O P E R A T I N G M A N U A L

HAPSITE® ER

Chemical Identification System

IPN 074-471-P1D

INFICON

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Definition of Note, Hint, Danger, Warning and Caution Paragraphs

NOTE: This is a note paragraph. Notes provide additional information about the current topic.

HINT: This is a hint paragraph. Hints provide insight into product usage.

DANGER

This is a Danger paragraph. Failure to heed these messages has a high likelihood of resulting in serious personal injury or even death!

WARNING

This is a Warning paragraph. It warns of actions that may cause physical injury.

WARNING - Risk Of Electric Shock

This Warning paragraph warns of the presence of electrical voltages which may cause physical injury.

CAUTION

This is a Caution paragraph. It cautions against actions which may damage the instrument or lead to the loss of data.

CAUTION

Heavy Object over 18 kg - To avoid muscle strain or injury, use mechanical lifting aides and proper lifting techniques. Get help when required.

Operating Manual Style Conventions

The following information describes the conventions used throughout this manual.

When holding down a key and then pressing another key, this is expressed as (for example) “Press Ctrl+C.”

It is assumed that the CD drive used is drive **d**. If using another drive, substitute the drive letter being used for “**d:**”.

It is assumed that the hard drive used is drive **c**. If using another drive, substitute the hard drive letter being used for “**c:**”.

Left-click means to press and release the left mouse button (LMB) and right-click means to press and release the right mouse button (RMB).

The HAPSITE software operates in the Windows environment using the Windows® Graphical User Interface (GUI). Actions in the HAPSITE software GUI that are common to the Windows GUI are not explained in detail in this manual. Refer to the Windows documentation supplied by Microsoft®.

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Chapter 1
Customer Support

1.1 How to Contact Customer Support

Please read the HAPSITE ER Operating Manual before contacting Customer Support. To contact support, please request:

- Technical Support - for information and questions regarding general operation or software assistance for the HAPSITE ER
- Applications Support - for information and questions regarding the ability of the HAPSITE ER to detect various compounds and for assistance creating calibration libraries
- Sales - for pricing requests and purchasing
- Service and Repair - for troubleshooting advice and for information on repairing HAPSITE ER

If experiencing a problem with your instrument, please have the following information readily available:

- The serial number for your instrument, located on the white sticker labeled **HAPSITE ER** inside the front panel door
- A description of your problem
- A summary of any corrective action that has been attempted
- The exact wording of any error messages

For current customer support phone numbers, please refer to Support at www.inficon.com.

1.2 Returning Your Instrument to INFICON

Do not return any component of the instrument to INFICON without first speaking with a Customer Support Representative.

Prior to returning the instrument, a Declaration of Contamination (DOC) form will need to be completed. The Customer Support Representative will provide the DOC form. All chemicals that have been analyzed by the HAPSITE ER should be reported on the DOC form in order for INFICON's service personnel to take the proper safety precautions when performing the repair. In certain cases, INFICON may require that the instrument be sent to a designated decontamination facility instead of the factory.

Once the DOC has been received, the Customer Support Representative will provide shipping instructions and a Return Materials Authorization (RMA) Number, which signifies that INFICON has authorized the return.

NOTE: Failure to follow these procedures will delay the repair of the instrument.

Chapter 2
Introduction

2.1 HAPSITE ER System

HAPSITE ER Chemical Identification System is designed to identify and quantify volatile organic compounds from the parts-per-million (PPM) to the parts-per-trillion (PPT) level. HAPSITE ER is a portable unit that collects and analyzes samples in the field using self-contained gas canisters and a chemically maintained vacuum source, while operating on battery power. The HAPSITE system can be operated with the front panel touchscreen or with a laptop computer. Near real time data will be displayed on the front panel touchscreen for immediate review.

NOTE: This manual is specifically for the HAPSITE ER. The terms “HAPSITE” and “HAPSITE ER” are used throughout this manual to refer to the HAPSITE ER.

2.1.1 HAPSITE ER and Accessories

HAPSITE ER . . . . . Also known as the Analytical Module (AM). HAPSITE ER contains the Gas Chromatograph and Mass Spectrometer, a vacuum chemical pump for portable operation, control electronics, battery, gases, keypad, display, and a battery charger

Air Sampling Probe . . . . . Consists of a hand-held sampling device, a heated inlet line, small display and buttons. The inlet line connects to HAPSITE ER and provides a flexible heated sample flow path

Service Module . . . . . Also known as the SM, consists of a turbo-molecular high-vacuum pump, roughing pump, battery-charger and power supply

Headspace Sampling System . . . Also known as the HSS, an accessory for the HAPSITE ER, used for testing volatile compounds in liquids and solids in vials

SituProbe™ . . . . . SituProbe is a water sampling device that provides portable field testing of water samples without the need for vials

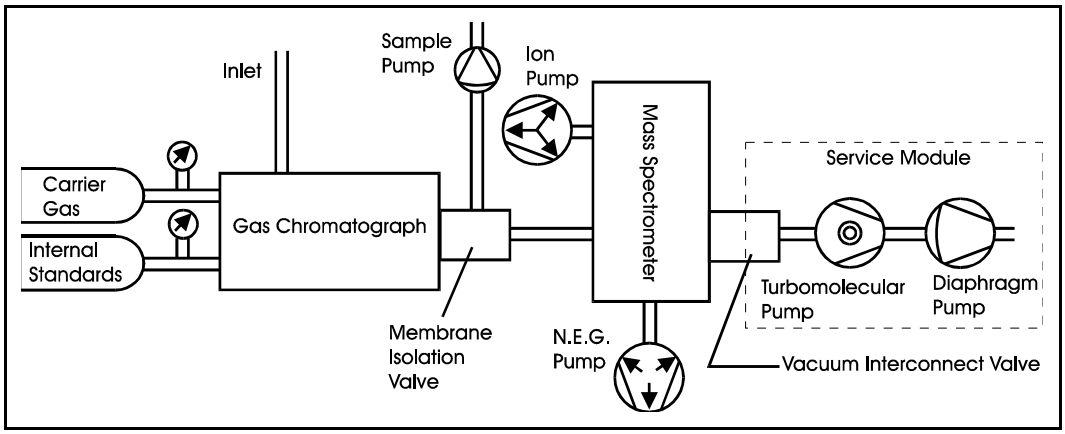
2.2 Specifications

Operating temperature range	5°C to 45°C (41°F to 113°F)
Dimensions (LxWxH)	46 cm x 43 cm x 18 cm (18 in. x 17 in. x 7 in.)
Weight	19 kg (42 lb) with battery
Battery Life	Approximately 2 to 3 hours (using the Air Probe)
Power Requirement	24 V(dc), 30 watts at normal operating conditions
Hard Drive	16 GB internal storage
Flash Drive	USB
Display	6.5 in. VGA color display with touch screen
Mass Range	41-300 amu (1-300 using SIM)
Scan Rate	up to 1000 amu/sec at 10 points per amu
Ionization Mode	70 eV Electron Impact
Carrier Gas	Nitrogen
Column Temperature Range	45°C to 200°C (113°F to 392°F)
Maximum Sample Moisture Content	8% by weight
pH Range of Sample	2 to 11
Boiling Point of Sample (approx)	<270°C (<518°F)
Vapor Pressure of Sample (approx)	0.01-250 mmHg
GC Column	5% diphenyl/95% dimethyl polysiloxane phase, 15 m x 0.25 mm i.d. x 1.0 μm df
SIM Channels	Option to enter mass fragments for up to 10 compounds
External Communications	802.11G wireless or direct Ethernet connection

2.3 Instrument Overview

A diagram of the major HAPSITE ER components is shown in Figure 2-1, including the pumps used to provide flow and vacuum. Service Module components are also identified in Figure 2-1. Service and HAPSITE Modules contain a Vacuum Interconnect Valve and electrical connectors through which vacuum systems join.

Figure 2-1 Major HAPSITE Subsystems



2.4 Description of Subsystems

HAPSITE combines two analytical techniques, gas chromatography and mass spectrometry, to separate and identify the organic components in a gas phase sample. The HAPSITE software also allows for the quantification of analytes.

HAPSITE is comprised of the following subsystems:

- Gas Chromatograph, see section 2.4.1
- Mass Spectrometer, see section 2.4.2 on page 2-5
- Vacuum System, see section 2.4.3 on page 2-6
- Electronic Systems, see section 2.4.4 on page 2-7
- Software Systems, see section 2.5 on page 2-8

2.4.1 Gas Chromatograph

Gas Chromatograph (GC) performs a time separation of the sample compounds. The separation order is primarily based on the volatility of the sample components.

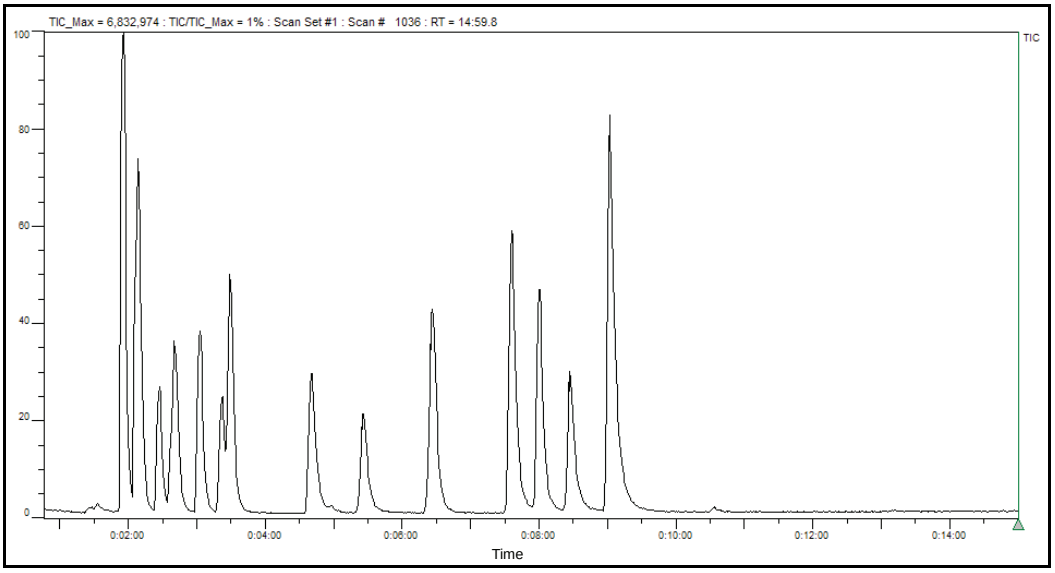
HAPSITE ER GC system utilizes nitrogen as the carrier gas to transport analytes through a column, of which the standard column is a narrow-bore fused silica tube 15 meters in length. The carrier gas is referred to as *mobile phase.* The inside of the column is coated with a thin layer of a material known as *stationary phase*.

The time needed by an individual compound to travel through the GC column to the detector is referred to as *retention time* (RT). If the GC conditions remain constant, the compound will elute from the column at the same retention time on every analysis.

HAPSITE ER uses internal standards to verify the performance of the Gas Chromatograph and Mass Spectrometer. The internal standard is composed of two volatile organic gases which are injected into the sample inlet flow. The internal standards' retention times and responses are used to ensure proper instrument performance.

A graph of eluting gases from the Gas Chromatograph is shown in Figure 2-2. This graph is called a Total Ion Chromatogram (TIC) and is plotted as a function of time (x-axis) verses response (y-axis).

