequence



- Select **Action | Run Sequence** to display the Run Sequence window.

**Figure 17.** Sequence Setup - Run Sequence Window



- Select **Start When Ready**.

8. Press the **Change Instruments** button to display the Change Instrument window. This is where you set up your instruments for an automatic injection or a manual injection.
9. Go to one of these topics: “[To perform automatic injections](#)” on page 21 or “[To perform manual injections](#)” on page 22.

❖ **To change the column arrangement**

1. Select **Change | Column Arrangement** if you want to change the displayed column labels. Some of the column descriptions are in [Table 1](#).

**Table 1.** Sequence Setup<sup>a</sup> Columns

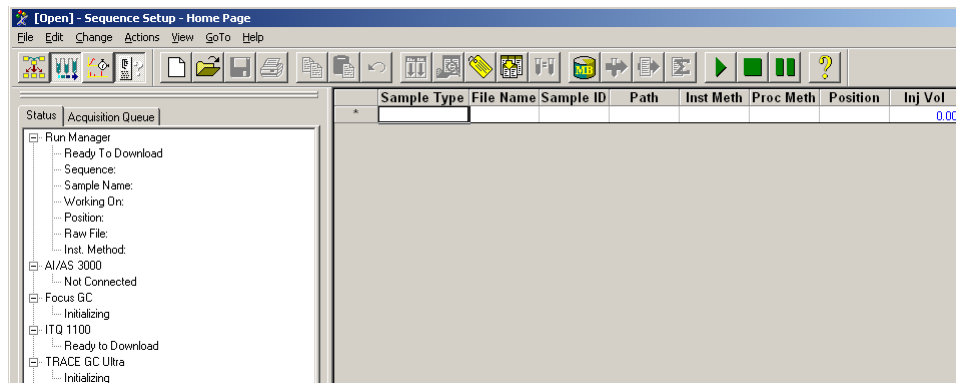
Item	Description
File Name	Name of the file where to save the sample data.
Inj Vol	Not used in this editor, but used instead in the AS method editor.
Inst Meth	The path and file name of the Instrument Method to be used for acquisition.
Path	The path to the raw file that Xcalibur creates for the sample data. Xcalibur creates this file with the extension *.raw. Double-click on this field to select a directory.
Position	The sample’s vial number. The format of the entry depends on the configured autosampler. AI/AS 3000 and TriPlus use simple integers.
Sample ID	An identifier unique to the sample. This field can also be used to import a barcode identifier.
Sample Type	Type of sample, selected from the following: <ul style="list-style-type: none"><li>• Unknown (the normal choice for qualitative analysis; all other types are only normally used for quantitative analysis)</li><li>• Blank</li><li>• QC (quality control)</li><li>• Standard Clear</li><li>• Standard Update</li><li>• Start Bracket</li><li>• End Bracket</li><li>• Standard Bracket</li></ul>

<sup>a</sup>More information about recording samples are in the online manuals.

❖ **To add a sequence**

1. Start entering information in the first blank row.

**Figure 18.** Sequence Setup: Sample Information



**Note** Press F2 on your computer to edit text already in a cell. Press F2 two times to see an edit dialog box.

2. Click in the File Name field and enter sample information, such as *Data01*.
3. Select a \*.*meth* file.

Click in the Inst Meth field and right-click in the field to display the drop-down menu, choose **Browse** to select an existing meth file to use for existing sample information.

❖ **To insert another row**

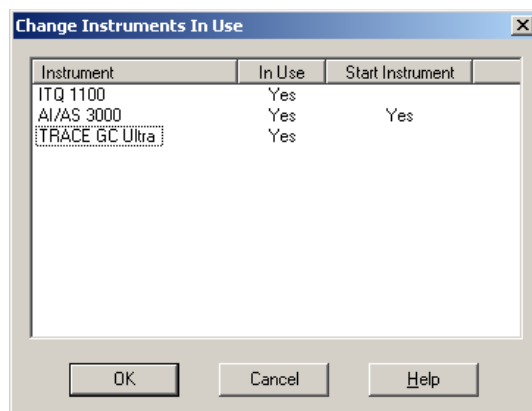
1. To insert a row within a list of samples you have already entered, right-click anywhere in the row below the row where you want to insert the new sample.
2. Choose **Edit | Insert Row** to open the Insert Row window.
3. Select **Yes** and return to the Sequence Setup window.

❖ **To perform automatic injections**

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

1. Configure the Change Instruments In Use window for automatic injections.
  - a. Select a sequence row and select the sample type.
  - b. Select **Actions | Run Sequence** to open the Run Sequence window.
  - c. Click the **Change Instruments** button to open the Change Instruments In Use window.

**Figure 19.** Sequence Setup: Change Instruments In Use (Automatic Injections)



- d. Make *Yes* display for each instrument (AS, GC, MS) listed in the In Use fields (Figure 19). However, if *Yes* is not listed, then click on the blank field to toggle *Yes* on.
  - e. Toggle *Yes* to display in the Start Instrument field for the AS. This makes the autosampler start as soon as all devices are ready.
  - f. Select **OK** to return to the Run Sequence window.
2. Prepare the injection.
    - a. Open and transfer the highest concentration test mixture.
    - b. Load the sample vial into position 1 of the autosampler.
  3. Start the run by clicking **OK** in the Run Sequence window (Figure 17).

#### ❖ To perform manual injections

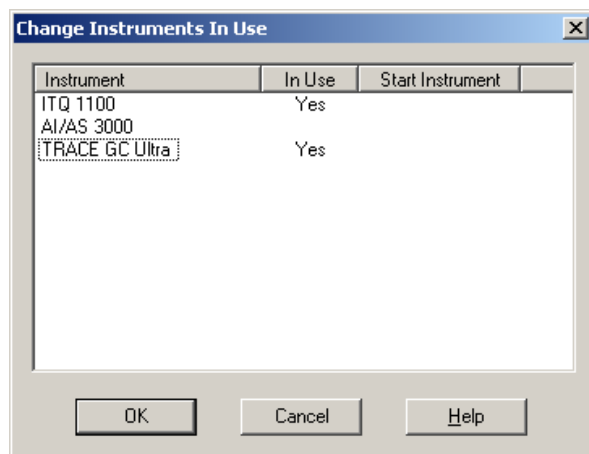
Manual injections are necessary for those not having or using an autosampler to run this method. Basically, make sure that the GC and MS listed in the In Use field do not read *Yes* in the Start Instrument field. If you do not want to use an instrument for the current sequence, click on the In Use *Yes* entry to change it to a blank space. Instruments with an In Use blank space are not available for the current sequence.

For example, if a sample is manually injected by a syringe into the GC/MS, the In Use entries for all instruments, except the GC/MS, must be a blank space.

All instruments used for the sequence submitted for processing, must display *Yes* in the In Use column.

1. Configure the Change Instruments In Use window for manual injections.
  - a. Select a sequence row and select the sample type.
  - b. Select **Actions | Run Sequence** to open the Run Sequence window.
  - c. Click the **Change Instruments** button to open the Change Instruments In Use window.

**Figure 20.** Sequence Setup: Change Instruments In Use Screen (Manual Injections)





- d. Toggle *Yes* to display in the In Use fields, for both the GC and MS. However, if *Yes* is not listed, then click on the blank field to toggle *Yes* on.
  - e. Make sure the GC and MS instruments start Instrument fields are empty (Figure 20). The operator or person making the injection will start the instrument.
  - f. Make sure the AS (if listed) does not say *Yes* in both the In Use and Start Instrument fields.
  - g. Select **OK** to return to the Run Sequence window.
2. Open the test compound that is in the GC/MS test kit.
  3. Select **OK** in the Run Sequence window (Figure 17) to start the run and return to the Sequence Setup window.
  4. Monitor the status View located in the Sequence Setup window until the instrument is “Waiting for Contact Closure.
  5. Prepare the injection.
    - a. Draw 1  $\mu\text{L}$  of the test compound into the supplied syringe. Be sure there are no bubbles in the syringe.
    - b. Draw in 1  $\mu\text{L}$  of air.
  6. Make the injection and start the GC.
    - a. Carefully, insert the needle into the injector port.
    - b. Wait three seconds and push the plunger.
    - c. Quickly, press the Start button located on the GC.
    - d. Remove the syringe.
  7. Watch the data while the sequence is running.

This is a good time to watch the data by selecting from one of the two views:

## 2 Running Your First Sample

Analyzing Data: Compounds with a Known Retention Time

- 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 Instrument Status** tab to view the list of the samples you have selected to run. Green items indicate the sequence is running.
8. Click the **Roadmap** button  to return to the Xcalibur Roadmap.
  9. Now you're ready to analyze your data. However, you'll need a thorough understanding of cursor actions, which are described in "Reviewing Cursor Actions in Browsers" on page 70.

### ❖ To analyze data

Go to any of the following topics:

- "Analyzing Data: Compounds with a Known Retention Time" on page 24
- "Analyzing Data: Compounds with a Known Ion Pattern" on page 32
- "Analyzing Data: Peak Height and Area" on page 35
- "Analyzing Data: Signal-to-Noise Ratio" on page 37

## Analyzing Data: Compounds with a Known Retention Time

When you're ready to analyze your data, use the Xcalibur browsers (Qual, Quan, and Library) to view the data file results.

**Note** See the online manuals for more detailed instruction.

Using Qual Browser you can answer the question, "Does this sample contain compound 'X'?" X being the test compound you used in the previous topic. Then we will determine the peak height, area, and signal-to-noise ratio.

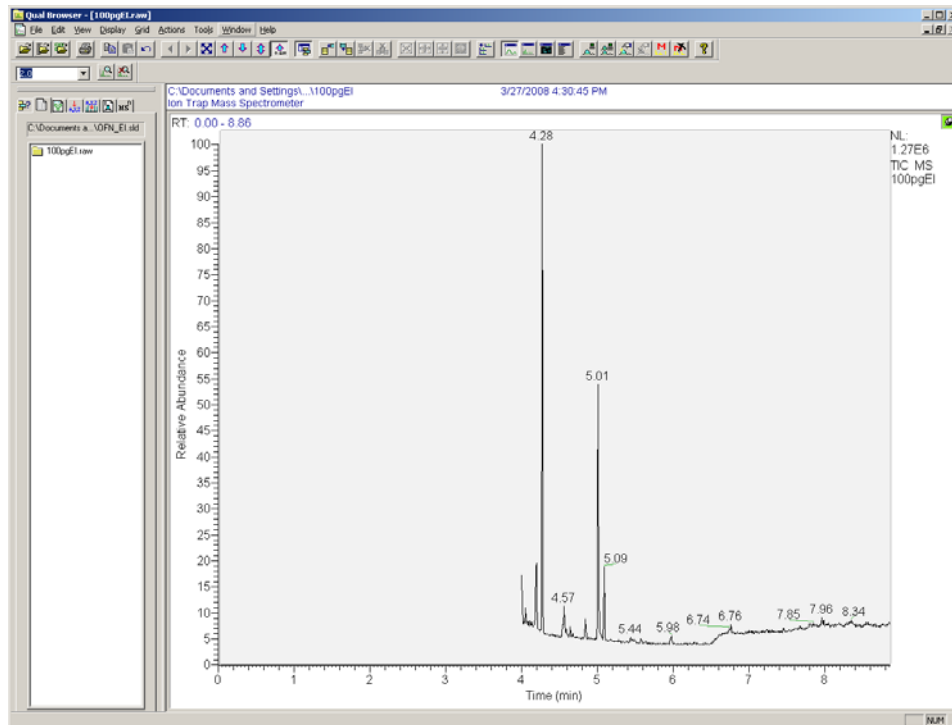
In this example, we used the `\Xcalibur\Data\Factory Test Data\100pgEI.raw` file, but you can use any `.raw` file. Preferably, use the one you just acquired in [Step 6, Make the injection and start the GC.](#), on page 23. If you did not acquire this sample, you can use the sample file located in `Xcalibur\Data\Factory Test Data\ 100pgEI.raw` or any `*EI.raw`.

Let's assume that you have previously carried out a GC run with a pure sample of the compound you are interested in, compound 'X', and consequently you know the retention time.

1. Open Qual Browser and select the `*.raw` file that contains the data for the sample you want to work on.
  - a. Select Qual Browser from the Roadmap.

- b. Choose **File | Open** and navigate to *Xcalibur\Data\Factory Test Data* to open the sample file *100pgEI.raw* or a \*.raw file containing the data you're interested in.

**Figure 21.** Qual Browser: 100pgEI.raw



Don't be surprised if the Qual Browser window looks different than [Figure 21](#). This is because 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 5 minutes, look at the mass spectrum recorded at that time in the chromatogram.

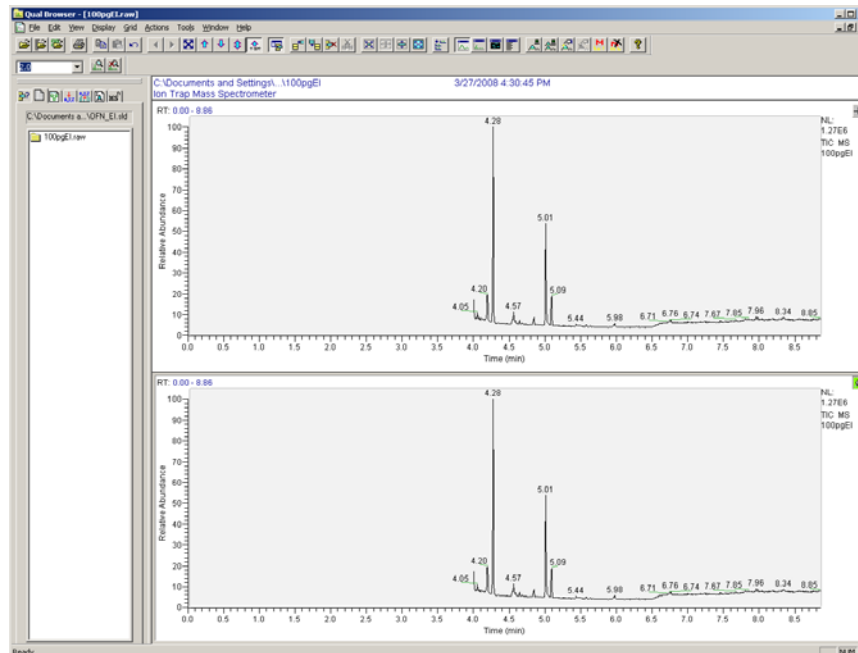
- a. Anchor your cursor in the chromatogram.