Figure 2-2 Total Ion Chromatogram



2.4.1.1 Membrane Isolation Valve

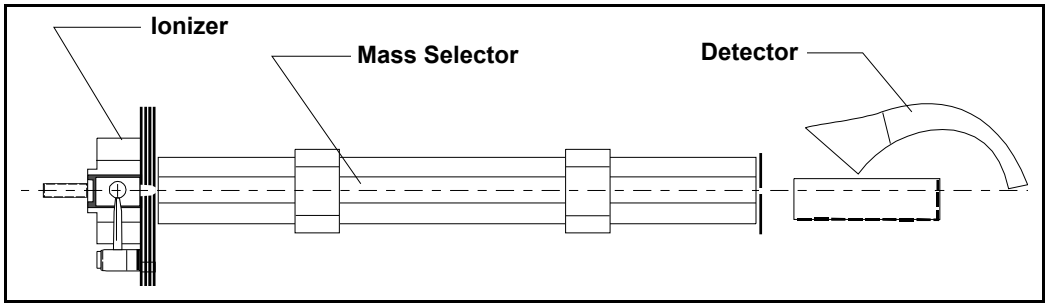
Gas eluting from the GC column passes through the membrane isolation valve. When the membrane isolation valve is opened, organic compounds are permitted to enter the Mass Spectrometer.

In the Survey mode of operation, in which air samples bypass the GC directly to the Mass Spectrometer, the sample pump draws the air sample directly across the membrane with the isolation valve in the open position.

2.4.2 Mass Spectrometer

The Mass Spectrometer is comprised of three basic physical systems: *ionizer*, *mass selector*, and *ion detector*. These are mounted together in a vacuum manifold which also includes: an inlet, two vacuum pumps, and a portion of the vacuum interconnect valve, as shown in Figure 2-1 on page 2-3. Figure 2-3 is a representation of the three sub-systems of the Mass Spectrometer.

Figure 2-3 Three Subsystems of the Mass Spectrometer



The inlet flow from the membrane isolation valve is brought directly to the *ionizer*. Within the ionizer, the compound introduced from the inlet flow is subjected to a bombardment of electrons which are boiled off the hot *filament*. Collisions with the energetic electrons remove one electron from some of the gas molecules, leaving them with a net positive charge. This process is termed *ionization*. Other gas molecules are fractured into smaller molecules, some of which are also ionized. The remaining stream of gas is pumped away by the vacuum pump system.

The ionized molecules, or ions, are driven from the ionizer toward the mass selector by the different voltages on the ion volume and focusing plates. As the ions move through the orifices in these plates, the ions are formed into a nearly parallel beam of mixed ions of nearly the same energy.

The mass selector (or mass filter) is a quadrupole analyzer. The quadrupole analyzer is comprised of four parallel rods, mounted with precise alignment and spacing. Opposing rods are electrically connected together. The two pairs of rods are connected to a radio frequency (RF) voltage 180° out of phase with each other. In addition, the two pairs of rods have a direct current (DC) voltage applied to them; positive on one pair, negative on the other.

The ion beam is directed down the center of the array of rods. At any specific combination of RF and DC fields, some ions are light enough to oscillate harmonically with the RF field. This oscillation causes them to increase in energy and in speed until the ions impact one of the rods and are neutralized. The DC field acts upon the heavier ions resulting in their movement from the center towards the rods. Once on the rod, the heavier ion is neutralized. At a specific combination of RF and DC fields, ions of a specific mass will be able to transit the rod structure and emerge at the exit where detection occurs.

When the ions emerge from the mass selector, the ions are directed to the detector. The active element of the detector is an electron multiplier. The electron multiplier responds to the arrival of each individual ion with a cascade of electrons, each of which generates more electrons. The result is a small burst of electrical current in response to each ion emerging from the mass selector. The signal from the electron multiplier is connected to the electronic amplifier and data-handling system outside the vacuum.

In order to determine the constituents of the gas mixture, the ratio of RF to DC field strengths is varied (swept) to permit progressively heavier ions to transit the mass selector. The sweep, or scan, over the full range of masses (from 1 to 300 amu) only takes about 100 milliseconds; the scan is usually repeated multiple times to statistically improve the quality of the data. This scanning produces the mass spectrum, a plot of the partial pressure or intensity of each mass.

The mass spectrum of the unknown compound is compared to a library of mass spectra. The HAPSITE ER identifies the unknown compound based upon this comparison.

2.4.3 Vacuum System

The Mass Spectrometer is operated in a vacuum for several reasons.

- The ions must travel 0.3048 m (12 in) from the ionizer through the quadrupole to the electron multiplier without colliding with another molecule (A collision would modify their trajectory and possibly their charge.)
- The sample gas must be free from interference from other unknown gases
- The hot filament, which generates the electrons, would be destroyed if operated at atmospheric pressure in the presence of oxygen

The vacuum is initially created by the turbo-molecular and diaphragm pumps in the Service Module. When a good vacuum is achieved, the pumps in HAPSITE ER are turned on and the vacuum interconnect valve is closed. At this point, the Service Module can be disconnected.

The two vacuum pumps of HAPSITE ER continue to provide the pumping necessary for operation. These two pumps are the non-evaporable getter (*NEG*) pump and the smaller sputter-ion pump. The NEG pump incorporates a special zirconium alloy, arranged in sintered disks, which aggressively adsorbs gas molecules when heated.

Over time, the sintered disks gradually become saturated with gas molecules, which causes the adsorption ability to drop. The instrument detects the resulting rise in operating pressure (loss of vacuum) and the software signals that the pump must be replaced.

The NEG pump can effectively remove active gases, but not noble gases. An ion pump is necessary to pump out noble gases, which would accumulate in the Mass Spectrometer. The accumulation would raise the Mass Spectrometer pressure and interfere with operation.

The turbo molecular pump in the Service Module is actually a compound pump, incorporating turbo molecular stages for high pumping speeds at low pressure, and molecular drag stages to provide good compression of the gas at higher pressures. However, even with drag stages, the turbo molecular pump is unable to exhaust gas into atmospheric pressure. An additional diaphragm roughing pump is provided for this purpose.

The diaphragm pump consists of four stages. The diaphragm pump draws the gas from the exhaust of the compound pump and sufficiently compresses exhaust gas in order to discharge the exhaust into the atmosphere.

2.4.4 Electronic Systems

The electronic systems in HAPSITE ER are considered in four groups:

- Mass Spectrometer Control, see section 2.4.4.1
- Gas Chromatograph Control, see section 2.4.4.2
- Main Processor, see section 2.4.4.3
- Interfaces, see section 2.4.4.4

2.4.4.1 Mass Spectrometer Control

The Mass Spectrometer control electronics include the programmable DC and RF power supplies for the mass selector, DC power supplies for the filament, electron multiplier, ion pump, and A/D converter for the signal from the electron multiplier.

2.4.4.2 Gas Chromatograph Control

The Gas Chromatograph (GC) control circuitry includes the power supplies for the solenoid valves, ovens and heated inlet line. It also controls the logic for all the valves and heaters of the GC system.

2.4.4.3 Main Processor

The main processor is supported by solid state memory and is located in the central electronics assembly. The main processor controls all the other electronic sub-assemblies for routine operation.

2.4.4.4 Interfaces

There are several input/output devices within HAPSITE ER. These include the front panel touchscreen, keypad and display, USB drive, crossover cable connection, wireless connection, probe, power and logic connections to the Service Module, Headspace Sampling System and SituProbe.

2.5 Software Systems

HAPSITE ER operates with two software systems:

- Control software accepts inputs from the touchscreen, keypad and other interfaces. It commands the operation and sequencing of all systems and subsystems. The control software allows a method to be started from the front panel. Design or modifications of a method require the use of HAPSITE ER IQ™ software on an external laptop.
- Analysis software analyzes the data from the Mass Spectrometer, accesses the libraries as required, and displays the results of the analyses on the front panel.

Additionally, HAPSITE ER Application software, ER IQ, is a Windows® XP, Windows 2000, and Windows 7 based system for laptop use. ER IQ is used to design and modify methods, view data, analyze results, and generate reports. The laptop is linked to HAPSITE ER via a specific crossover cable or wireless connection. This linkage permits data and methods to be uploaded from HAPSITE ER. It also allows for new or modified methods to be downloaded to HAPSITE ER.

Chapter 3
HAPSITE Components and Assemblies

3.1 Ship Kit Packing Lists

3.1.1 930-850-G9, G12 Ship Kit Contents

The following items are provided in a typical 930-850-G5, G8 HAPSITE Ship Kit.

Box 1 Contents

- ❑ . 036-0015 . . . . . Shoulder Strap
- ❑ . 074-290 . . . . . Instruction Sheet (Shoulder Strap)
- ❑ . 059-0329 . . . . . Quick Disconnect Stem
- ❑ . 070-0972 . . . . . Plunger Contact (Bag of 4)
- ❑ . 074-490-P1. . . . Quick Use Guide
- ❑ . 074-5009-G1. . . Manual CD
- ❑ . 074-5012-G1. . . Basic Front Panel Training CD
- ❑ . 600-1319-P2. . . Ethernet Cable
- ❑ . 930-021-G1. . . . Gasket Kit
- ❑ . 930-022-G1. . . . Tool Kit
- ❑ . 930-716-G1. . . . Concentrator Tube (Tri-Bed)
- ❑ . 930-0221-G1. . . Concentrator Nut and Ferrule
- ❑ . 930-0231-G1. . . Probe Nut and Ferrule
- ❑ . 930-2020-G1. . . Cap Kit ER
- ❑ . 930-4652-P1. . . Permanent Marker
- ❑ . 930-612-P1. . . . USB Flash Drive

Special Cords for International Ship Kits
Extra Cords for SM and Battery Charger (Qty. 2)

	Ship Kit	Location . .	Cord
❑ .	930-850-G5. . . .	USA	N/A
❑ .	930-850-G8. . . .	Australia . .	068-0393

Box 2 Contents

❑ . . . . .930-470-G1 Battery Charger

Box 3 Contents

❑ . . . . 24 V Power Supply (see table)

Power Supply	Ship Kit	Usage
930-469-P1	930-850-G5	110 V USA
930-469-G4	930-850-G18	230 V Australia

Box 4 and 5 Contents

❑. . . . . In two separate boxes,
Battery Pack NiMH (930-4061-G1)

3.1.2 930-850-G10, G11 Ship Kit Contents

The following items are provided in a typical 930-850-G6, G7 HAPSITE Ship Kit.

Box 1 Contents

- ❑ . . 036-0015 . . . . . Shoulder Strap
- ❑ . . 074-290 . . . . . Instruction Sheet (Shoulder Strap)
- ❑ . . 059-0329 . . . . . Quick Disconnect Stem
- ❑ . . 070-0972 . . . . . Plunger Contact (Bag of 4)
- ❑ . . 074-490-P1 . . . Quick Start Guide
- ❑ . . 074-5009-G1 . . Manual CD
- ❑ . . 600-1319-P2 . . Ethernet Cable
- ❑ . . 930-021-G1 . . . Gasket Kit
- ❑ . . 930-022-G1 . . . Tool Kit
- ❑ . . 930-249-G2 . . . Concentrator Cover
- ❑ . . 930-251-G1 . . . Concentrator Tube (Tenax®-TA)
- ❑ . . 930-716-G1 . . . Concentrator Tube (Tri-Bed)
- ❑ . . 930-0221-G1 . . Concentrator Nut and Ferrule
- ❑ . . 930-0231-G1 . . Probe Nut and Ferrule
- ❑ . . 930-2020-G1 . . Cap Kit ER
- ❑ . . 930-4652-P1 . . Permanent Marker
- ❑ . . 930-612-P1 . . . USB Flash Drive

Special Cords for International Ship Kits

Extra Cords for SM and Battery Charger (Qty. 2)

Ship Kit.	Location . . .	Cord
❑ . . 930-850-G6 . . .	Europe	068-0151
❑ . . 930-850-G7 . . .	UK	068-0388

Box 2 Contents

❑ . . . . .930-470-G1 Battery Charger

Box 3 Contents

❑ . . . . 24 V Power Supply (see table)

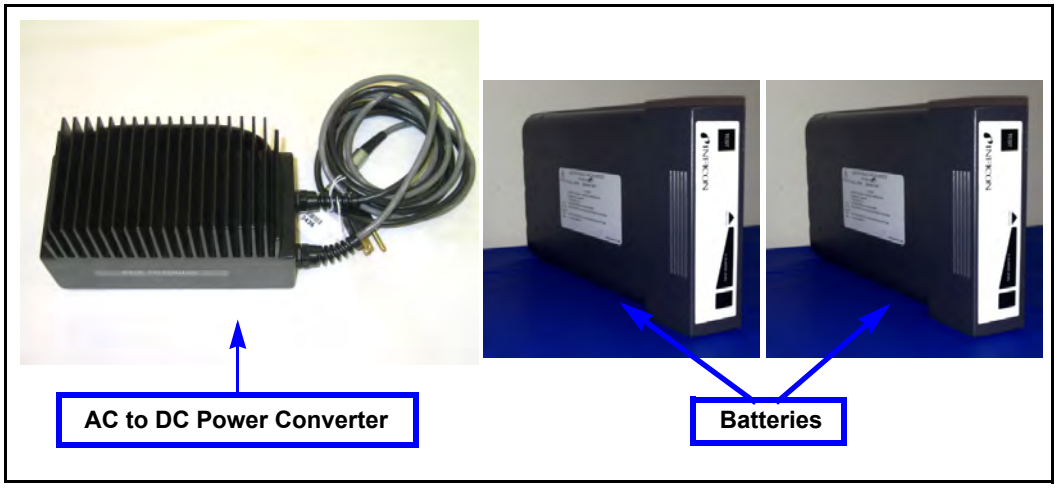
Power Supply	Ship Kit	Usage
930-469-P2	930-850-G10	230 V European
930-469-G3	930-850-G11	230 V UK

Box 4 and 5 Contents

❑. . . . . In two separate boxes,
Battery Pack NiMH (930-4061-G1)

3.1.3 Ship Kits Box 3 and 4

Figure 3-1 USA 24V Power Supply (AC To DC Power Converter) - Box 3 and Battery (2 Shipped) - Boxes 4 and 5



A laptop computer and its accessories will be shipped. The ship kits for the laptops will vary; the items in the laptop ship kit is based upon the type of laptop ordered. The laptop kits will include the ER IQ Software CD and NIST Library Install CD.

3.2 Basic Assembly

CAUTION

HAPSITE ER must be operated a minimum of every 3 weeks. Recommended storage is in Extended Standby.

Figure 3-2 HAPSITE Parts for Basic Assembly

3.2.1 Attaching the Probe

The probe attaches on the top of HAPSITE ER. The probe has two connections: a LEMO® communication line and a Valco connector.

1. Remove the silver LEMO port cap from the HAPSITE ER by pulling it outwards. Store the port cap for future use. (See Figure 3-3.)

Figure 3-3 Silver LEMO Port

2. Unscrew the Valco connector port cap. Store the port cap for future use. (See Figure 3-4.)

Figure 3-4 Valco Connector

3. Align the red dots on the LEMO communication line with the red dots on the port. Insert the line into the port. (See Figure 3-5.)

Figure 3-5 Aligning Red Dots

4 Insert the Valco connector into the top of HAPSITE ER. Screw the Valco connector into place. (See Figure 3-6.)

Figure 3-6 Valco Connector

NOTE: Save all of the port caps for further use.These caps are necessary when decontaminating HAPSITE ER. Spare caps are provided in the Ship Kit.

3.2.2 Installing the Gas Canisters

CAUTION

Do not open the front panel in a contaminated area.

The carrier and internal standard gas canisters must be installed inside HAPSITE ER prior to sampling. See section 2.4.1, Gas Chromatograph, on page 2-3 for information on the gas canisters. Follow the instructions below to install the gas canisters into the spring-loaded slots inside the unit.

1 Open the panel by placing thumbs on the top of panel and pulling downwards. This technique avoids damaging the sealing gasket with fingernails. (See Figure 3-7.)

Figure 3-7 Opening the Front Panel

2 Insert a yellow banded internal standard canister into the bottom round opening. This opening is marked with a yellow stripe. (See Figure 3-8.)

Figure 3-8 Inserting Internal Standard Canister

3 Press the **PUSH** lever while inserting the internal standard canister. (See Figure 3-9.)

Figure 3-9 PUSH Lever

4 Once inserted, press in the canister and PUSH level together, then release the **PUSH** lever. (See Figure 3-10.)

Figure 3-10 Push Lever

5 Gently pull on the internal standard canister outwards. It should remain fastened inside the HAPSITE ER. (See Figure 3-11.)

Figure 3-11 Internal Standard Installation Verification

CAUTION

Closing the front panel when the canisters are not properly installed may damage HAPSITE ER and/or canisters.

6 Insert a purple banded carrier gas canister into the bottom round opening. This opening is marked with a purple stripe. (See Figure 3-12.)

Figure 3-12 Inserting the Carrier Gas

7 Press the **PUSH** lever while inserting the carrier gas canister. (See Figure 3-13.)

Figure 3-13 Pressing the PUSH Lever

8 Once inserted, release the **PUSH** lever. (See Figure 3-14.)

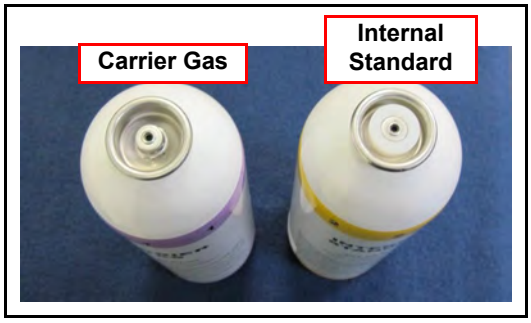
Figure 3-14 Releasing the PUSH Lever

9 Gently pull the carrier gas canister outwards. It should remain fastened inside HAPSITE ER. (See Figure 3-15.)

Figure 3-15 Carrier Gas Installation Verification

NOTE: The position of the gas canisters should not be interchanged. To prevent improper placement, the internal standard canister has a Teflon® ring which surrounds the inner stem on the top of the can. Do not force the canisters into the wrong location as this will contaminate and/or damage HAPSITE ER. (See Figure 3-16.)

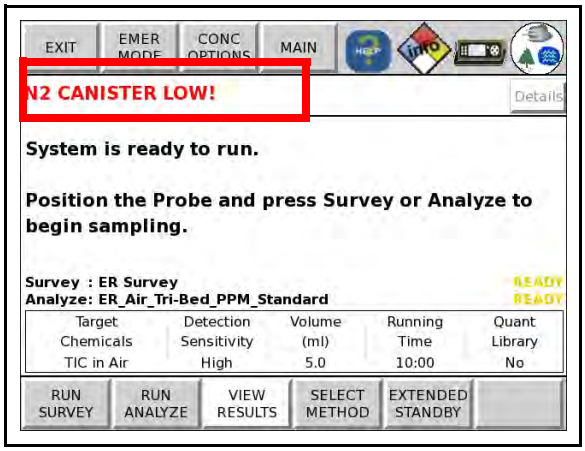
Figure 3-16 Inner Stem of Canisters



3.2.2.1 How to Remove a Gas Canister

Removing the gas canisters is advised when HAPSITE ER has been placed into Extended Standby. Also, the gas canister will need to be replaced when the canister is low. A low canister warning will be displayed on the front panel when the canister needs replacement. (See Figure 3-17.) Follow the instructions below to remove a gas canister.

Figure 3-17 Canister Replacement Warning



1 Press the **PUSH** lever located to the right of the canister. (See Figure 3-18.)

Figure 3-18 Pressing the Lever

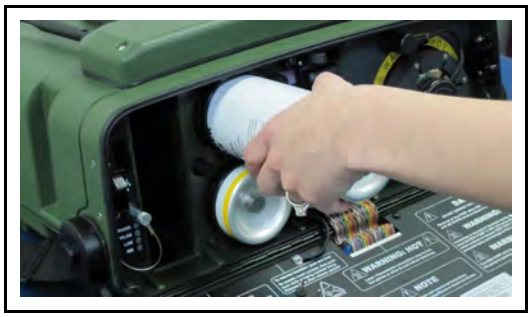
2 The canister will release. (See Figure 3-19.)

NOTE: A slight twist on the canister may be required.

Figure 3-19 Canister Release

3 Remove the canister. (See Figure 3-20.)

Figure 3-20 Remove the Canister



The carrier gas canister will need to be replaced after approximately 12 hours of use. The internal standard canister will need to be replaced after 3 days of continuous use. These numbers are guidelines and will vary.

WARNING

Do not refill canisters. Bodily injury may result. Canisters are designed to be disposable and may fail if filling is attempted.

CAUTION

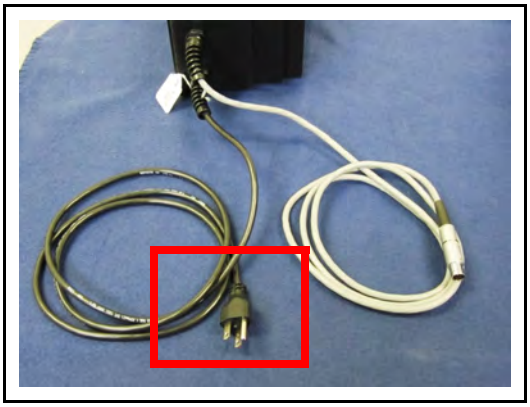
Closing the front panel when the canisters are not properly installed may damage HAPSITE and/or canisters.

3.2.3 Connect the Power Supply

HAPSITE ER uses an AC to DC power converter power supply. This power supply connects to HAPSITE ER and a power outlet.

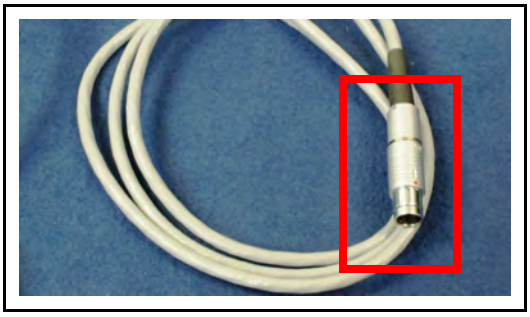
1. The connection with the black cord is fitted with a standard power plug. Plug this cord into a power outlet. (See Figure 3-21.)