## 2 Running Your First Sample

Analyzing Data: Compounds with a Known Retention Time

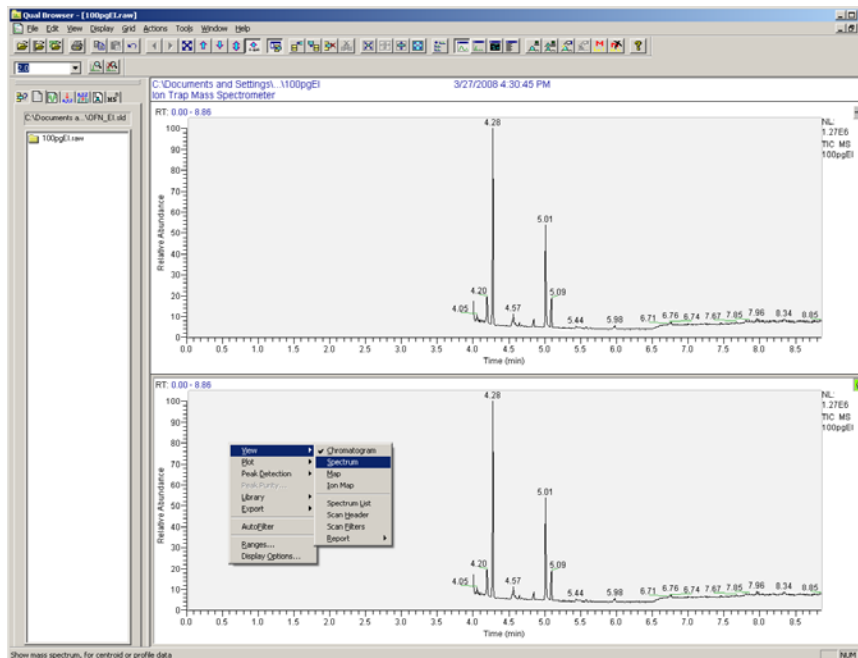
- b. Click the **Insert Cell** button  to open a new cell containing the same information as the existing cell.

**Figure 22.** Qual Browser: Displaying two chromatograms



- c. Select the lower cell by clicking on the pin icon in the upper right corner of the window.

**Figure 23.** Qual Browser: Chromatogram drop-down menu





- d. Choose **View | Spectrum** from this menu 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 vs.  $m/z$  that is a mass spectrum. Initially, you'll see the first mass spectrum.

3. Zoom in on the time period of interest.

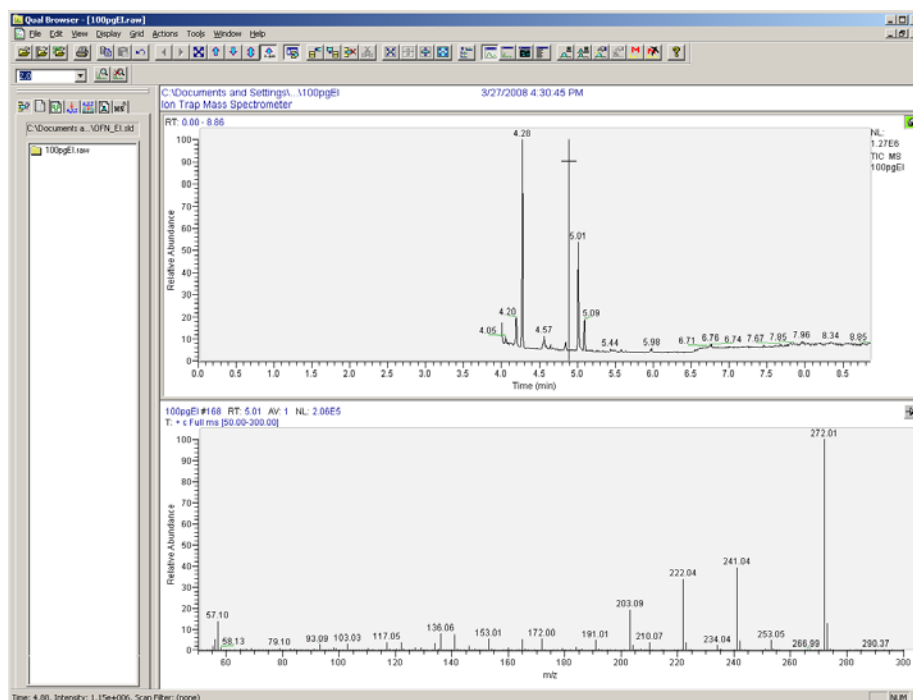
Although the full TIC chromatogram is currently displayed in the upper cell, only the retention time around three or four minutes is of particular interest. Therefore, zoom in on that part of the chromatogram and view it in more detail.

There are two ways of doing this; using mouse functions or using range functions.

#### ❖ To use mouse functions

1. Click the pin icon that is located in the top right corner of a chromatogram cell, so it is green (pinned).

**Figure 24.** Qual Browser: Chromatogram using Mouse



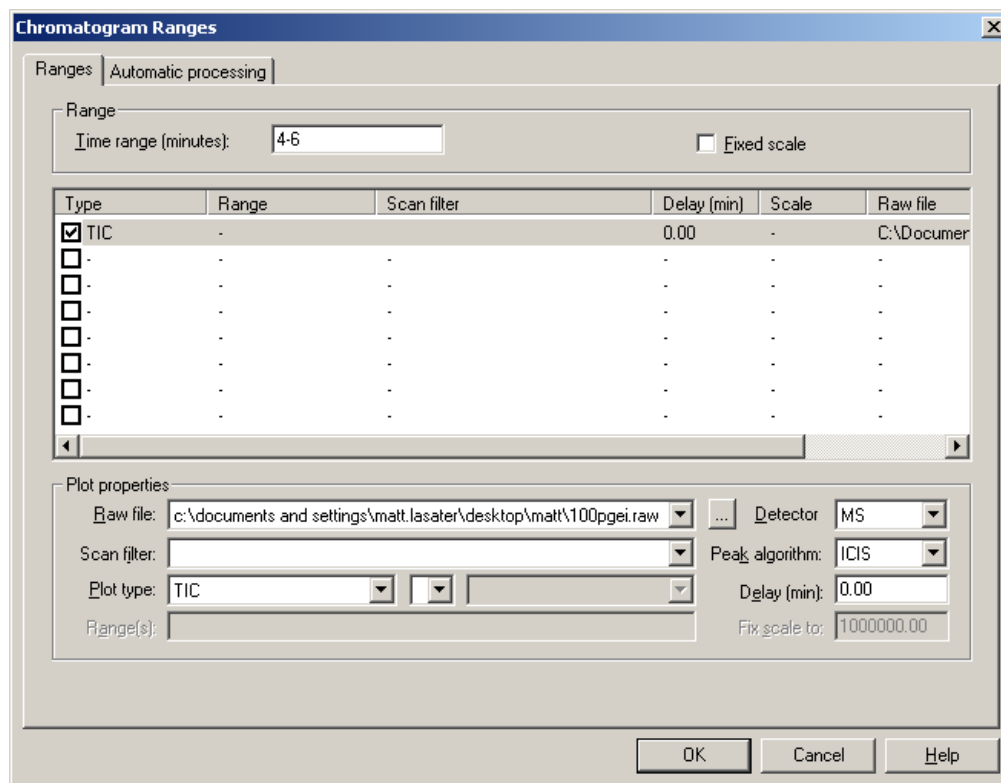
2. Position the cursor at the starting time you are interested in, at a position close to or on the baseline.
3. Click and drag the cursor parallel to the time axis to the end of the period required.

Notice that a line is drawn on the screen as you do this. As the cell redisplay, notice that only part of the chromatogram within the line you have just drawn.

## ❖ To use range functions



1. Right-click on the chromatogram to display the context-sensitive menu and choose Ranges to display the Chromatogram Ranges window.
2. Enter the time range of interest in the Time Range field such as 4 to 6 minutes.

Figure 25. Qual Browser: Chromatogram Ranges



3. 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 icon shown in the top right corner of the mass spectrum cell and click on it. The icon 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 desired 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 therefore be made up of mass peaks resulting from the sample compound plus mass peaks resulting from background contamination. Therefore, 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. Choose **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 will usually 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 drawn on the screen as you do this.

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 at  $m/z$  207, and 281. The removal of 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.

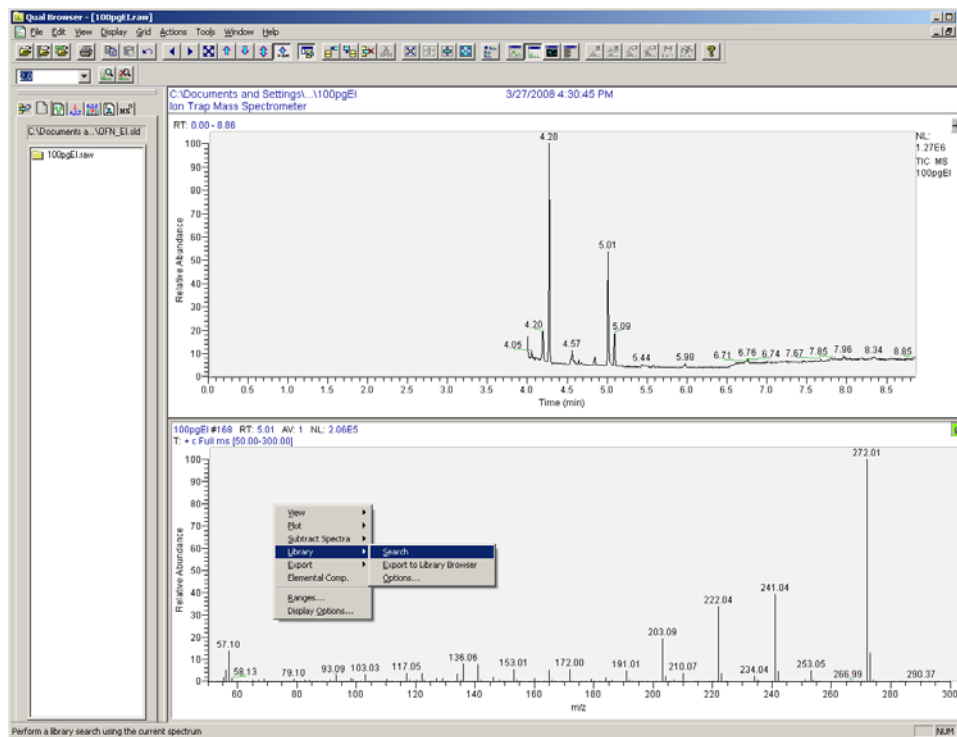
**Note** Right-mouse click in a window to view pull-down menus.

## 2 Running Your First Sample

Analyzing Data: Compounds with a Known Retention Time

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

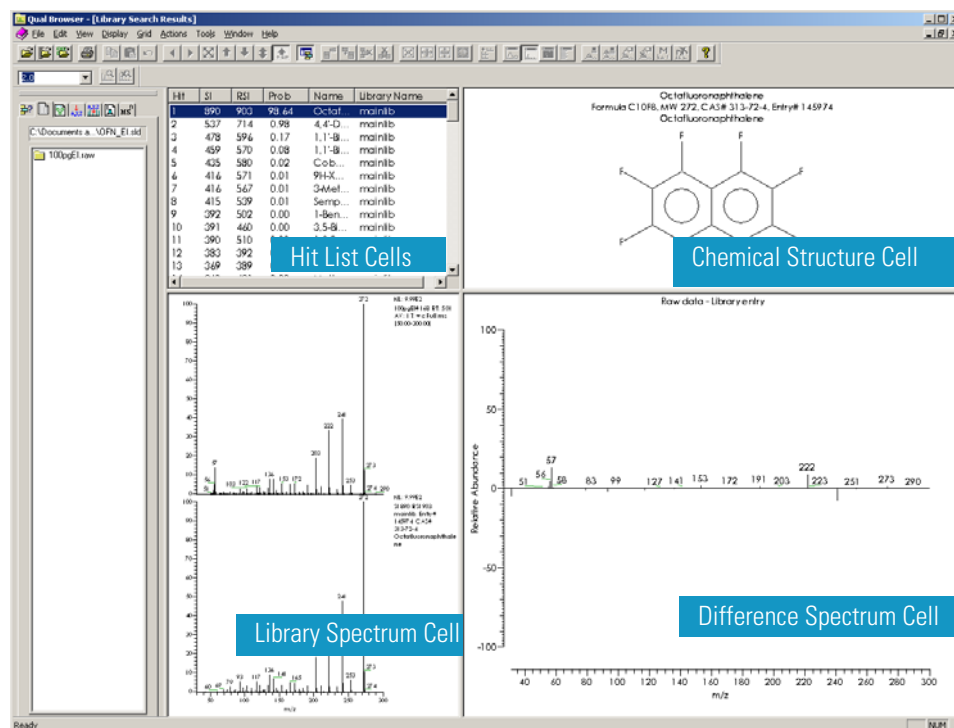
**Figure 26.** Qual Browser: Library Search Menu



- b. If you have the optional NIST library installed, look in the Hit List Cell for the most likely compounds in decreasing order of match probability.

If the test compound is not one of the top hits, you may only have the demonstration library loaded. The full NIST library is an option. Check which libraries are available for search by selecting the Library Options pull-down menu.

**Figure 27.** Qual Browser: Library Search Results





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

## Analyzing Data: Compounds with a Known Ion Pattern

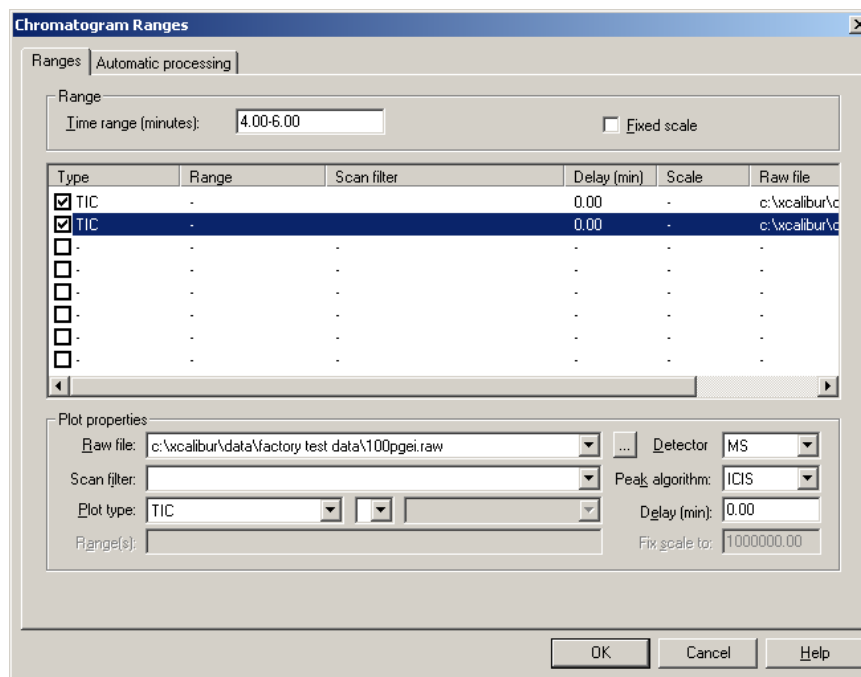
Using Qual Browser you can answer the question, “Does this sample contain compound ‘x’? X being the test compound you used in the “Running Methods” on page 18. Then we will determine the peak height, area, and signal-to-noise ratio.