Figure 3-21 Black Cord



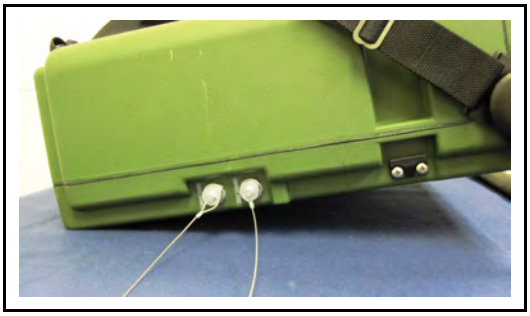
2. The connection with the gray cord is fitted with a LEMO connection. (See Figure 3-22.) When facing the front panel, this cord will plug into the left side of HAPSITE ER.

Figure 3-22 HAPSITE Power Port



3. Remove the silver plugs from HAPSITE ER. Store the plugs for future use. These plugs will be necessary when decontaminating the unit. (See Figure 3-23.)

Figure 3-23 Removing the Silver Plugs



4 Align the red dots on the LEMO connection with the red dots on HAPSITE ER. Insert the connection into the power port. (See Figure 3-24.)

Figure 3-24 Aligning Red Dots

3.2.4 Connecting the Laptop

HAPSITE ER has two possible configurations for connecting a laptop computer:

- via the black crossover cable
- via the wireless connection

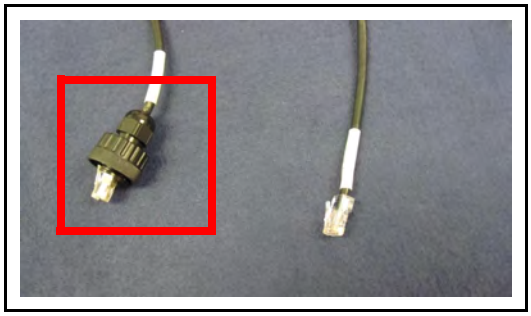
3.2.4.1 Connect Laptop with Black Crossover Cable

1 Unscrew the cap on the port which is located on the top, left-hand side of the HAPSITE ER. (See Figure 3-25.)

Figure 3-25 Crossover Cable Port

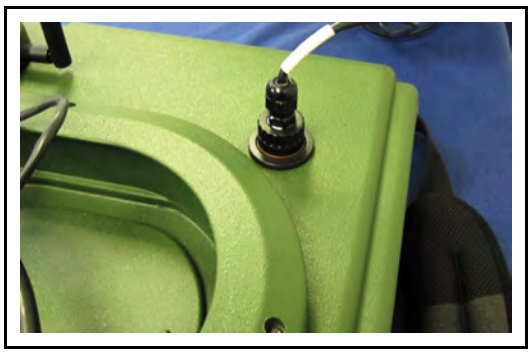
2 The crossover cable has two ends. One end has a screw top on the modular connector. This end will connect to HAPSITE ER. (See Figure 3-26.)

Figure 3-26 Crossover Cable



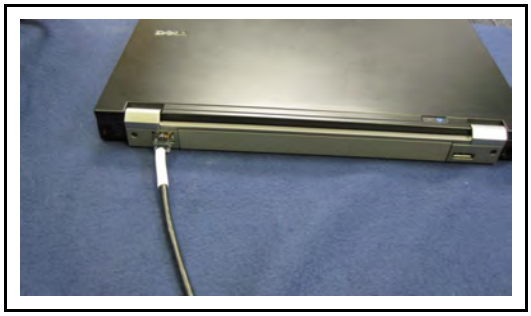
3 Plug the modular connector with the screw top into HAPSITE ER port. Screw the plug into place. (See Figure 3-27.)

Figure 3-27 Modular Connector



4 Plug the opposite end into the laptop. (See Figure 3-28.)

Figure 3-28 Plugging in the Laptop



5 Once connected, the crossover cable communication between HAPSITE ER and laptop computer will be enabled.

NOTE: To troubleshoot or set up communications for a new laptop, see section 3.2.4, Connecting the Laptop, on page 3-14.

3.2.4.2 Connect Laptop with Wireless Connection

Refer to Chapter 5, Communications and Touch Screen Options for information on enabling the wireless connection.

3.3 Battery

The battery provides power to HAPSITE ER when portability is desired. Under optimum conditions, the battery has a two hour life. The battery can be charged using the battery charger. Alternately, it can be charged in the HAPSITE ER when it is connected to external power. However, the battery will charge more slowly when charging inside HAPSITE ER.

3.3.1 Battery Charger

The auxiliary battery charger (part number 930-470-G1) uses AC power to charge up to three HAPSITE batteries in 15 hours or less.

CAUTION

The battery charger is not sealed against moisture, debris, or contamination.

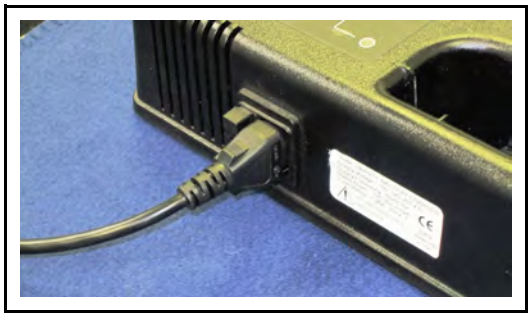
The battery charger operates from a range of nominal AC voltages from 100 to 230 V(ac). It will continue to operate without internal damage at a voltage as low as 90 V(ac) and as high as 253 V(ac). The frequency can be from 50 to 60 Hz. The battery charger draws 120 W when fully loaded.

The battery charger is designed for indoor use at ambient temperatures from 5°C to 35°C (41°F to 95°F). The battery charger is not designed for exposure to contaminants, as it cannot be decontaminated.

3.3.2 Battery Charger Connections and Startup

1. Plug the power cord into the connector at the right rear of the battery charger. (See Figure 3-29.)

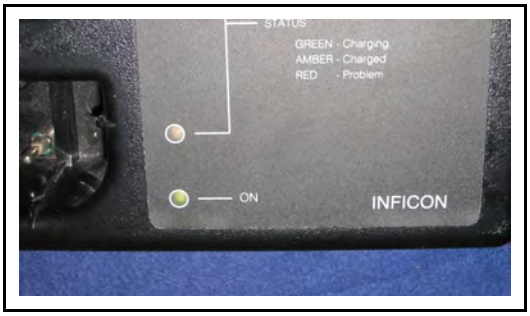
Figure 3-29 Plugging in the Power Cord for the Battery Charger



2 Plug the battery charger into a grounded outlet.

3 The **ON** indicator on the battery charger will illuminate. The battery charger does not have a power switch. (See Figure 3-30.)

Figure 3-30 ON Indicator



4 As the battery charger performs a self-test, all the indicators will turn amber.

5 The indicators for the empty receptacles will then turn green. If a receptacle contains a battery, its indicator will turn red.

6 All lights except for the **ON** indicator will extinguish. No further warm-up is required; it is ready to charge batteries.

3.3.3 Loading the Battery Charger

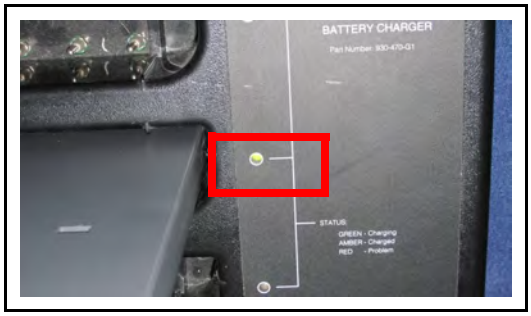
The battery charger receptacles are identical and batteries in any state of charge can be loaded.

1 Place the discharged battery into one of the charging receptacles. (See Figure 3-31.)

Figure 3-31 Placing Battery into Charging Receptacle

2 The respective indicator will turn green and charging will commence immediately. (See Figure 3-32.)

Figure 3-32 Charging Indicator



CAUTION

Do not use excessive force when placing the battery in the battery charger.

CAUTION

Do not charge batteries in a moving vehicle.

3.3.4 Understanding the Battery Charger Indicators

Each battery receptacle is associated with an indicator light which can be illuminated in the colors listed below.

Green . . . . . The battery is being charged. If a battery with a severely depleted charge is inserted, the green light will flash. If it flashes for more than 10 minutes, the battery will not accept a charge and should be replaced. The actual state of the battery charge can be assessed by using the **TEST** button on the battery. A fully discharged battery will charge in approximately 15-20 hours.

Amber . . . . . The battery is fully charged. The rate of charge has been reduced to a maintenance level. The battery can remain in charger indefinitely.

Red . . . . . The receptacle and/or the battery, if one is installed is experiencing a problem. A flashing red light indicates that the charger cannot communicate with the battery.

Off . . . . . The receptacle is ready to charge a battery. If the indicator remains extinguished when a battery is inserted, the battery is severely depleted. In this case, leave the battery in the receptacle and unplug the power cord. Reconnect the power cord and the battery will start to charge.

3.3.4.1 Testing Battery

1 To test a battery, press the **TEST** button on the end of the battery. (See Figure 3-33.)

Figure 3-33 Battery TEST Button

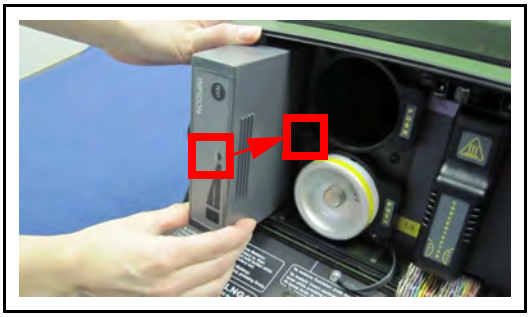
2 In the elongated triangle, green lighted numbers will be displayed. The highest illuminated number indicates the remaining percentage of battery charge, which is reported in 20% increments.

NOTE: If **OVER** is illuminated, the battery is fully charged.

3.3.5 Installing the Battery

1 Insert a fully charged battery by sliding it into the rectangular opening to the left of the gas canisters. The battery should be inserted with the release arrow pointing towards the release button. (See Figure 3-34.)

Figure 3-34 Inserting Battery



2 Push firmly and listen for the battery to click into place. (See Figure 3-35.)

Figure 3-35 Installing Battery

3 Once in place, gently pull the battery outwards to ensure that the battery is securely fastened.

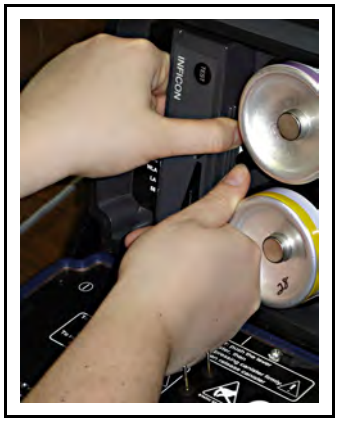
3.3.6 Removing the Battery

1 Firmly push in the battery until a faint click is heard. (See Figure 3-36.)

Figure 3-36 Removing the Battery

2 Push in the **Release** button, the black round button to the right of the battery. (See Figure 3-37.)

Figure 3-37 Release Button



3 Pull the battery out of its compartment while pressing the release button.

CAUTION

Do not expose the battery compartment to rain or other foreign material. Ensure that the area is dry and contaminant-free before opening the front panel.

3.3.7 Replacing the Concentrator

HAPSITE ER is shipped with the concentrator already installed. The concentrator will only need to be replaced if it becomes chipped or cracked, or the concentrator becomes saturated with use. If the concentrator does not cleanout after numerous cleanout methods, this may be indicative of a chipped or cracked concentrator.

1 Open the front panel of HAPSITE ER and remove the black cover labeled **CONCENTRATOR**. (See Figure 3-38.)

Figure 3-38 Removing the Concentrator Cover

WARNING

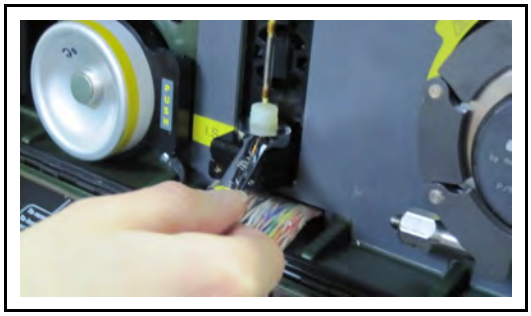
The elbow fittings may be hot. Allow these fittings to cool before continuing.

WARNING

Excessive force and/or tightening can cause the fragile glass to break. Tighten nuts to finger-tight only.

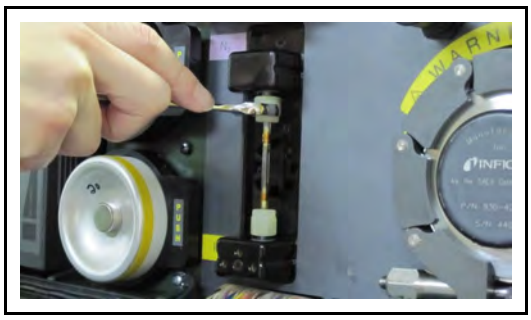
2 Using the 7/16 in. wrench, turn the bottom nut a 1/4 turn counterclockwise. (See Figure 3-39.)

Figure 3-39 Turning the Bottom Nut with Wrench



3 Using the 7/16 in. wrench, turn the top nut a 1/4 turn clockwise. (See Figure 3-40.)

Figure 3-40 Turning the Bottom Nut with the Wrench

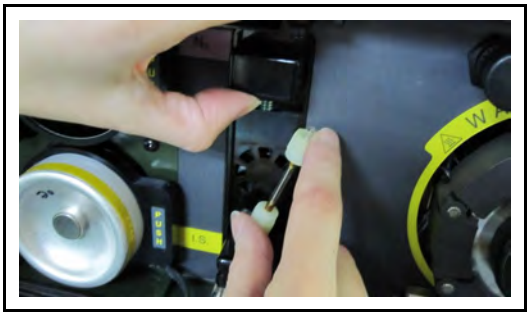


4 With fingers, continue to loosen the nuts on the top and bottom of the concentrator until the concentrator is unscrewed. (See Figure 3-41.)

Figure 3-41 Loosening the Concentrator Nuts

5 Lift the top elbow. Gently lift and angle the concentrator out of the fixture. (See Figure 3-42.)

Figure 3-42 Inserting the Concentrator



WARNING

The elbow fittings may be hot. Allow for these fittings to cool before continuing.

6 Carefully, remove the concentrator from the bottom elbow. Avoid losing the ferrules which are located inside the nuts. (See Figure 3-43.)

Figure 3-43 Removing the Concentrator

7 Dispose of the damaged concentrator according to local procedure. Please be aware that the concentrator contains glass.

WARNING

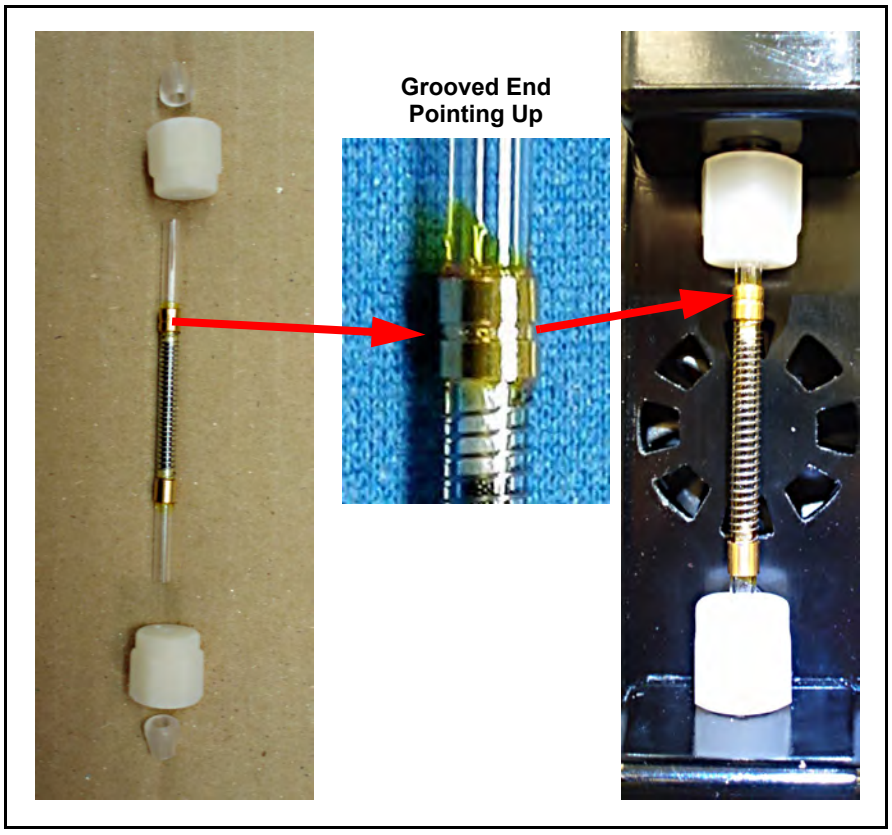
The concentrator contains glass. Wear appropriate personal protection equipment when handling a broken concentrator.

8 Remove the new concentrator from the storage vial and unwrap it.

9 Ensure that a Teflon® ferrule is installed into the threaded end of each plastic nut with the wide end of the cone facing toward the center of the concentrator. (See Figure 3-44.)

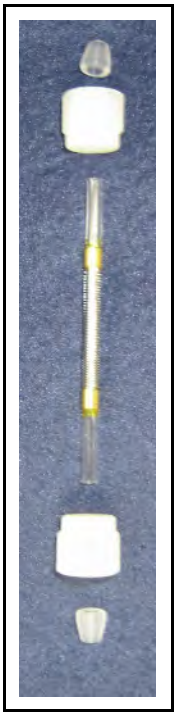
10 The Tri-Bed concentrator is directional. The Tri-Bed concentrator must be installed with the smooth metal sleeve pointing downwards and the grooved metal sleeve pointing upwards. (See Figure 3-44.)

Figure 3-44 Proper Tri-Bed Concentrator Orientation



11 The Tenax Concentrator does not have a specific orientation. (See Figure 3-45.)

Figure 3-45 Tenax Concentrator

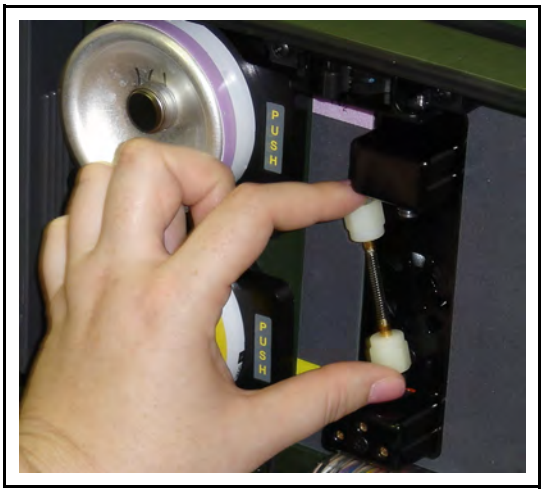


12 Place the Tri-Bed concentrator:

12a **Tri-Bed concentrator**: While holding the nut and ferrule in place, carefully place the smooth metal sleeve end of the Tri-Bed concentrator into the lower elbow fitting.

12b **Tenax concentrator**: While holding the nut and ferrule in place, carefully place either end of the concentrator into the lower elbow fitting. (See Figure 3-46.)

Figure 3-46 Placing Concentrator in the Bottom Elbow



13 Insert the top of the concentrator:

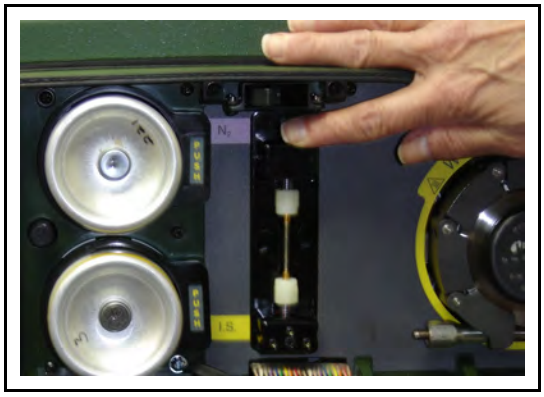
13a **Tri-Bed concentrator**: Carefully lift up on the top elbow fitting and insert the end of the concentrator with the grooved metal sleeve into this fitting. (See Figure 3-47.)

13b **Tenax concentrator**: Carefully lift up on the top elbow fitting and insert either end of the concentrator into this fitting. (See Figure 3-47.)

Figure 3-47 Inserting the Top of the Concentrator

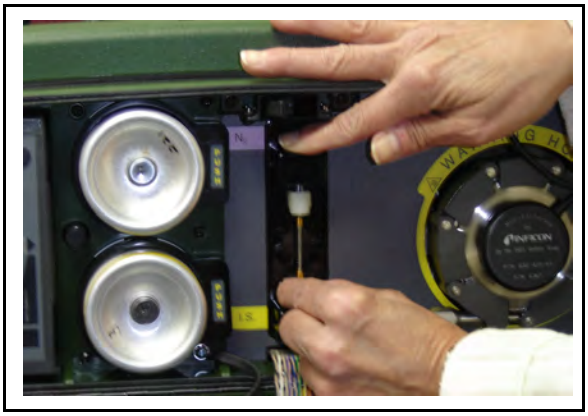
14 Keep the concentrator aligned between the two elbow fittings while gently pressing down on the top elbow fitting. (See Figure 3-48.)

Figure 3-48 Pressing Down on Elbow Assembly



15 While maintaining steady pressure on the top elbow fitting, finger-tighten the bottom nut of the concentrator until tight. (See Figure 3-49.)

Figure 3-49 Tightening the Top and Bottom Nut



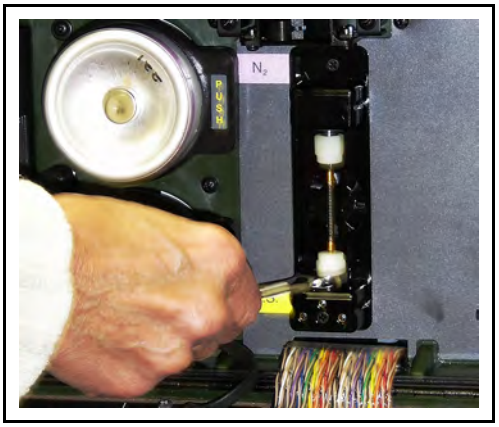
16 While continuing to maintain steady pressure on the top elbow, finger-tighten the top nut until tight.

WARNING

Excessive force and/or tightening can cause the fragile glass to break.