In this example, we used the *Xcalibur\Data\100pgEI.raw* file you just acquired in [Step 6, Make the injection and start the GC.](#), on [page 23](#).

In this example, let’s assume that you already have some knowledge of the mass spectrum of the compound of interest, compound 'X', and consequently 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 therefore this ion represents a “marker” for the compound.

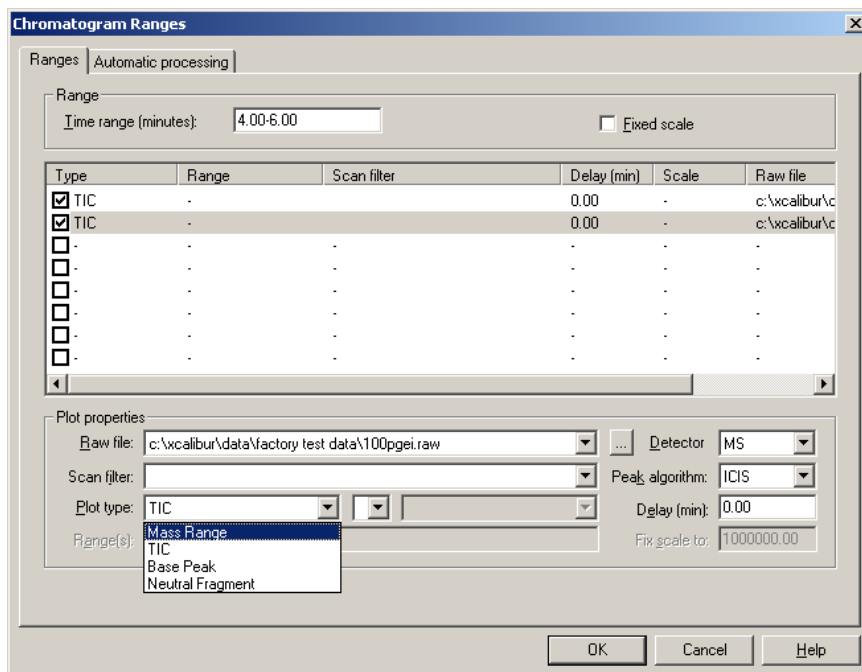
1. Open Qual Browser.
  - a. Set up the cells so you have only one cell: a chromatogram. Pin the cell and then select **Grid | Delete Row** from the menu. You can also anchor the cursor in the cell you wish to delete and click the  icon.
  - b. Reset the time range to the full range by selecting Zoom Reset  from the toolbar.
2. Add a mass range chromatogram.
  - a. Select the chromatogram cell and then right-click your mouse to display the context sensitive menu.
  - b. Select **Ranges** to open the Chromatogram Ranges window.

**Figure 28.** Qual Browser: Opening the Chromatogram Ranges Window



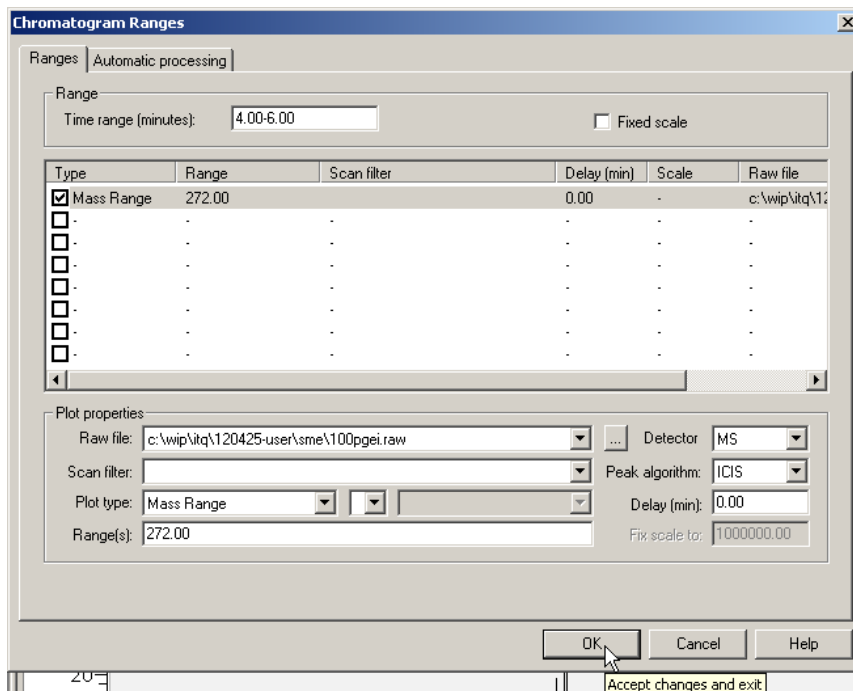
- c. Add another plot by clicking the checkbox located in the Type column.
- d. Select **Mass Range** from the Plot Type field.

**Figure 29.** Qual Browser: Selecting Mass Range



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

**Figure 30.** Qual Browser: Entering a Mass Range

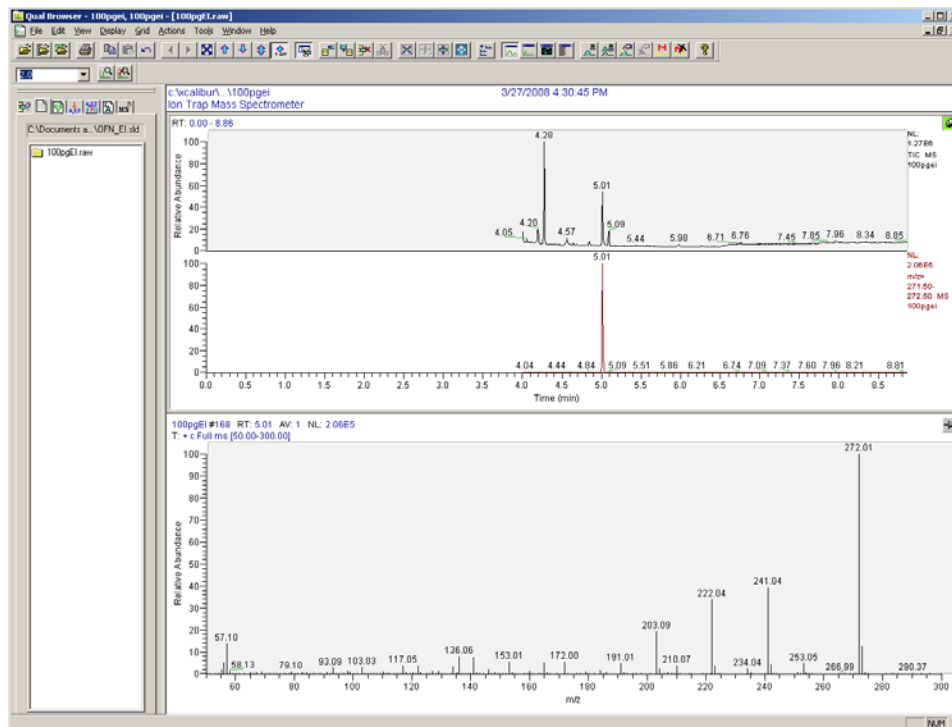


## 2 Running Your First Sample

Analyzing Data: Compounds with a Known Ion Pattern

- 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 31.** Qual Browser: Displaying a Mass TIC and Mass Range Chromatogram



The result in this example shows that the peak at retention time 5.01 minutes is of particular interest because it includes  $m/z$  272, the molecular ion from the test compound.

3. View the mass spectrum.

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

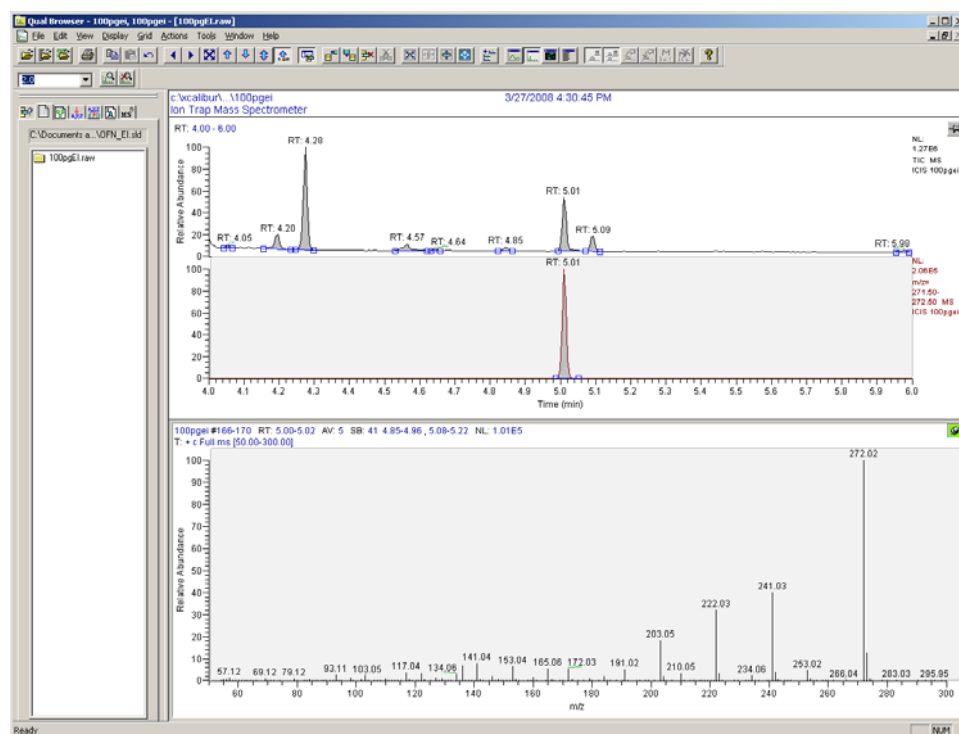


## Analyzing Data: Peak Height and Area

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 an important feature of quantitation.

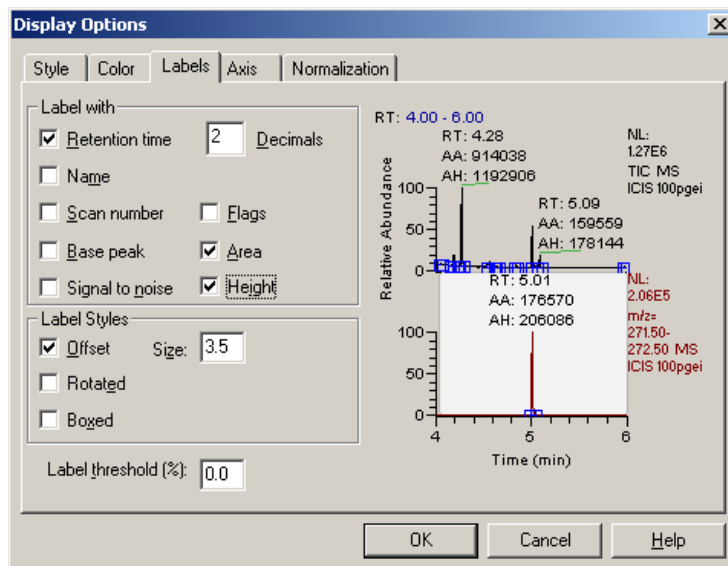
1. Open Qual Browser to open a \*.raw file that you stored from the Sequence Setup window.
2. Zoom in on the part of the chromatogram that is of particular interest.
  - a. Right-click on the chromatogram and choose **Peak Detection | Toggle Detection in All Plots** from the menu. Individual peaks are shaded and the extent of each peak is shown in blocks on the baseline.

Figure 32. Qual Browser: Peak Detection



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

**Figure 33.** Qual Browser: Display Options | Labels



- c. Click the **Labels** tab.
- d. Select both the **Area** and **Height** checkboxes.
- e. Click **OK** to return to the chromatogram.

## Analyzing Data: Signal-to-Noise Ratio

Determine if you want to use Qual Browser or the Signal-to-Noise Test to determine the peak's signal-to-noise ratio. The signal-to-noise ratio is a good measure of the performance of the system because it defines the smallest amounts of compound that can be detected and quantified. If the signal-to-noise ratio is low, true peaks (signals) resulting from the presence of very small amounts of material can be lost in the background noise.

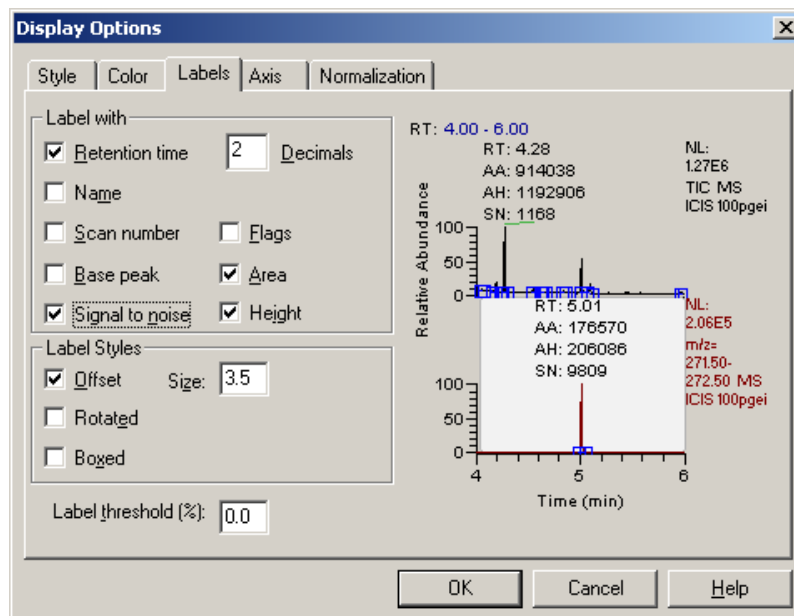
Low signal-to-noise ratios can result from:

- Poor column quality
- A dirty ion source
- Poor quality carrier gas
- Inadequate sample cleanup (extraction)
- Poor chromatography techniques

### ❖ To use Qual Browser to determine 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. Choose **Display Options** to open the Display Options window.

**Figure 34.** Qual Browser: Display Options | Labels | Signal-to-Noise



- c. Click the **Labels** tab.
- d. Select the **Signal-to-Noise** checkbox.

## 2 Running Your First Sample

### Analyzing Data: Signal-to-Noise Ratio

- e. Click **OK** to return to the chromatogram.
2. Choose the baseline noise range.
3. Click the **Peak Detection Settings** tab located in the Info bar.
4. Pin the chromatogram cell by clicking in the top right corner.
5. Click on the chromatogram plot on which you wish to measure the signal-to-noise. It will turn gray.
6. Check the **Manual Noise Region** in the Info bar.
7. Enter a noise range near the peak. Avoid choosing a region with a peak in it.
8. Click **Apply** to display the RMS (root mean square) signal-to-noise calculation.
9. Look for a red line in the chromatogram to view the noise range you chose.

#### ❖ To use the Signal-to-Noise Test

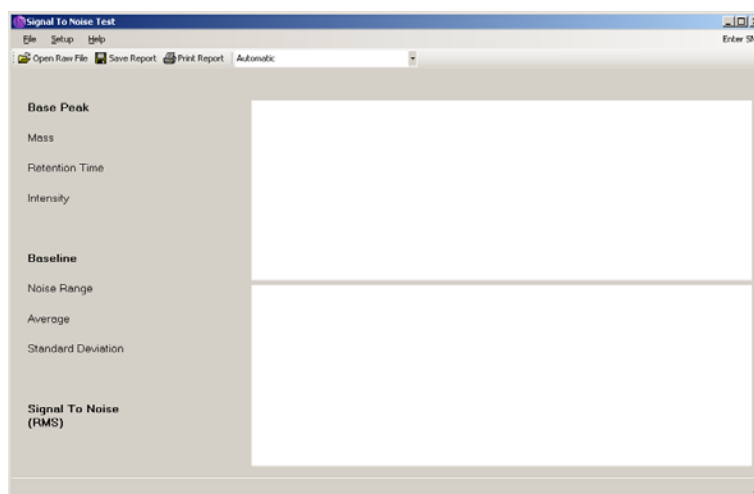
1. Use the Signal-to-Noise Test, which is provided with all versions of Xcalibur.

A shortcut for the Signal-to-Noise Test is located on the desktop. The Signal-to-Noise Test may also be added to the Tools menu of the Xcalibur Roadmap. Select **Tools | Add Tools** and specify the program location as *C:\Program Files\Thermo\Signal To Noise Test 1.1\SignalToNoiseTest.exe*.

2. Run the Signal-to-Noise Test by double-clicking the shortcut located on the desktop to open the Signal to Noise Test window.

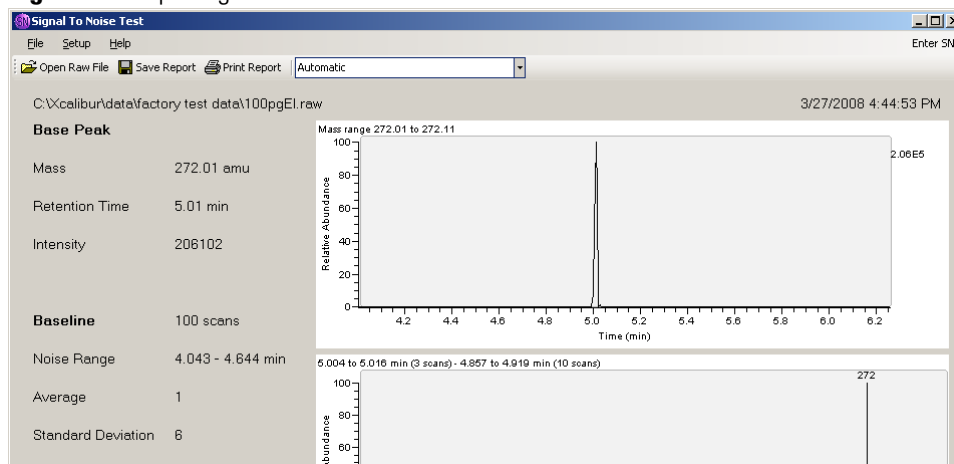
You can also run it from *C:\Program Files\Thermo\Signal To Noise Test 1.1\SignalToNoiseTest.exe* if the icon is not available.

**Figure 35.** Opening the Signal-to-Noise Test Window



- a. Select **File | Open Raw File** and select the *100pgEI.raw* file or the data file of interest. Xcalibur begins processing the file upon opening.

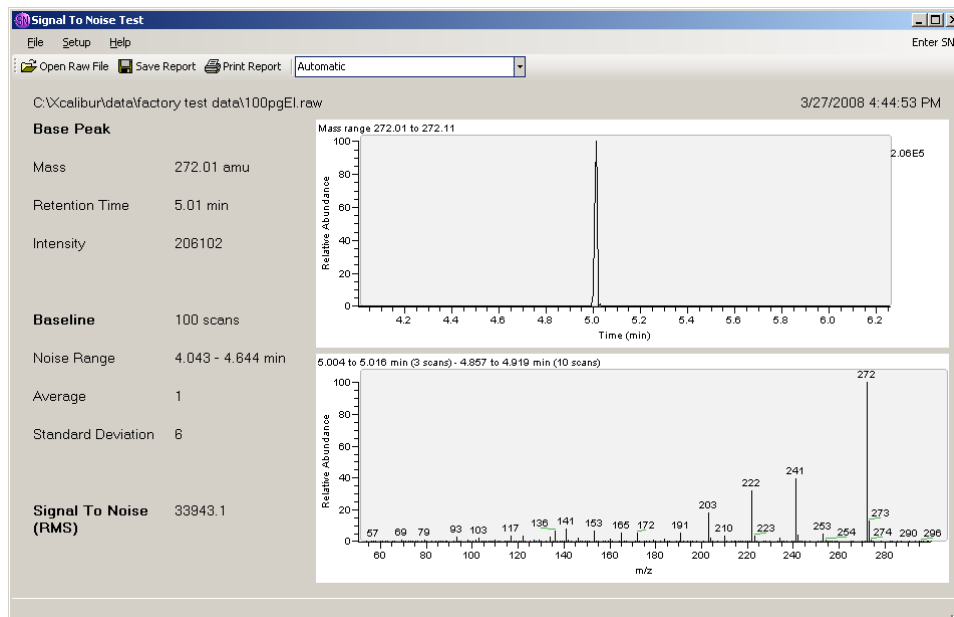
**Figure 36.** Opening a Raw File



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

- b. Select **Custom** from the list box. In the custom mode, you may choose the mass and the retention time to use.

**Figure 37.** Using Custom Mode



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

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

## **2 Running Your First Sample**

Analyzing Data: Signal-to-Noise Ratio

## Using the Options

This chapter discusses the Ion Trap Series options and how best to use them.

### Contents

- MSn Scan Mode
- Chemical Ionization (CI Mode) Options
- ACE Options
- DDS Options
- PQD Options
- Variable Damping Gas Option

**Table 2.** Ion Trap Series Options<sup>a</sup> for ITQ Instruments

Options	ITQ 700 Series	ITQ 900 Series	ITQ 1100 Series
Mass Ranges	10-700 amu	10-900 amu	10-1100 amu
MSn Scan Mode	*	*	standard
ACE (Automatic Collision Energy)	*	*	standard
DDS (Data Dependency Scanning)	*	*	standard
PQD (Pulsed Q Dissociation)	*	*	standard
Chemical Ionization (CI Mode)	*	*	*
Probe System (DIP/DEP)	*	*	*
Variable Damping Gas	*	*	*

<sup>a</sup>Available as an upgrade option. Ask your dealer for the upgrade.

## MSn Scan Mode

MSn is a term used synonymously with the terms MS/MS, MSMS, and MS/MS/MS. Multiple stages (MSn) of mass spectrometry are the core strength of an ion trap instrument. In the ion trap, the initial capture of the ions is called the first MS stage. In an MS/MS experiment, this initial population of ions is reduced to a precursor ion, which is then excited and fragmented through collision-induced dissociation (CID). This isolation and fragmentation is the second stage of MS. An MS/MS/MS experiment would be the same as an MS/MS experiment, but with the isolation and subsequent fragmentation of one of the fragments from the second MS stage. The ion trap can perform a maximum of five MS stages.

Each isolation and fragmentation stage makes it increasingly easier to separate a compound away from the background matrix because the probability that the matrix shares a mass and also fragments in the same way as the analyte is very small. Even if the matrix interferes after one stage of isolation and fragmentation, another stage is usually enough to isolate the analyte signal from the background. The superb selectivity of the MSn technique is very useful for quantitation in a heavy matrix. Detection and quantitation of sub-picogram levels of target compounds in matrices, such as milk, tissues, soils, and sludges, has been achieved. MSn may also be used for structural elucidation and other research techniques. This powerful tool comes standard on the ITQ 1100 system and is an available option for the ITQ 700 and ITQ 900 instruments.

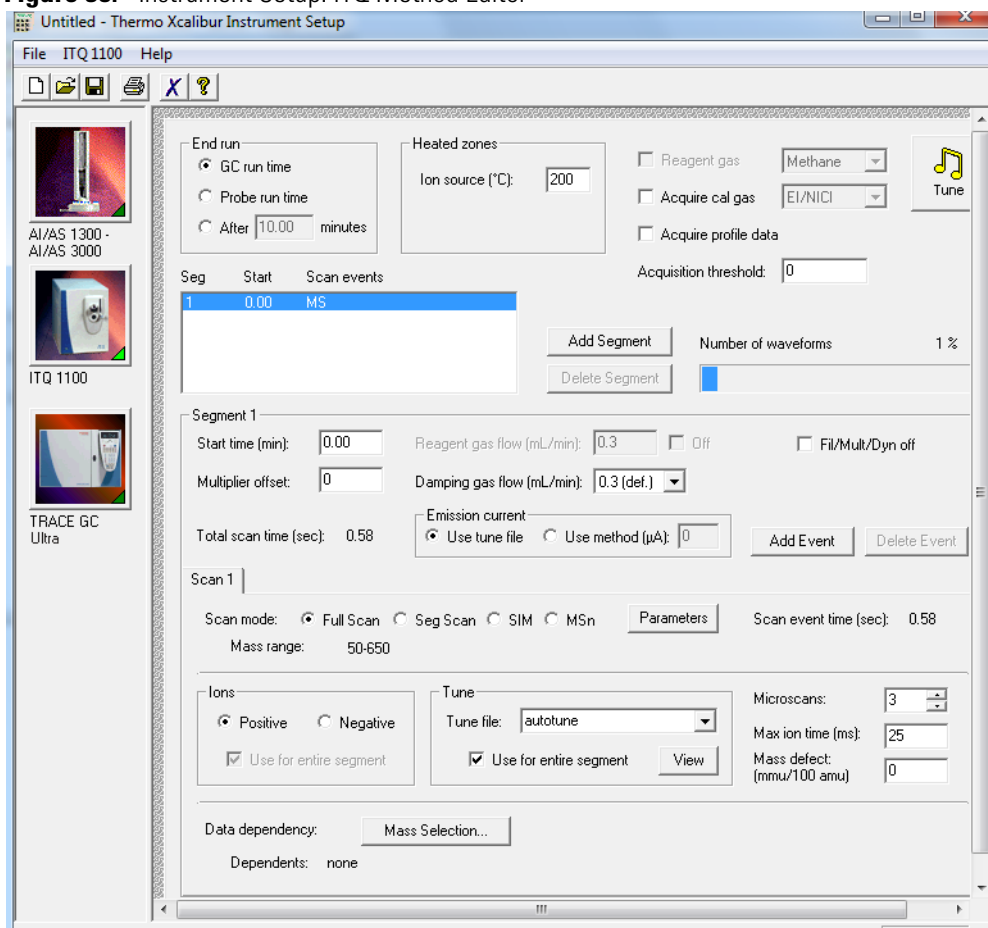
To activate ACE, DDS, and PQD options, set the method to MSn scan mode and click the **Parameters** button to set the parameters in the MSn Parameters window.



❖ To run an MSn method

1. Select Instrument Setup from the Xcalibur Home Page to display the Instrument Setup window.
2. Click the mass spectrometer icon to display the mass spectrometer method editor.

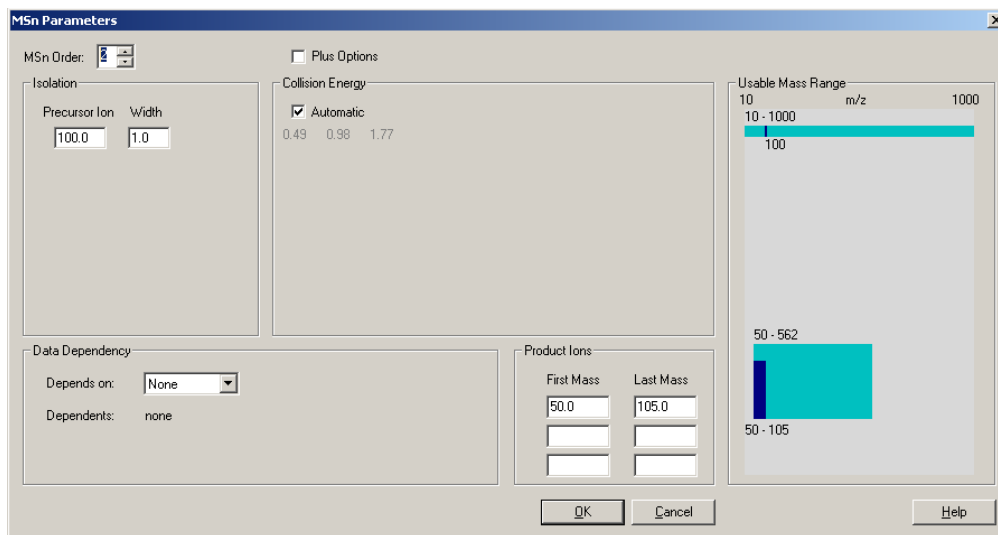
Figure 38. Instrument Setup: ITQ Method Editor



3. Set the scan mode to *MSn*.

4. Click the **Parameters** button to open the MSn Parameters window and configure the parameters needed to run the MSn experiment.

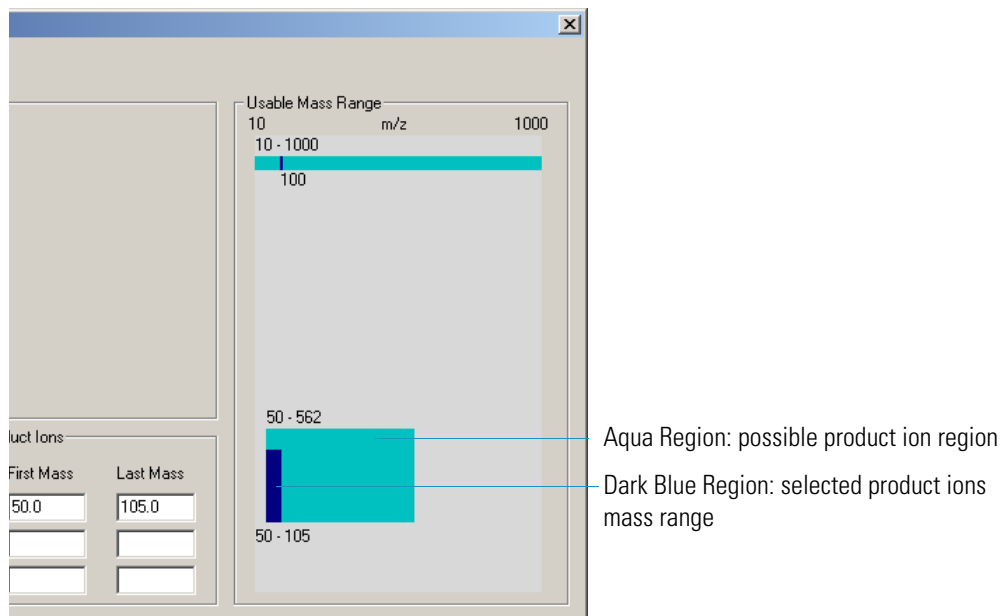
**Figure 39.** Opening the MSn Parameters Window



- a. Select an MSn order by setting the order of the MSn experiment to 2 if you are running an MS/MS experiment or 3 if you are running an MS/MS/MS experiment. Each additional stage of MS increases the MSn order by one. For each MS stage, you must specify the mass of the precursor in the isolation. In this example, the precursor ion is mass 100 and will be isolated to a 1 amu width. So, ions with a mass between 99.5 and 100.5 will stay in the trap and all other ions will be ejected during isolation.
  - b. Set the Collision Energy parameters. Specify the collision energy or select the **Automatic** checkbox to have the software automatically estimate the collision energy. To maintain full control over the collision energy, deselect the **Automatic** checkbox and enter a collision energy value. The three-grayed out collision energy values displayed in [Figure 39](#) are the values that the automated collision energy uses. If you are using PQD, there will only be one collision energy value displayed. You can generally get the highest fragmentation efficiencies using an experimentally determined value for the collision energy. However, determining the best collision energy can be time consuming, requiring multiple injections and manual examination of the data. The value that is estimated automatically may be sufficient for analysis.
5. Set the Product Ions parameters by entering the product ions' first and last mass range. In GC/MS, the product mass-to-charge ratio is nearly always less than the precursor mass. As a result, the last mass of the product ion range should rarely be a few amu above the precursor. The first mass should be as low as necessary to capture the product ions.