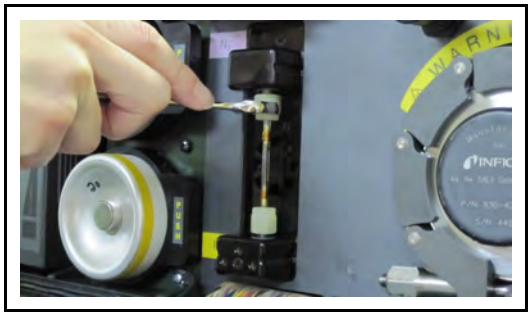
17 Using a 7/16 in. wrench, turn the bottom nut approximately 1/4 of a turn clockwise until tight. (See Figure 3-50.)

Figure 3-50 Using Wrench to Tighten Bottom Nut



18 Using a 7/16 in. wrench, turn the top nut approximately 1/4 of a turn counter clockwise until tight. (See Figure 3-51.)

Figure 3-51 Using Wrench to Tighten Top Nut



19 When **gentle** upward pressure is applied to the top elbow, the elbow should not move. If the elbow moves, the concentrator is not properly seated. Repeat section 3.3.7, Replacing the Concentrator, on page 3-21.

20 The concentrator cover contains two metal contacts. Inspect the contacts to verify that they fit snuggly onto the concentrator collars, ensuring electrical contact, without placing uneven strain on the glass concentrator tube. (See Figure 3-52.)

Figure 3-52 Inspecting Concentrator Cover

21 Place the black concentrator cover over the concentrator and elbow assembly. The cover should fit easily; force is not required if the concentrator is properly installed. (See Figure 3-53.)

Figure 3-53 Concentrator Cover

NOTE: If the cover does not easily fit over the concentrator, do not force it. Check to ensure that the concentrator is correctly installed with the concentrator fully seated into both elbows and the nuts properly tightened for a secure fitting.

22 Close the front panel.

3.3.8 Probe Nut Assembly

The ferrules inside the probe nut are installed in the probe when shipped. It may be necessary to replace the ferrules if they become misshapen due to frequent use.

The orientation of the ferrules in the probe nut is critical for proper sampling when attaching a bag sample or VX/R-33 Conversion Tube. Verify that the orientation of the ferrules is correct prior to sampling.

1 Using a guide (i.e., a small screwdriver or a plastic pen cap with pocket clip extension), place the metal probe nut over the guide's narrow end. The threads on the nut should be facing upwards.

NOTE: Verify that the guide is clean to prevent the introduction of contaminants into the HAPSITE ER system.

2 Place the small, back ferrule over the narrow end of the guide with the beveled side facing upwards. (See Figure 3-54.)

3 The cone-shaped ferrule should be placed over the bevel with the narrow end facing upwards. (See Figure 3-54.)

4 Carefully remove the nut assembly from the narrow end of the guide. Gently tap the nut to seat the ferrule properly into the nut.

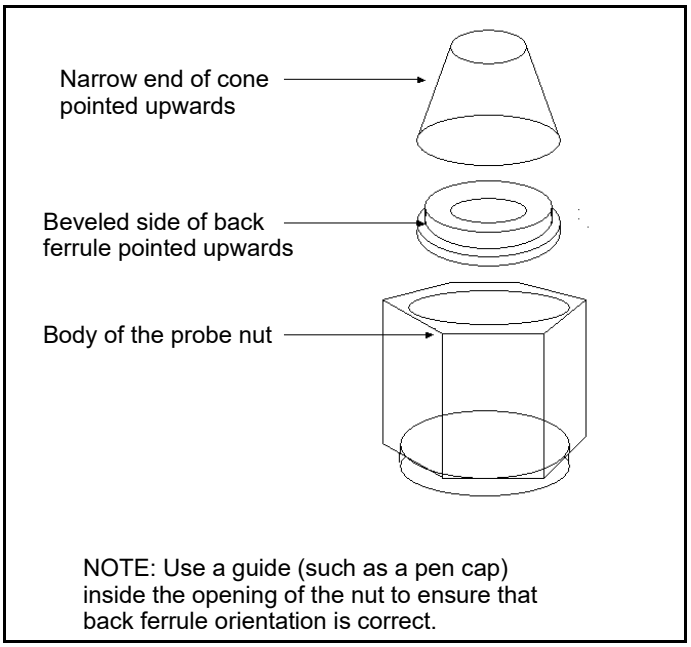
5 Thread the nut-ferrule assembly onto the probe.

6 Finger-tighten the nut-ferrule assembly into place.

WARNING

Correct ferrule orientation is critical to avoid leaks of hazardous or toxic material

Figure 3-54 Diagram of Proper Ferrule Orientation in the Probe Nut



3.3.9 Attaching a Bag Sample

When collecting samples, various sampling bags can be used. This procedure outlines the steps used to attach a Tedlar® bag.

WARNING

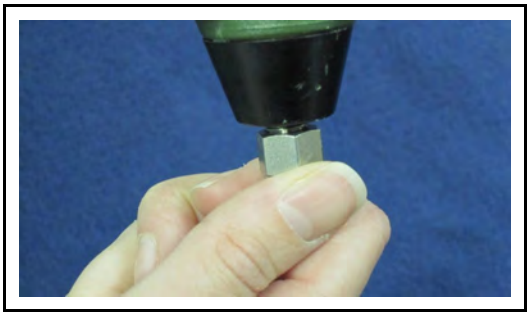
Ensure that the bag's valve remains closed when it is not attached to the probe.

WARNING

To avoid inhalation of bag's sample, attach an exhaust tube to the HAPSITE ER exhaust port. Vent the exhaust to a safe area.

1. Before attaching a Tedlar bag to the probe, refer to section 3.3.8, Probe Nut Assembly, on page 3-29 to ensure proper ferrule orientation in the probe nut.
2. Prepare the Tedlar bag sample. Avoid filling bag more than 80% full. Verify that the white valve is closed on the Tedlar bag.
3. Loosen the nut on the probe by turning the nut counter-clockwise up to two complete revolutions. (See Figure 3-55.)

Figure 3-55 Loosening Probe



4. Guide the white cylindrical stem of the bag valve assembly into the opening of the probe nut. (See Figure 3-56.)

Figure 3-56 Inserting the White Stem

5. Firmly push the stem into the probe nut. Two clicks will be heard when the bag is properly seated into the probe nut.
6. Finger-tighten the probe nut by turning the nut clockwise. (See Figure 3-57.)

Figure 3-57 Finger Tightening the Probe

7 When the front panel displays **Collect Sample Now**, open the Tedlar bag by turning the valve one complete counter-clockwise revolution. (See Figure 3-58.)

Figure 3-58 Opening the Tedlar Bag

8 When the sampling period is finished, close the bag by turning it one clockwise revolution until tight.

9 Unscrew the probe nut up to two revolutions. (See Figure 3-59.)

Figure 3-59 Unscrew the Probe

10 Pull out the Tedlar bag to detach. (See Figure 3-60.)

Figure 3-60 Detaching the Tedlar Bag

11 Finger-tighten the nut by turning the nut clockwise. (See Figure 3-61.)

Figure 3-61 Finger-Tighten the Nut

3.3.10 VX/R-33 Conversion Tube

This procedure describes how to prepare HAPSITE to sample VX or RVX using the VX-G conversion tubes (part numbers 930-4292-G1 and 930-4293-G1).

To detect VX or RVX, the VX-G conversion tube must be inserted into the probe head or thermal desorption tube.

The process of detecting VX or RVX with HAPSITE requires the conversion of VX or RVX (high boiling point chemicals) to what is referred to as the G analog. The VX or RVX molecule is broken at the sulfur bond when it comes into contact with a silver fluoride pad. The result is the formation of a volatile chemical ethyl methylphosphonofluoridate in the case of VX, or isobutyl methylphosphonofluoridate in the case of RVX. These compounds are chromatographed and detected by HAPSITE as VX-G or RVX-G.

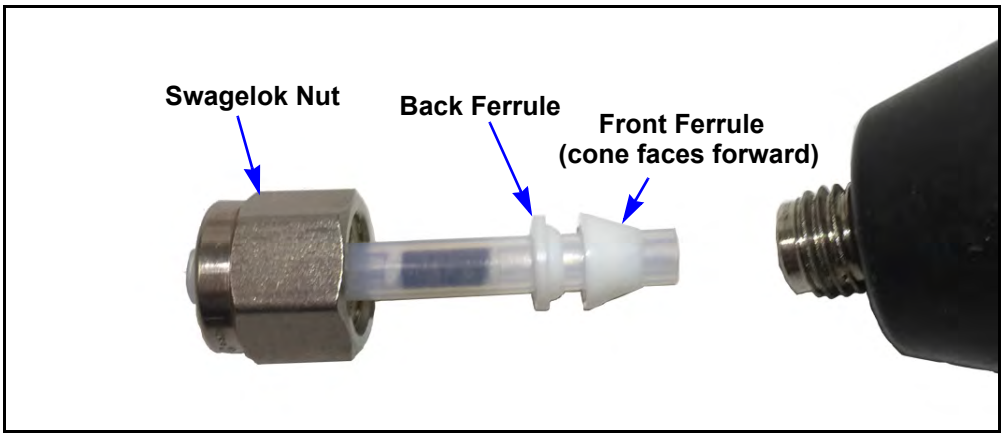
NOTE: G agents can be detected with the VX conversion pad in place. However, if other G agents are suspected, it would be best to also run the sample without the conversion tube in place.

NOTE: Sulfur mustard cannot be detected with the conversion tube in place.

3.3.10.1 Air Probe Sampling

The HAPSITE probe has a 3/16 in. Swagelok® nut installed at the end of the probe. Inside this nut is a ferrule. The ferrule consists of two pieces, a front and back ferrule. These must be in place and in the proper orientation. See Figure 3-62 for proper orientation.

Figure 3-62 Ferrule Location



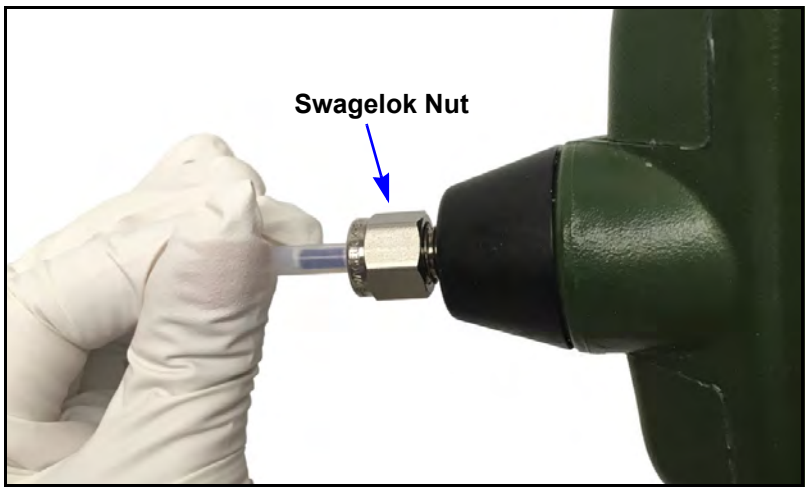
NOTE: If the nut is removed, ensure that the ferrules are not dropped. It is critical that both ferrules are in place and in proper orientation to ensure a leak-free fit around the VX-G conversion tube. See Figure 3-62.