In [Figure 39](#), the first mass is 50 and the last mass is 105. Narrower mass ranges result in faster scan speeds. So, if your product ions are far apart in mass and you need faster scanning, try using several narrow product ion ranges instead of one contiguous wide one. The possible product ion mass range is graphically represented by the larger aqua colored region surrounding the dark blue product ions bar (see [Figure 40](#)).

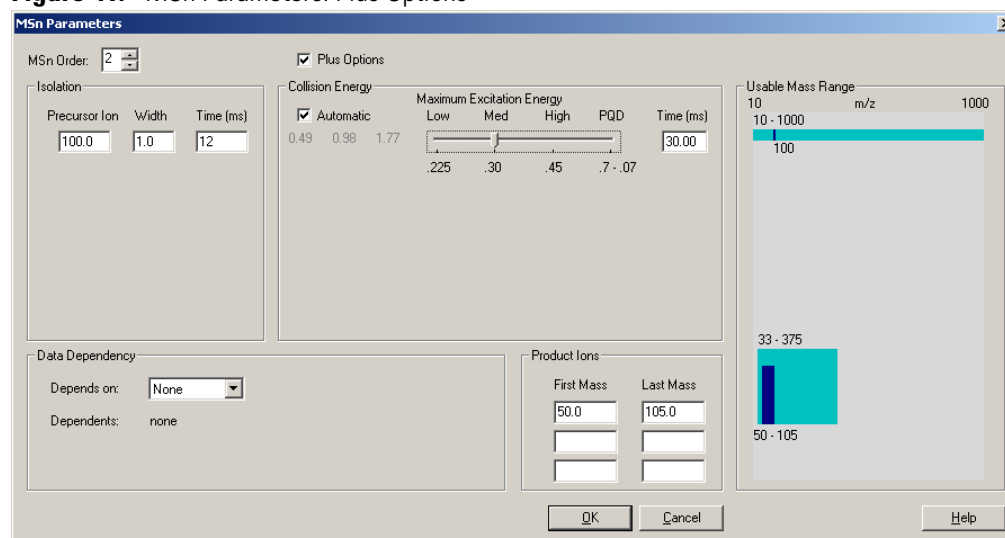
**Figure 40.** MSn Parameters: Usable Mass Range



The dark blue bar indicates the selected product ion mass range. In this example, the allowable range is 50-562 amu, and the selected range is 50-105 amu. The lower mass range depends on the trapping voltages applied to the ion trap. The trapping voltages can be adjusted in the Plus Options.

6. Select **Plus Options** to access more advanced parameters.

**Figure 41.** MSn Parameters: Plus Options



This selection allows you to set the time that the isolation and collision voltages are applied. However, the default values are nearly always sufficient. Additionally, the maximum excitation energy, also known as  $q$ , is accessible. The default maximum excitation energy is set to 0.45. However, this value sets the minimum allowable mass range to  $\frac{1}{2}$  the value of the precursor ion. If lower mass ranges are required, then this value must be reduced.

As can be seen in [Figure 41](#) on [page 46](#), reducing the maximum excitation energy from 0.45 to 0.30 lowers the minimum allowable mass to 33, which is  $\frac{1}{3}$  the precursor ion's mass. If the maximum excitation energy is lowered to 0.225, then the lowest allowable mass would drop to  $\frac{1}{4}$  of the precursor ion mass. Lowering the maximum excitation energy reduces the amount of energy that can be deposited in the precursor ion during CID and reduces the fragmentation efficiency. The final maximum excitation energy option is PQD (see "[PQD Options](#)" on [page 55](#)). This option allows the minimum allowable mass to be significantly less than any of the other excitation energy options. However, the fragmentation efficiency is significantly lower.

## Chemical Ionization (CI Mode) Options

Chemical ionization is a softer ionization technique than the standard electron ionization (EI). CI operates by having a relatively high pressure of reagent gas in the ionization region. Because less energy is deposited into the analyte during ionization when using CI, less fragmentation occurs. CI can be used to produce positive ions through protonation or negative ions through electron capture. Positive CI works well with compound containing atoms such as nitrogen or oxygen. Negative CI is effective on compounds with highly electronegative atoms, like fluorine and chlorine. Because this ionization technique is more selective, especially negative CI, the matrix background may be reduced.



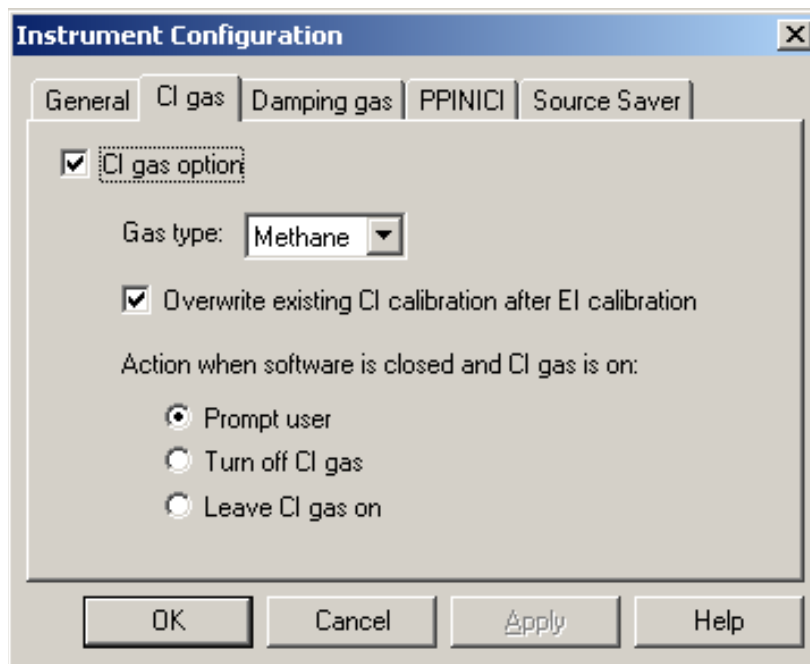
**WARNING FLAMMABLE OR CORROSIVE GAS HAZARD.** CI typically uses flammable gases, such as methane, or corrosive gases, such as ammonia. Care must be taken to ensure the safe use of the CI reagent gases.

CI can be used for quantitation. Additionally, because the ion population is focused into the molecular ion, MS<sub>n</sub> can give better quantitative results. The method software controls the reagent gas flow so that any time the data system activates the analytical method, a precise flow of the CI reagent gas is delivered to the mass spectrometer. In addition, proprietary pulsed positive ion negative ion chemical ionization (PPINICI) allows for the acquisition of both positive and negative chemical ionization data in a single segment. Without this option, positive CI must be performed in a separate segment from negative CI. This restriction prevents the simultaneous acquisition of positive and negative CI at the same GC elution time without the PPINICI option.

❖ **To set CI options**

1. Configure the instrument for CI gas in Instrument Configuration.
  - a. Open the Instrument Configuration window and click the **CI gas** tab.

**Figure 42.** Activating CI Gas

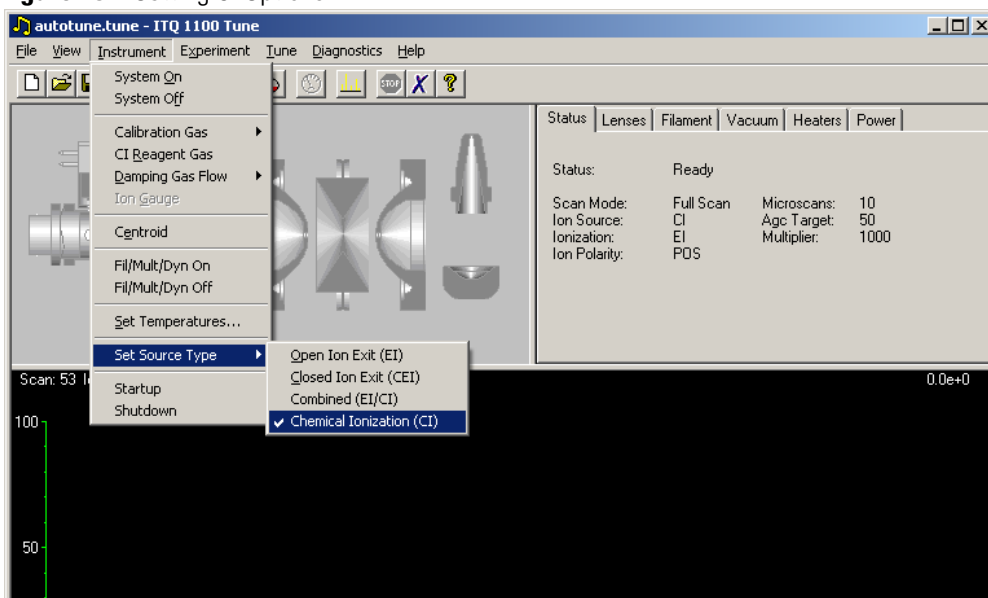


- b. Select **CI gas option**.
  - c. Once this option is activated, you may select the reagent gas type. The default values of the other options are usually acceptable. Please consult the online help for a discussion of these other choices.

2. Tune the instrument for CI.

After the CI option is activated in Instrument Configuration, the instrument must be tuned for use with CI.

**Figure 43.** Setting CI Options



- a. Begin by selecting the type of ion volume that is in the instrument. In order to run CI, either the CI ion volume or the combined EI/CI ion volume must be selected. Because of the pressure requirements for a successful CI, a CI ion volume needs to be more enclosed than an EI ion volume. The CI ion volume is optimal for CI. The combination EI/CI ion volume has a slightly larger conductance limit for the reagent gas, which decreases the CI ionization effectiveness. However, standard EI ionization can occur with the combined EI/CI ion volume.

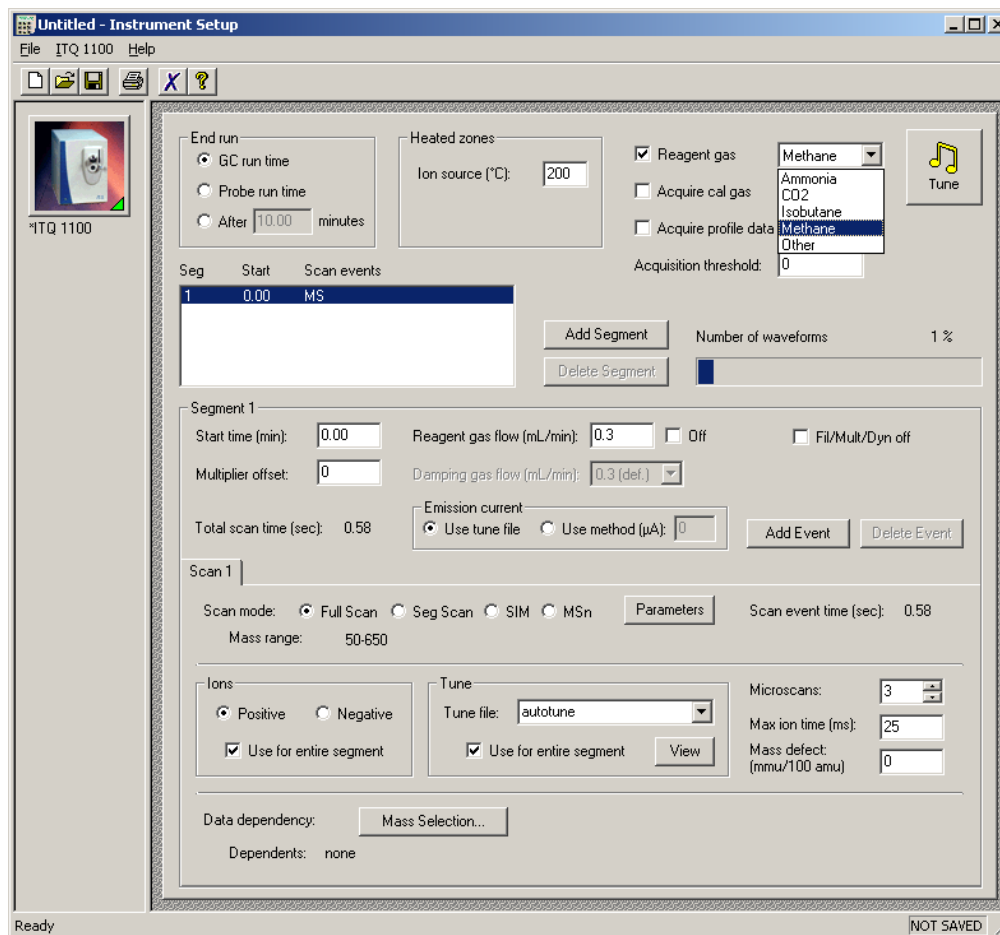
You must turn on the CI reagent gas before tuning in CI. If the CI ion volume is selected, then only the CI autotune is available. If the combined EI/CI ion volume is selected and the CI reagent gas is OFF, then only the EI autotune is available.

After tuning the system and saving the tune files then set up the method parameters in Instrument Setup.

3. In Xcalibur, click the Instrument Setup icon.

4. Click the mass spectrometer image to open the instrument's method editor.

**Figure 44.** Configuring the Method Editor for CI



- a. Select the **Reagent Gas** checkbox and select the reagent gas type.
- b. Set the reagent gas flow rate, and the tune files to use for your analytical method. If you have an EI/CI ion volume installed, then you can collect data in both EI and CI for a given injection. However, because the reagent gas must be pumped away for EI operation, you must have EI and CI acquisitions in separate segments. If PPINICI is enabled, then you may elect to have scan events use different ion polarities when CI is on.