If the nut and ferrules on the HAPSITE probe are in place, they do not need to be removed. The VX-G conversion tube can be inserted into the nut opening using the following procedure:

1 Loosen the Swagelok nut on the end of the probe approximately 1/4 to 1/2 turn. See Figure 3-63.

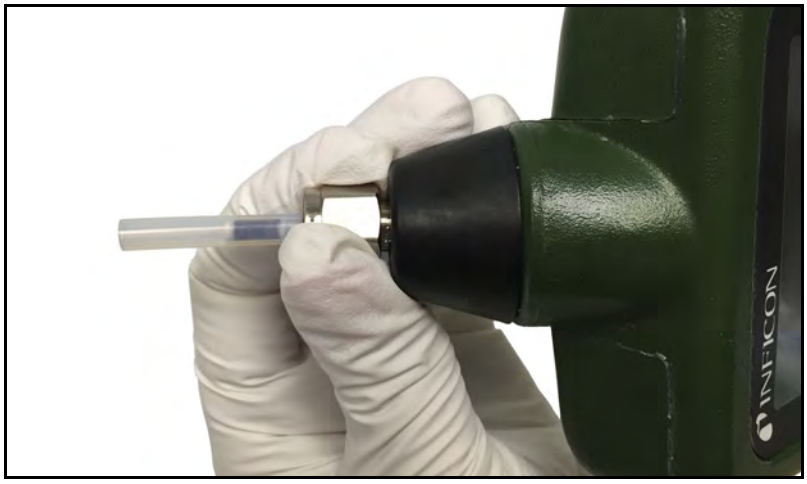
2 Insert the VX-G conversion tube into the Swagelok nut. Ensure the tube is firmly seated into the front ferrule. This positions the nut approximately 1/2 in. from the end of the tube inserted in the probe and 1 inch from the sampling end of the tube. See Figure 3-63.

Figure 3-63 Inserting the Conversion Tube



3 Tighten the Swagelok nut finger tight. Pull gently on the conversion tube, to ensure it is held firmly in place. (See Figure 3-64.)

Figure 3-64 Tightening the Swagelok Nut



NOTE: The VX-G conversion tube must be replaced after eight hours of exposure to light and air, or after exposure to VX or RVX.

The silver fluoride pads in the tube are light sensitive and are degraded by exposure to nitrogen containing compounds in air. The tubes must be stored in their original sealed container to maximize their shelf life.

CAUTION

To maintain the maximum shelf life of one year from manufacture date, store tubes sealed in their original packaging when not in use.

3.3.10.2 Thermal Desorption Tube Sampling

1 Fasten a 6 mm VX-conversion tube to the inlet end using a short segment of Tygon tubing, as shown in Figure 3-65.

2 Connect the thermal desorption tube in the proper orientation (flow direction arrow on the tube should point towards the sampling pump (see Figure 3-65)) to a small portable sampling pump. The air sample will be drawn through the conversion tube and onto the TD tube.

Suggested sampling flow rates are 20-100 mL/min. Suggested sample volumes are 100-1000 mL. Larger volumes should be tested for breakthrough, see **Thermal Desorber Sampling** in the Operating Manual for details.

After sampling is complete, remove the VX conversion tube from the TD tube. Continue analysis of TD tube as described in **Section 4.2** of the TDSS Operating Manual.

Figure 3-65 Sampling Pump and TD Tube

3.4 Helpful Guidelines

DON'T…	DO…
◆ Ship with a battery installed. ◆ Draw liquid into the instrument. ◆ Go into a potentially explosive environment without an LEL meter and safety checks. HAPSITE ER is not intrinsically safe. ◆ Pressure wash HAPSITE ER or immerse in water. ◆ Sample strong acids (below pH 2) or strong bases (above pH 11). ◆ Use force when assembling any HAPSITE ER system components. ◆ Modify default methods without changing their name. ◆ Sample for Sulfur Mustard (HD) with the VX conversion tube installed. ◆ Abort an Analyze (GC/MS) method during a sample run. ◆ Over-tighten the concentrator nuts. ◆ Block the exhaust vent on HAPSITE ER. ◆ Use the NEG pump and Service Module pumps together. ◆ Use expired internal standard gas. ◆ Attach a bag sample without first checking the ferrules in the probe nut.	◆ Leave a battery installed when operating, even when external power is connected. ◆ Run a background blank once per week or more. ◆ Use Extended Standby instead of powering off HAPSITE ER. ◆ Place appropriate caps over openings before decontaminating. ◆ Use 5% to 10% bleach solution or local SOP to decontaminate HAPSITE ER. ◆ Only use thumbs to open the front panel. ◆ Attempt to reboot as a first step to troubleshooting operational problems. ◆ Screen samples with the Survey method to reduce the risk of saturation. ◆ Use the VX conversion tube for identification (and quantification) of VX and R-33. ◆ Take a training course. ◆ Contact INFICON at HAPSITE.Support@INFICON.com, 800.223.0633 for help.

Chapter 4
Operating HAPSITE ER in Portable Mode

4.1 Starting HAPSITE ER in Portable Mode

Portable Mode refers to using HAPSITE ER without the Laptop computer.

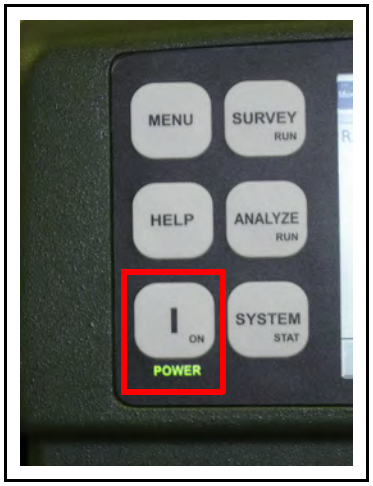
Required Materials

- HAPSITE (Analytical Module)
- Internal Standard Gas Canister
- Carrier Gas Canister
- Charged Battery
- AC to DC Power Converter Power Supply
- Probe

Procedure

1. Assemble HAPSITE ER as shown in section 3.2, Basic Assembly, on page 3-5.
2. Press the **POWER** button on the front panel. The word **POWER** will illuminate. Powering on HAPSITE ER takes one (1) to two (2) minutes. (See Figure 4-1.)

Figure 4-1 Power Switch



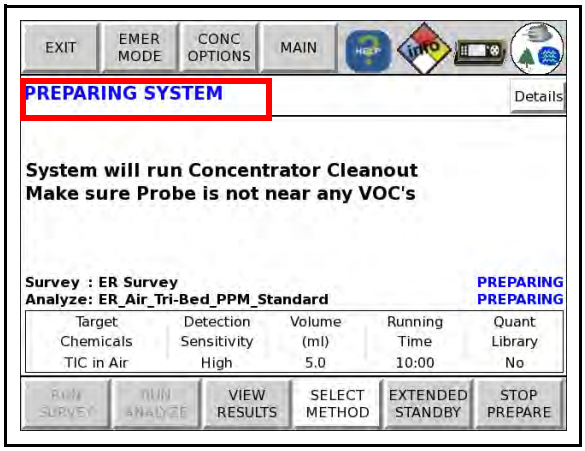
NOTE: Power on HAPSITE ER while connected to AC power. Using battery power to turn on and heat HAPSITE ER will consume over 40% of the battery's charge.

3. HAPSITE ER will boot in approximately one minute and will sense which sample configuration (i.e., concentrator) has been installed. It will begin to prepare the default method for this sample configuration.

4 HAPSITE ER will begin to prepare various components. These components include heating the HAPSITE and accessory heaters, running AutoTune (see Step 8 on page 4-3), powering the NEG, and if necessary, running concentrator cleanout.

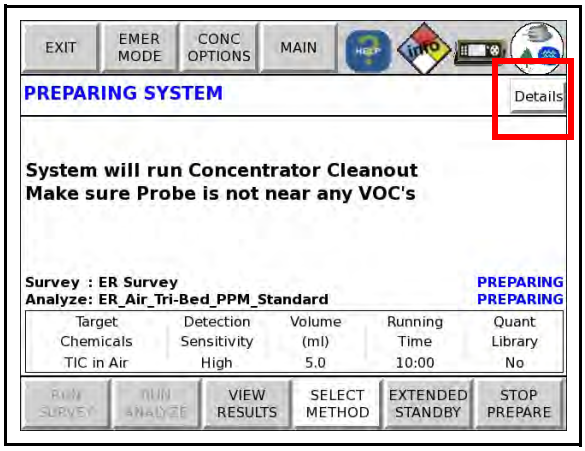
5 During the preparation period, the front panel will display the **PREPARING SYSTEM** message. Depending upon the chosen default method, this screen may show **PREPARING ANALYZE** or **PREPARING SURVEY**. This message will occur when the methods have different temperature setpoints. (See Figure 4-2.)

Figure 4-2 Front Panel Preparing System



6 To view the preparation details' progress, touch the **Details** button. (See Figure 4-3.)

Figure 4-3 Details Button



7 The progress of the preparation is shown by a bar graph. If a component is in the process of being prepared, it will be shown in blue. When a component is ready, it will be shown in green. If a component is going to be prepared, but the preparation process has not started, it will be shown in yellow. If the system is not ready, the items that need to be prepared will be shown in red. (See Figure 4-4.)

Figure 4-4 Preparation Bar Graph

8 When the heating sequence is completed, the software will check the mass spectrometer tune and automatically make any necessary adjustments. The automatic tune adjustment is called AutoTune. If AutoTune fails, see section 9.4, Performing Manual Tune, on page 9-7.

9 As part of the preparation, a concentrator cleanout will be run when the concentrator is installed. This cleanout will heat the concentrator to 180°C to remove residue. The cleanout will occur when the unit has been turned on, taken out of Extended Standby, the concentrator has been changed or the concentrator has been saturated.

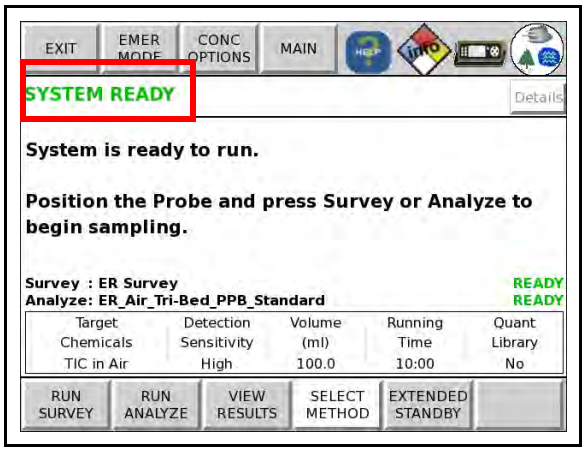
NOTE: If a concentrator cleanout is not desired due to an emergency, see section 4.1.1, Emergency Mode (EMER MODE), on page 4-6.

NOTE: A concentrator cleanout can also be skipped, although skipping the concentrator cleanout is not recommended and may lead to poor results. See section 4.1.2, Concentrator Options (CONC OPTIONS), on page 4-8.

10 Hold the probe in a clean environment for the duration of the cleanout. If the concentrator cleanout is not successful, see section 4.1.3, Concentrator Cleanout Failure, on page 4-11.

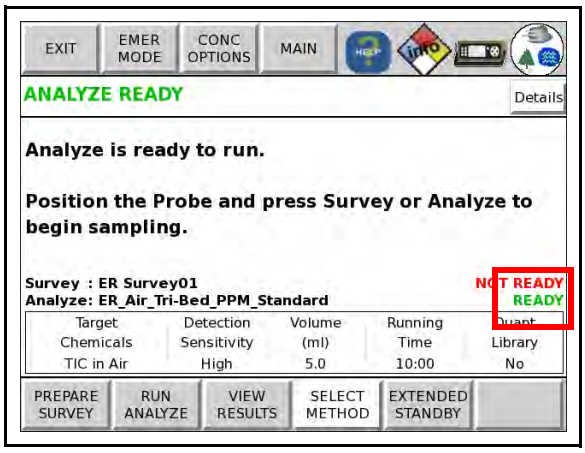
11 When HAPSITE ER is ready to run samples, a green **SYSTEM READY**, **SURVEY READY** or **ANALYZE READY** message will display. (See Figure 4-5.)