**CAUTION BURN HAZARD.** PPINICI requires the use of a special high speed dynode power supply. Activating PPINICI with the standard dynode supply may damage the instrument. This damage is not covered under the standard warranty.



## ACE Options

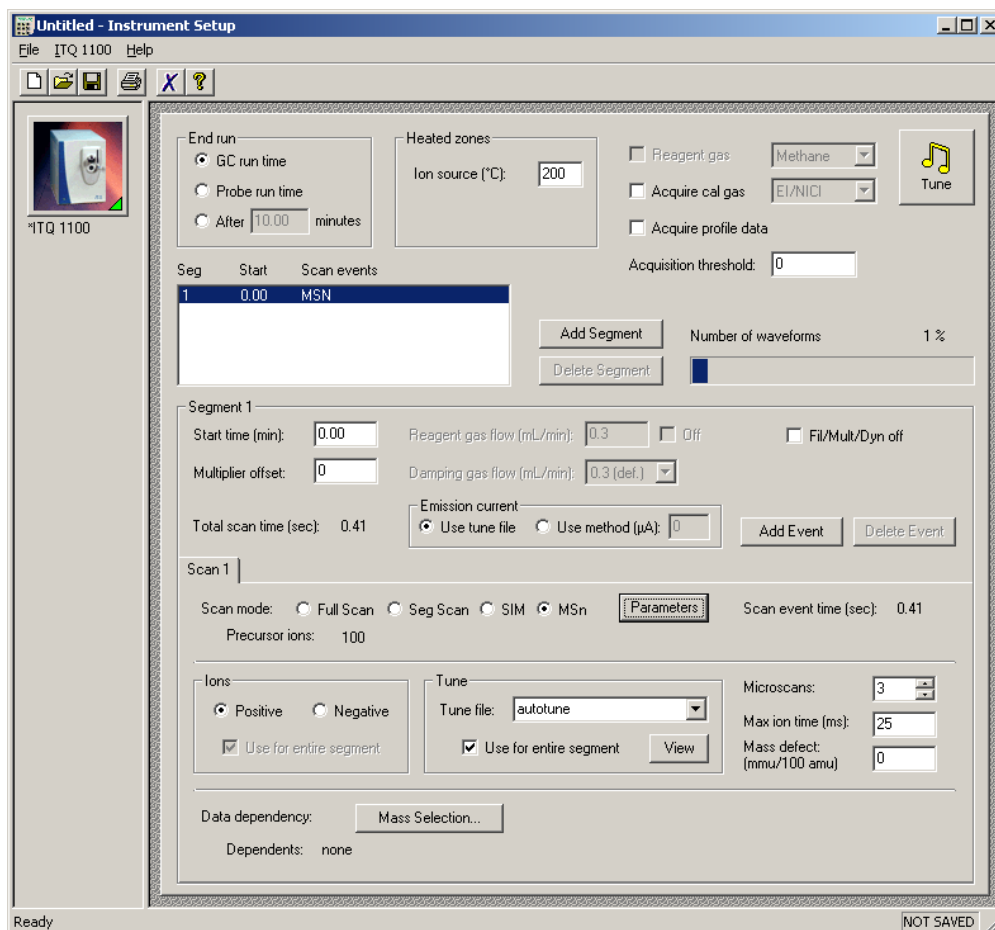
ACE (Automatic Collision Energy) is an MSn scan optional upgrade. ACE automatically calculates an estimated optimal collision energy based on the operating parameters of the scan. Because of differences in the ease of which ions are fragmented, this calculation is an estimated value. ACE runs three energies in a single scan to ensure optimal fragmentation and product ion production. The optimal energy no longer needs to be determined for an MSn run. Use when desiring a fixed collision energy, ACE calculates the estimated collision energy, which is a starting point for further optimization.

For the ITQ, we have introduced automated collision energy (ACE), which greatly simplifies MSn optimization. Determining the collision energy setting required to ensure maximal product ion generation typically means performing a number of separate experiments using different collision energy settings. The results of these experiments would then have to be manually evaluated to determine which setting resulted in the greatest product ion intensities. Any changes to the experimental parameters, such as column flow rates, required a repeat of the optimization. ACE automatically calculates an estimated collision energy based on the operating parameters of the scan. ACE runs three energies in a single scan to ensure fragmentation and product ion production. ACE is used for qualitative and semi-quantitative MSn analyses. A fixed collision energy will be more optimal for quantitative work, however. If you want to run at a fixed collision energy, the estimated collision energy given by ACE is a good starting point.

❖ To set up an ACE method

1. In Xcalibur, click the Instrument Setup icon.
2. Click the mass spectrometer icon to open the mass spectrometer method editor.

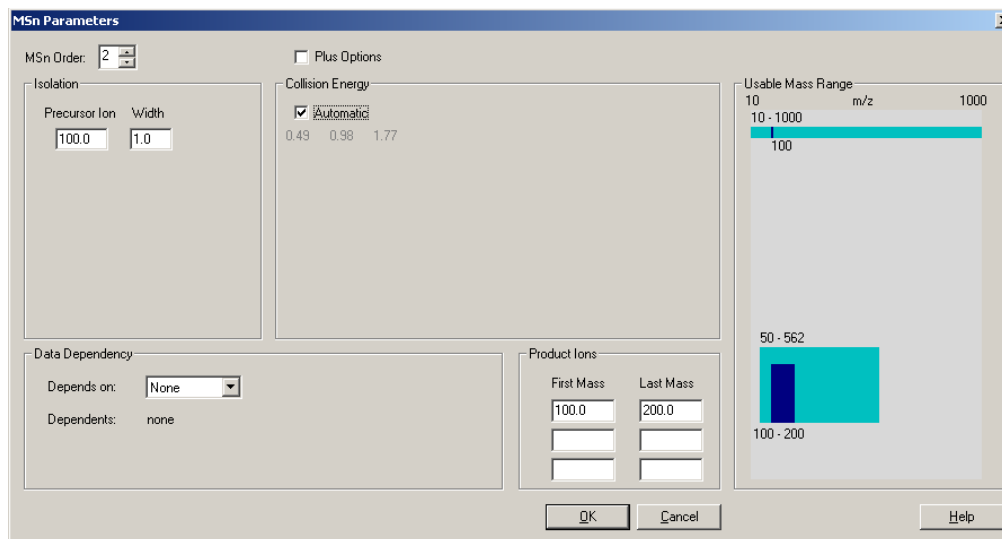
Figure 45. Configuring the Method Editor for MSn Options



3. Select MSn as a scan mode because ACE is an MSn scan option.

4. Click the **Parameters** button to open the MSn Parameters window.

**Figure 46.** Configuring ACE Options in the MSn Parameters Window



5. Select the **Automatic** option in the Collision Energy box from within instrument setup.
6. Click **OK** to return to the method editor and save the method.

## DDS Options

DDS (Data Dependency Scanning) is an MSn optional upgrade. It is also a powerful tool for dynamically changing qualitative analyses. The data dependent algorithms probe mass spectra for ions from a full scan event that match a mass selection criteria to create an intensity sorted, dependent mass list that is used for subsequent scan events. Data dependency allows MSn methods to be written automatically with no advance knowledge on what specific precursor ions may be encountered during an analysis. This allows for qualitative methods to be developed rapidly. For example, the selection criteria for a simple data dependent method may be to isolate and fragment the largest ion from full scan event. A user benefits from library searchable full scan data and the additional qualitative data from the MS/MS spectra.

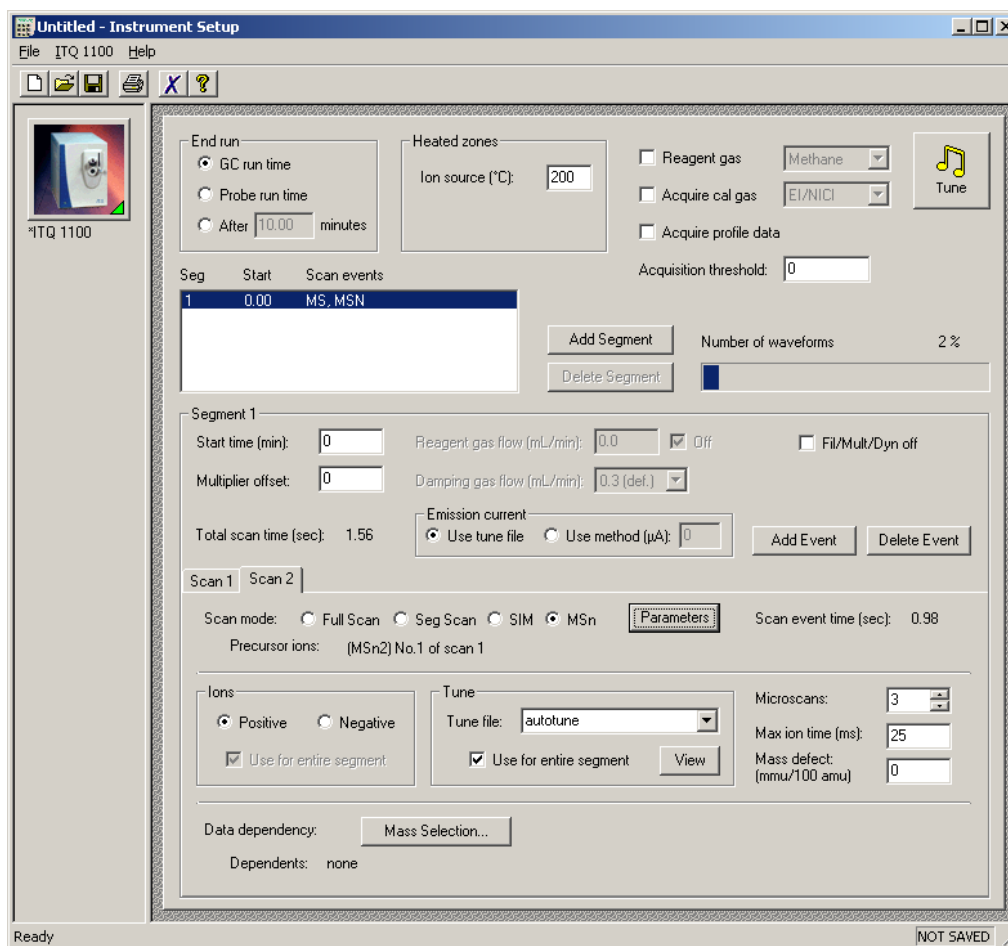
DDS allows MSn methods to be written without knowing in advance what specific precursor ions may be encountered during an analysis, so additional qualitative data may be obtained without spending time running additional analyses and methods. For example, a simple data dependent method may include a full scan event followed by a dependent scan event performing MS/MS on the most intense ion from the previous scan. A data dependent scan can not be the first scan in a segment and the DDS scan event must be an MSn event. A scan can be dependant on any scan that occurred previous. For example, the third scan event in a segment may be dependant on either the first or second scan event.

There are many ways to modify which precursor ion the data dependent scan selects for MS/MS. For example, the ion selected for isolation may be the most intense, or within a certain mass range, or may be dynamically excluded for a time because that mass had already been selected, or may be required to exceed a certain intensity. The array of options when using DDS is discussed more fully in the online help.

❖ **To set up a DDS method**

1. In Xcalibur, click the Instrument Setup icon.
2. Click the mass spectrometer icon to open the mass spectrometer method editor.

**Figure 47.** Configuring the DDS Options

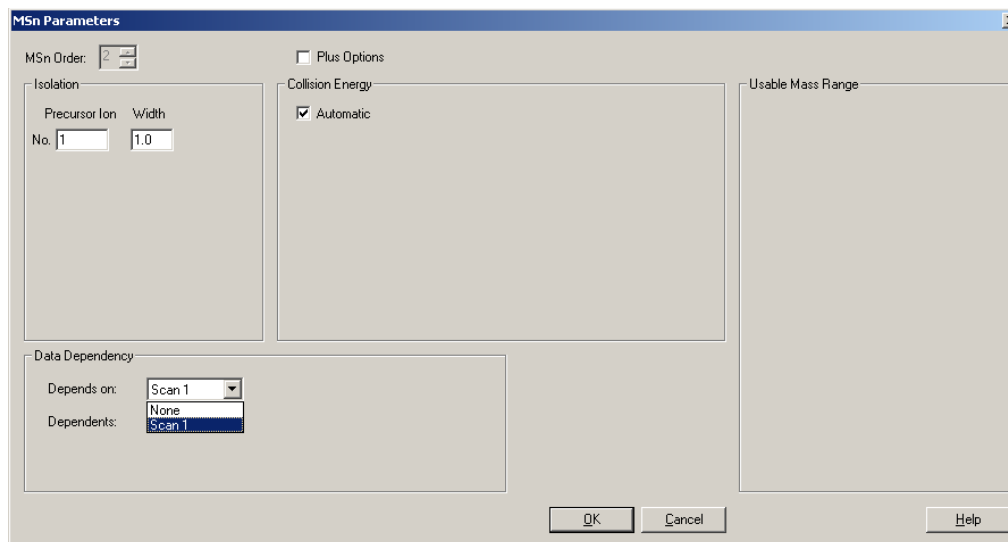


3. Go to a second (or later) scan event that has an MSn scan mode.

**Tip** Click the **Add Event** button to add another scan event tab.

4. Click the **Parameters** button to open the MSn Parameters window.

**Figure 48.** Configuring DDS Options in the MSn Parameters Window



5. Select the scan's Data Dependency. In this example, the DDS scan is based on the results of scan 1 and will select the most intense ion from scan 1, then isolate and fragment it.
6. Click **OK** to return to the method editor and save the method.

## PQD Options

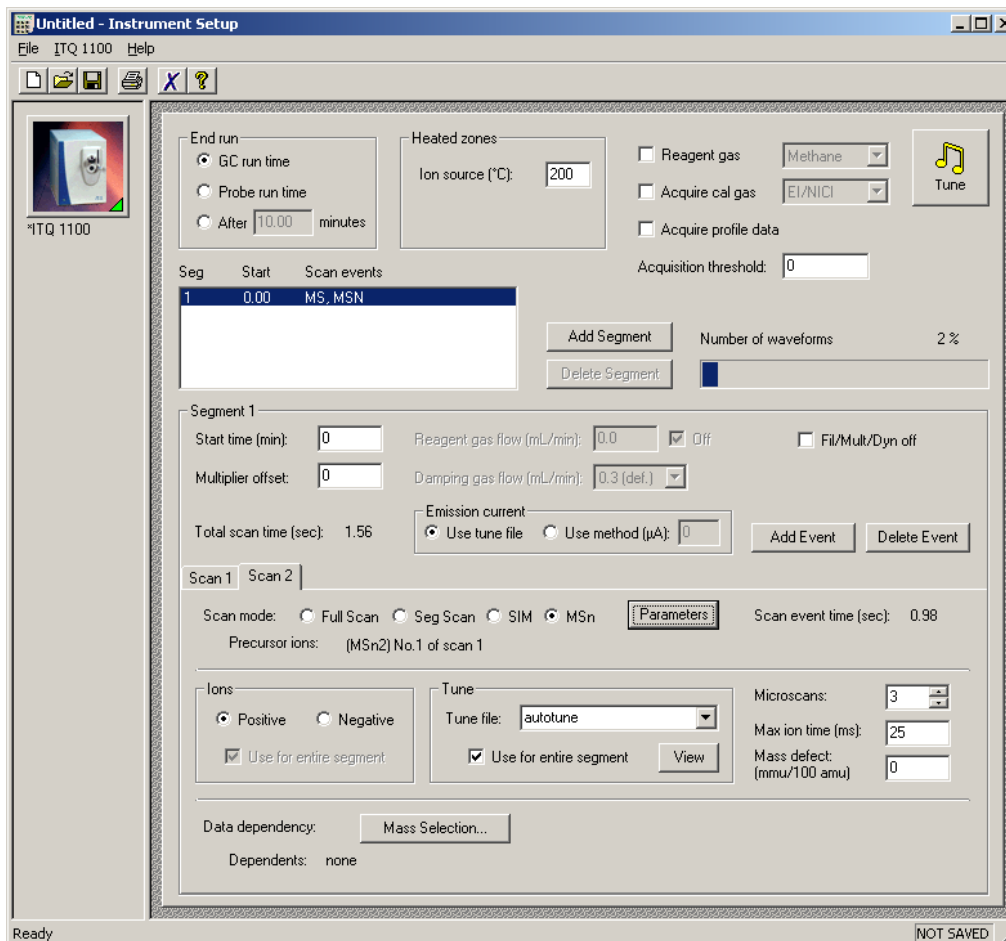
PQD (Pulsed Q Dissociation) is a technique exciting the precursor at high energy for a short time. It is also useful as a structure elucidation qualitative tool. PQD is used to generate spectral data that are qualitatively similar to data produced using standard collision induced dissociation (CID). The key difference is that PQD increases the overall spectral quality, particularly in low mass range, which lets you see low  $m/z$  fragments that are usually excluded from CID spectra. PQD also helps you access higher energy dissociation channels. PQD is a novel fragmentation mechanism that involves precursor ion activation at high  $q$ , a time delay to allow the precursor to fragment, then a rapid pulse to low  $q$  where all fragment ions are trapped. The product ions can then be scanned out of the ion trap and detected.

PQD is used to generate spectral data that are qualitatively similar to data produced using standard CID. PQD allows for the observation of lower masses that are usually excluded from CID spectra. PQD also helps you access higher energy dissociation channels. PQD is a novel fragmentation mechanism that involves precursor ion activation at high  $q$ , which is also called maximum excitation energy. After activation of the precursor ion, a time delay occurs to allow the precursor to fragment, then a rapid pulse to low  $q$  where all fragment ions are trapped. The product ions can then be scanned out of the ion trap and detected. The fragmentation efficiency is not as high as a standard CID method, which makes PQD worse for quantitative and semi-quantitative methods. This methodology is used to generate qualitative results from MS/MS where low mass ions are needed or to access high energy fragmentation pathways for research purposes.

❖ To set up a PQD method

1. In Xcalibur, click the Instrument Setup icon.
2. Click the mass spectrometer icon to open the mass spectrometer method editor.

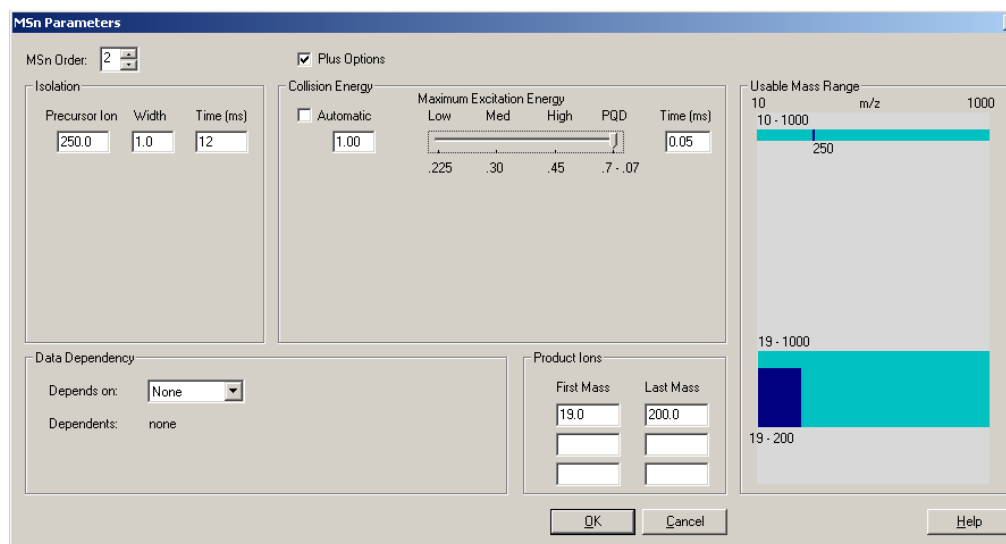
Figure 49. Configuring PQD Options



3. Select MSn as a scan mode because PQD is an MSn scan option.

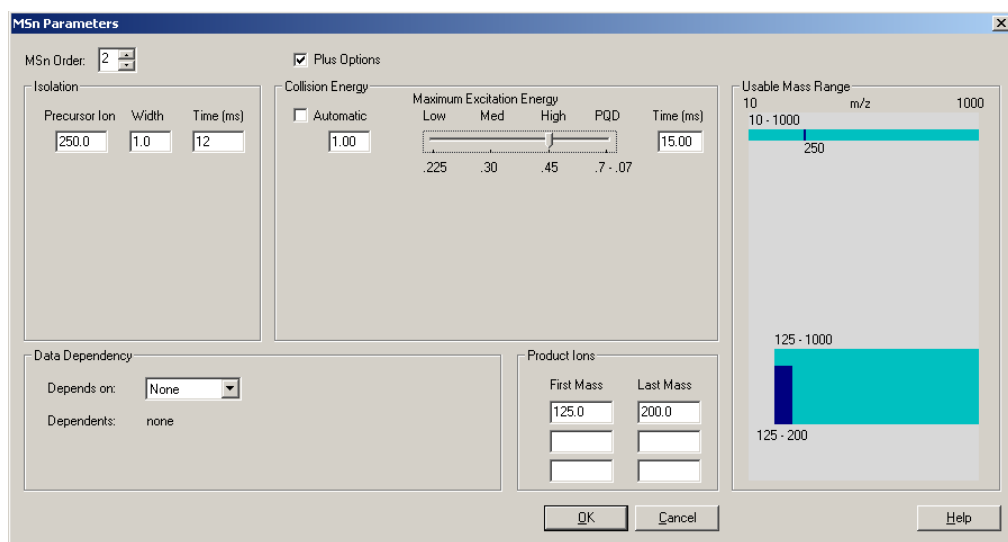
- Click the **Parameters** button to open the MSn Parameters window.

**Figure 50.** Configuring PQD Options in the MSn Parameters Window



- Select the **Plus Options** box to open the Maximum Excitation Energy selection.

**Figure 51.** Setting the High Maximum Excitation Energy ( $q$ )



If the maximum excitation energy is set to 0.225, the minimum mass product ion that can be seen is  $\frac{1}{4}$  the precursor ion. When the maximum excitation energy is set to 0.30, the minimum mass is  $\frac{1}{3}$  of the precursor ion and when the maximum excitation energy is set to 0.45, the minimum mass is  $\frac{1}{2}$  the precursor ion's mass (Figure 51 on page 57).

When the maximum excitation energy is set to 0.45, the precursor ion is mass 250 (Figure 51), and the minimum product ion is 125. However, when PQD is selected, the minimum mass is only 19 amu as illustrated in Figure 50. If you do not want to optimize the collision energy for your particular experiment, try using the Automated Collision Energy option. Activate this by selecting the **Automatic** box in the Collision Energy group.

6. Click **OK** to return to the method editor and save the method.

## Variable Damping Gas Option

Variable damping gas allows computer control over the damping gas pressure in the ion trap mass analyzer. By increasing the rate of the damping gas flow, the damping gas pressure increases proportionally. The default flow is 0.3 mL/min, which corresponds to a pressure of approximately 0.13 Pa (1 mTorr) inside the ion trap. Increasing this flow increases sensitivity at the expense of resolution. Higher flow rates also affect the dissociation efficiency. If you use the automated collision energy option, then the effect of higher damping gas flows is accounted for when ACE calculates the energy required for fragmentation. Changing the damping gas flow may be useful when trying to achieve the maximum signal from the trap.

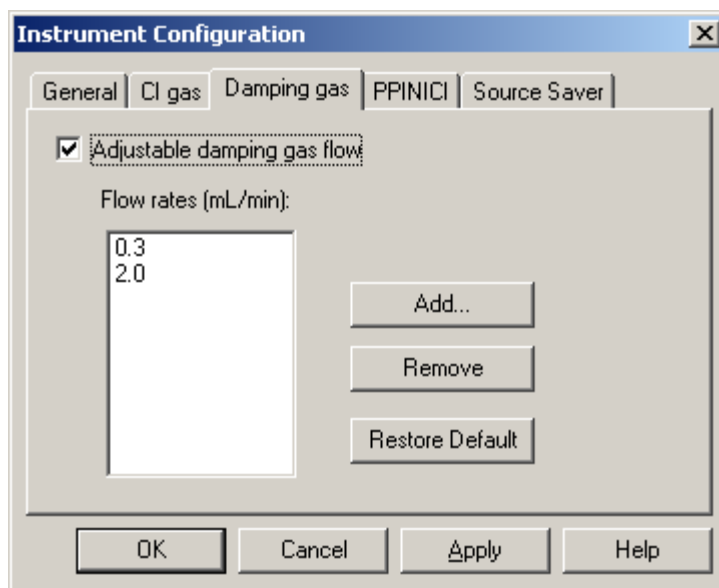
### ❖ To use variable damping gas

1. Configure the instrument for damping gas flow rates in Instrument Configuration.
  - a. Run Instrument Configuration.
  - b. Double-click the instrument icon you are configuring to open the Instrument Configuration window.



- c. Click the **Damping Gas** tab to configure variable damping gas flow rates. The ion trap can be configured for up to six damping gas flow rates, including the 0.3 mL/min default.

**Figure 52.** Configuring Variable Damping Gas Flow Rates

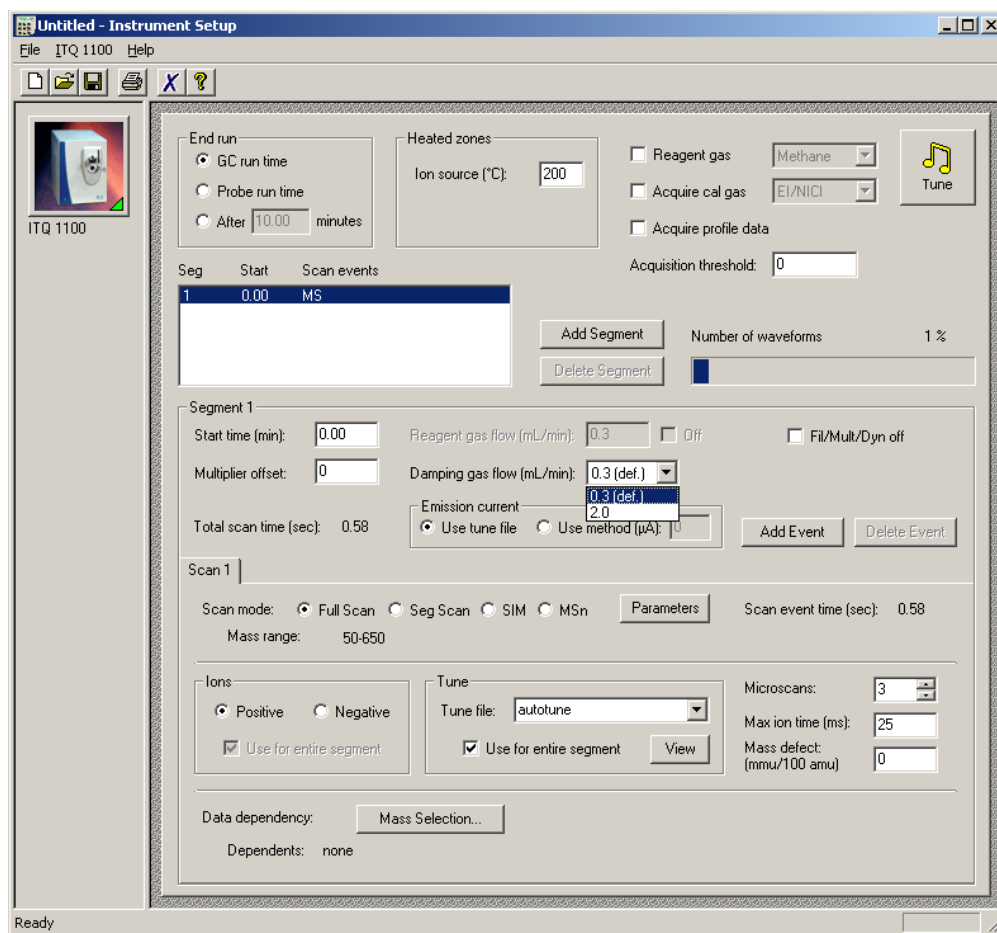


As seen in [Figure 52](#), the instrument has the variable damping gas option installed and set to use either 0.3 or 2.0 mL/min of helium into the trap. Click the **Add** button to use additional flow rates. Once the flow rates are in the instrument configuration, configure your methods to use one of these flows while using the method editor in Instrument Setup.

2. In Xcalibur, click the Instrument Setup icon.

3. Click the mass spectrometer icon to open the mass spectrometer method editor.

**Figure 53.** Configuring the Method Editor for Variable Damping Gas



- Click the **Tune** button if you need to tune the instrument. Before using a flow rate, it is strongly recommended that you tune the instrument at the gas flow rate you will be using when collecting data.
- Select the damping gas flow you wish to use.

Save the method.

## Additional Help

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

### Contents

- [Assembling Swagelok Fittings](#)
- [Using a Swagelok Tee or Cross](#)
- [Pressure Testing the TRACE GC Ultra Inlet](#)
- [Automatic Tune Flow Chart](#)
- [Calibrating the RF Frequency](#)
- [Baking Out the Source](#)
- [Reviewing Cursor Actions in Browsers](#)

## Assembling Swagelok Fittings

### Tools Needed



- Swagelok® Fitting
- Wrench set (open end), 5/16-in., 7/16-in., 9/16-in., 1/2-in.,



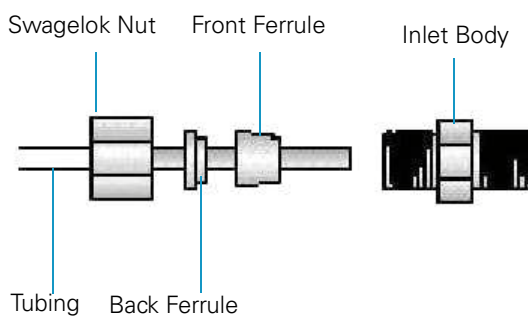
### Frequency

Fixing leaks

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 [Figure 1](#). 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.

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 1](#).

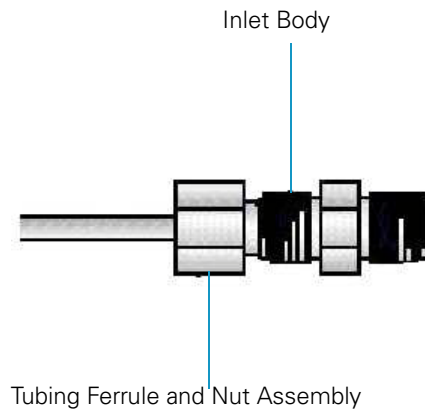
**Figure 1.** Swagelok Ferrule and Nut Assembly



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

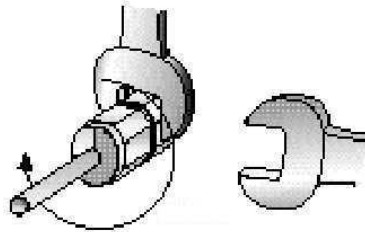
2. Place a swagelok back ferrule over the tubing with the smaller side facing the open end of the tubing.
3. Place a swagelok front ferrule over the tubing with the smaller side facing the open end of the tubing.
4. Push the ferrules down into the swagelok nut.
5. Insert the tubing into the swagelok inlet as far as it will go as shown in [Figure 2](#).

**Figure 2.** 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 3](#). 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 3.** Tightening Swagelok Fittings



## Using a Swagelok Tee or Cross

### Tools Needed



- Ruler or measuring tape
- Swagelok Fittings
- Swagelok Plugs
- Tubing Cutter



### Frequency

Fixing 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.

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. Refer to [“Assembling Swagelok Fittings”](#) on [page 62](#).
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.

## Pressure Testing the TRACE GC Ultra Inlet

Use this procedure to determine if any leaks exist in the inlet or carrier flow module prior to performing a column evaluation. This procedure is written for the TRACE GC Ultra. If you have a TRACE 1300, TRACE 1310, or FOCUS GC, refer to your GC user documentation for the correct procedure.

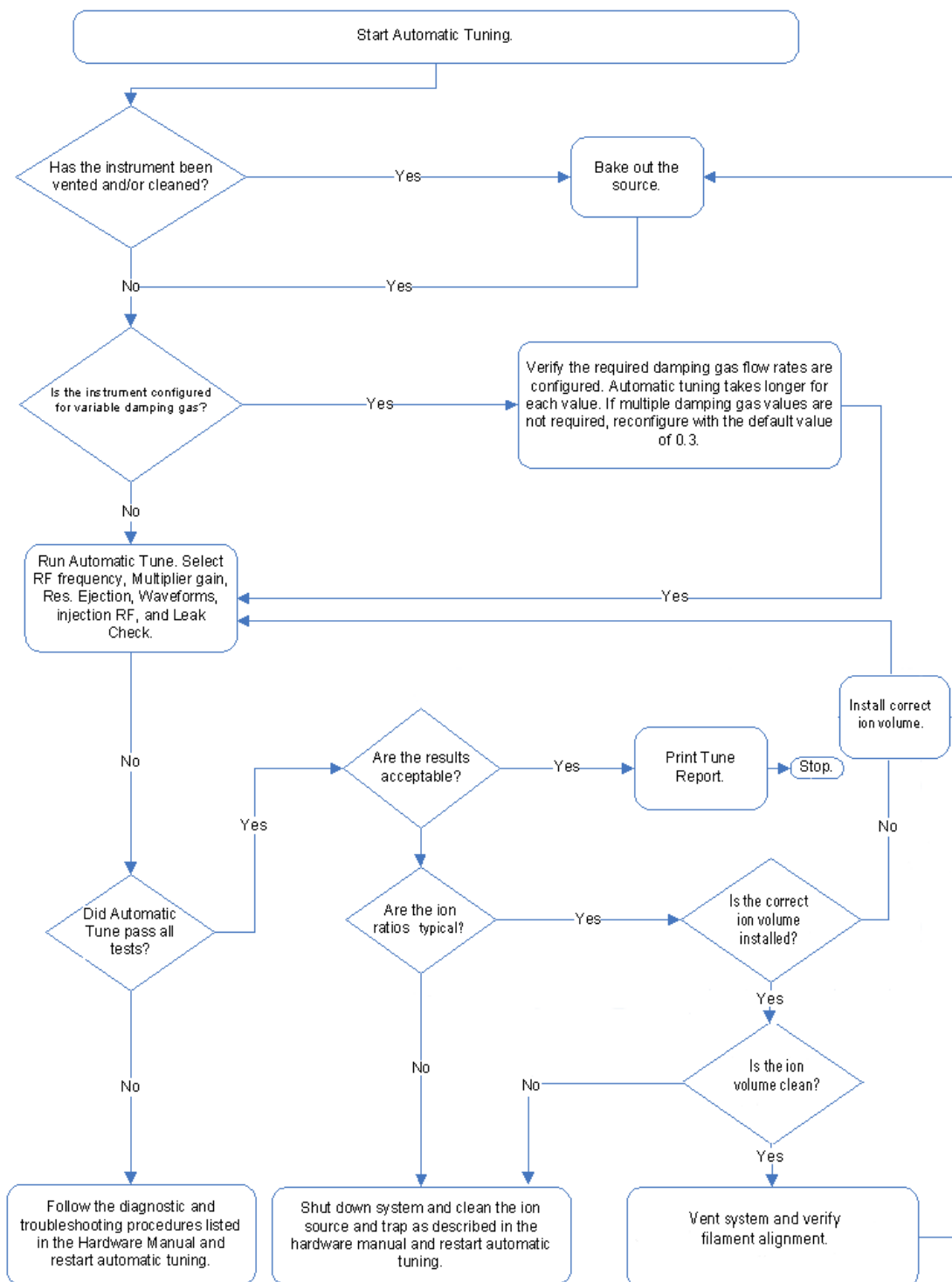
1. Install an injector nut with an aluminum plug onto the GC inlet.
2. Tighten it using a 6 mm wrench.
3. Press the **Left or Right Carrier** button and put the inlet in the constant pressure mode.
4. Put the septum purge and split vent valve in the *OFF* position.
  - a. Press the **Valve** button located 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 for the display to indicate it is off.
5. 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.
  6. Turn the inlet pressure off and monitor the pressure. The pressure should not change more than 1 psi (7 kPa) over 3 minutes.
  7. Determine if a leak exists.
    - a. Use a suitable leak detector, if the pressure indicates a gradual decrease. 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 <1mL) 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 3 minutes may indicate a defective flow module.
  8. 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.
  9. Remove the injector nut with plug and continue with the column installation.

## Automatic Tune Flow Chart

Refer to this chart to determine when to use various tuning features.

**Figure 4.** Automatic Tune Flow Chart



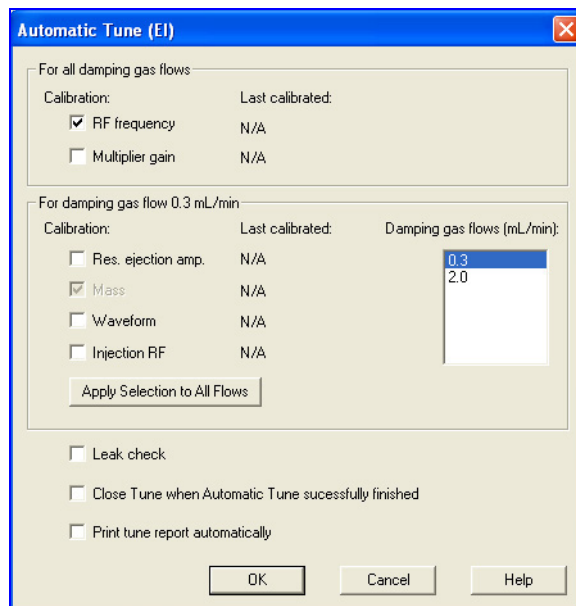


## Calibrating the RF Frequency

Use this procedure to adjust the RF Frequency. However, 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. Select **Tune | Automatic Tune** to open the Automatic Tune window.

**Figure 5.** Adjusting the RF Dip Calibration



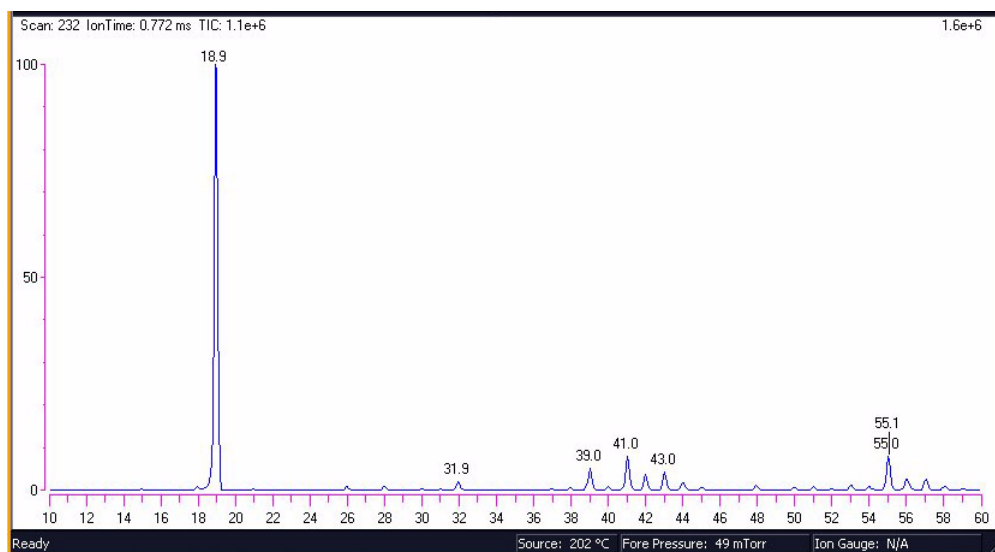
3. Select the **RF Frequency** option.
  4. Uncheck all other options.
  5. Click **OK** to adjust the RF Calibration automatically and return to the Tune window.
- Ion Trap Series User Guide

## Baking Out the Source

Use this procedure to bake out the source to reduce background. This is especially useful after a system has been cleaned.

1. After startup, open the Tune window and set the source temperature to 200 °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. This will usually be displayed as  $m/z$  19.

**Figure 6.** Air/Water Spectra  $m/z$  19



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

4. Increase the source temperature and MS transfer line to 275 °C. As the source temperature rises, the pressure will begin to increase.
5. Allow the source to remain at 275 °C until the fore pressure begins to decrease to a pressure equal to or below the fore pressure noted in the previous step.

**Note** Operating the system at an elevated source temperature for an extended period of time with an air leak will oxidize and contaminate the source.

6. Set the source temperature and transfer line to the desired operating temperature.
7. Once the operating temperature has been reached, allow the system 1 hour to stabilize.
8. 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 icon 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.

1. Unpin an active cell by clicking once on the pin icon.
2. Make a cell active by clicking anywhere within the cell.

Xcalibur highlights the cell with a gray border. Click on its pin icon 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 1](#)).

**Table 1.** 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 2](#)).

**Table 2.** 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.

# Glossary

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

## Numerics

$\mu$  micro ( $10^{-6}$ )

$\Omega$  ohm

## A

**A** ampere

**ACE** automatic collision energy

**ac** alternating current

**amu** atomic mass unit

**ADC** analog-to-digital converter

**ASCII** american standard code for information interchange

## B

**baud rate** data transmission speed in events per second.

## C

$^{\circ}\text{C}$  degrees Celsius

**CD-ROM** compact disc read-only memory

**CE** (F. Conformité Européenne) European conformity. Mandatory european marking for certain product groups to indicate conformity with essential health and safety requirements set out in european directives.

**cfm** cubic feet per minute

**CI** chemical ionization

**CID** collision induced dissociation

**CIP** carriage and insurance paid to

**cm** centimeter

**cc or  $\text{cm}^3$**  cubic centimeter

**CPU** central processing unit (in a computer)

## D

**Da** Dalton

**DAC** digital-to-analog converter

**dc** direct current

**DDS** data dependency scanning

**DEP™** direct exposure probe

**DIP** direct insertion probe

**DS** data system

**DSP** digital signal processor

## E

- EI** electron ionization  
**ESD** electrostatic discharge  
**eV** electron volt  
**EN** european conformity

## F

- f** femto ( $10^{-15}$ )  
**°F** degrees Fahrenheit  
**FCC** federal communication commission  
**FOB** free on board  
**ft.** foot  
**FSE** field service engineer  
**FTP** file transfer protocol

## G

- g** gram  
**G** giga ( $10^9$ )  
**GB** gigabytes 1024 MB (billion)  
**GC** gas chromatograph  
**GC/MS** gas chromatograph / mass spectrometer  
**GND** electrical ground  
**GPIB** general-purpose interface bus  
**GUI** graphical user interface

## H

- HV** high voltage  
**Hz** hertz (cycles per second)

## I

- ICIS™** interactive chemical information system  
**IEC** international electrotechnical commission  
**IEEE** institute of electrical and electronics engineers  
**in.** inch  
**I/O** input/output

## K

- k** kilo ( $10^3$ , 1000)  
**K** Kelvin  
**kb** kilobyte 1024 bytes (thousand)  
**kg** kilogram  
**kPa** kilopascal  
**kVA** kilo volt amperes (1000 VA)

## L

- L** liter  
**LAN** local area network  
**lb** pound  
**LED** light-emitting diode

## M

- m** meter; milli ( $10^{-3}$ )  
**M** mega ( $10^6$ )  
**MB** megabyte or 1,024 kb (million)  
**M<sup>+</sup>** molecular ion  
**min** minute  
**mL** milliliter  
**mm** millimeter

**MS** scan power:  $MS^1$ , mass spectrometer

**m/z** mass-to-charge ratio

## N

**n** nano ( $10^{-9}$ )

## P

**p** pico ( $10^{-12}$ )

**Pa** Pascal

**PCB** printed circuit board

**PID** proportional / integral / differential

**PN** part number

**P/P** peak-to-peak voltage

**PPINICI** pulsed positive ion negative ion chemical ionization

**ppm** parts per million

**PQD** pulsed  $q$  dissociation

**psig** pounds per square inch, gauge

## Q

**$q$**  maximum excitation energy

## R

**RAM** random access memory

**RF** radio frequency

**RMS** root mean square

**ROM** read-only memory

**RS-232** industry standard for serial communications

## S

**s** second

**SCSI** small computer system interface

**SIM** selected ion monitoring

**SI** international system of units

**S/N** signal to noise ratio

## T

**TIC** total ion current

**TCP/IP** transmission control protocol / Internet protocol

**Torr** torr

## U

**URL** uniform resource locator

**USB** universal serial bus

## V

**V** volt

**V ac** volts alternating current

**V dc** volts direct current





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