Figure 4-5 System Ready



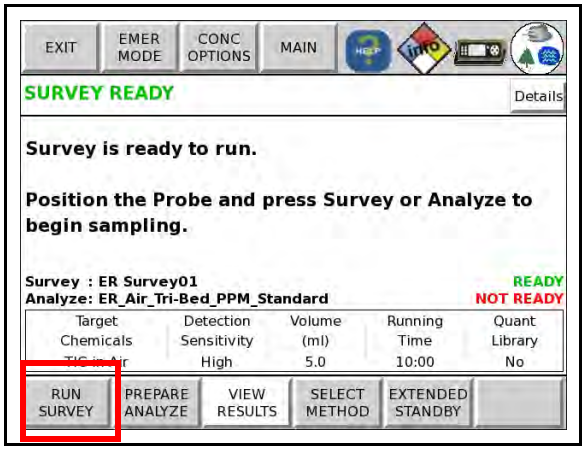
NOTE: If the methods have different temperature setpoints, the method that has been prepared to run will have a green **READY** message next to the method name.

Figure 4-6 Ready Message



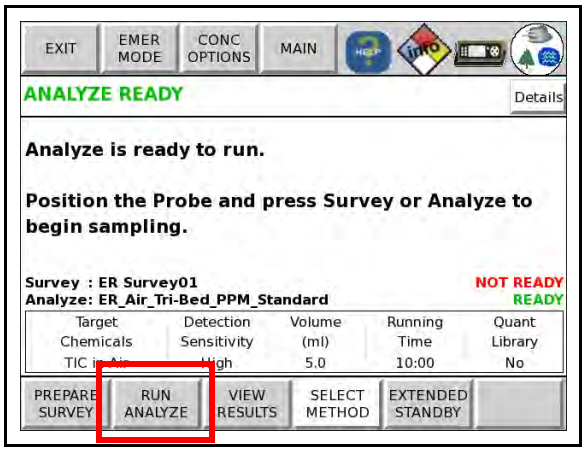
12 If **SURVEY READY** is displayed, touch **RUN SURVEY** or push **SURVEY RUN**. (See Figure 4-7.)

Figure 4-7 Survey Ready



13 If **ANALYZE READY** is displayed, touch **RUN ANALYZE** or push **ANALYZE RUN**. (See Figure 4-8.)

Figure 4-8 Analyze Ready



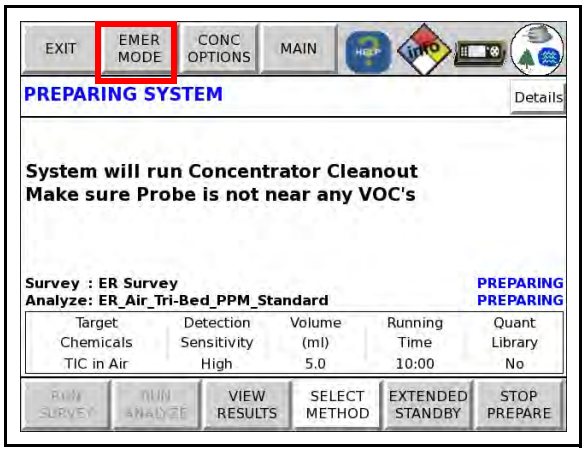
NOTE: If the system is preparing a **SURVEY** run and an **ANALYZE** method is desired, touch the **PREPARE ANALYZE** button. Likewise, if an **ANALYZE** method is being prepared and a **SURVEY** is desired, touch the **PREPARE SURVEY** button.

4.1.1 Emergency Mode (EMER MODE)

In an emergency, the concentrator cleanout can be bypassed to allow for faster startup. This is not recommended for everyday use. While Emergency Mode is active, the concentrator cleanout will continue to be skipped until Emergency Mode is exited. To place the system into Emergency Mode:

1 Touch **EMER MODE** while the **PREPARING SYSTEM** message is displayed. (See Figure 4-9.)

Figure 4-9 Emergency Mode

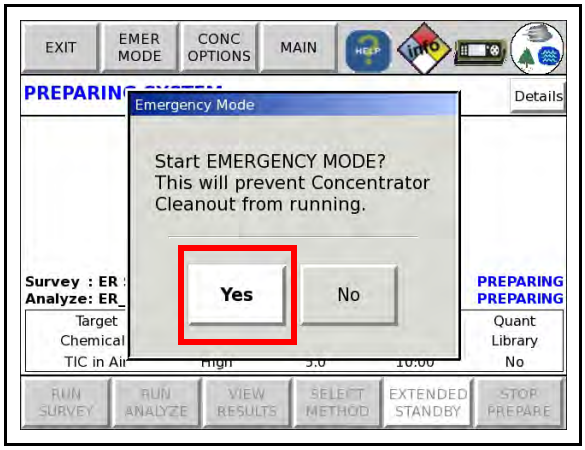


2 Alternately, use the arrow keys to highlight the **EMER MODE** button and push **OK SEL**. (See Figure 4-10.)

Figure 4-10 Arrow Keys

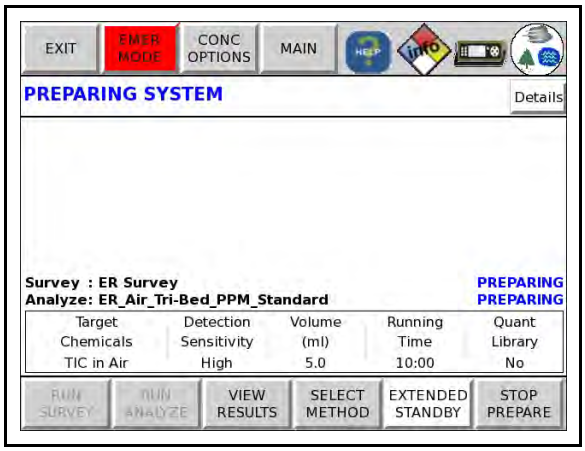
3 A confirmation message will be displayed. Touch **Yes** or push **OK SEL** to continue. (See Figure 4-11.)

Figure 4-11 Emergency Mode Confirmation



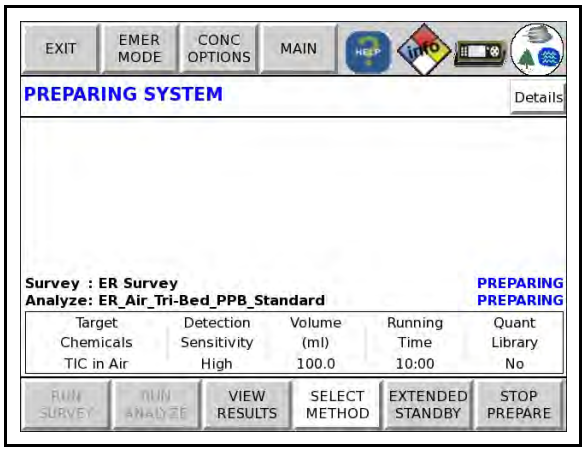
4 The **EMER MODE** button will turn red when Emergency mode is activated. (See Figure 4-12.)

Figure 4-12 Emergency Mode Active



5 To exit Emergency Mode, touch the **EMER MODE** button. Alternately, use the arrow keys to highlight the **EMER MODE** button and push **OK SEL**. The **EMER MODE** button will turn gray. (See Figure 4-13.)

Figure 4-13 EMER Mode Inactive



6 The HAPSITE ER will run a concentrator cleanout and prepare for general (non-emergency) use. See section 4.1, Starting HAPSITE ER in Portable Mode, on page 4-1.

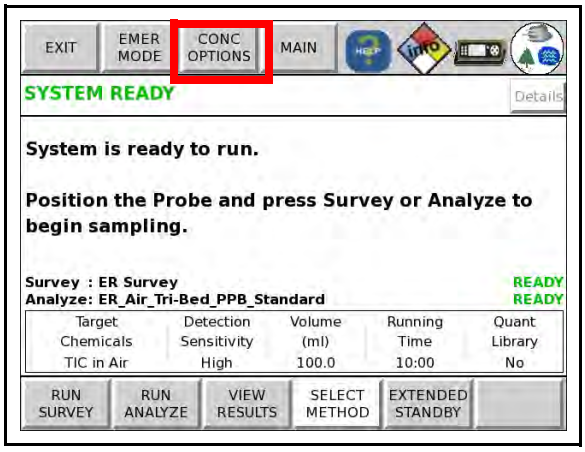
4.1.2 Concentrator Options (CONC OPTIONS)

The **CONC OPTIONS** button has two selections: **Concentrator Cleanout** and **Skip Conc Cleanout**. When **Concentrator Cleanout** is selected, the HAPSITE ER will run a manual cleanout. When **Skip Conc Cleanout** is selected, HAPSITE ER will bypass the concentrator cleanout once while the HAPSITE ER is preparing.

4.1.2.1 Concentrator Cleanout

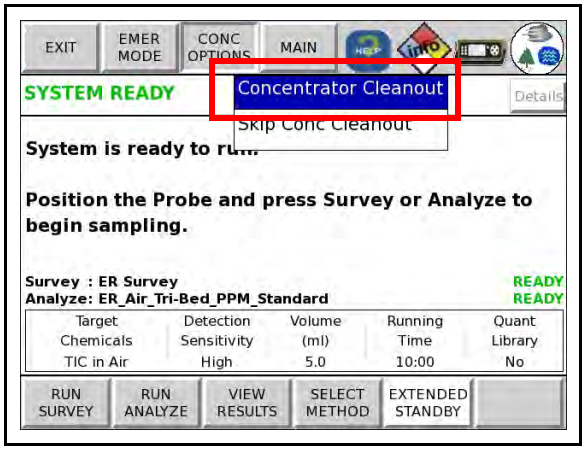
1 Touch **CONC OPTIONS** or use the **arrow keys** to highlight the **CONC OPTIONS** button and push **OK SEL**. (See Figure 4-14.)

Figure 4-14 Concentrator Options



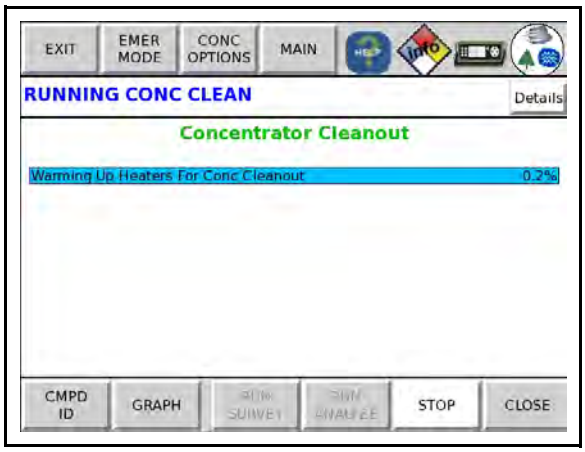
2 Touch **Concentrator Cleanout** or highlight **Concentrator Cleanout** using the **arrow keys**. Push **OK SEL**. (See Figure 4-15.)

Figure 4-15 Concentrator Cleanout



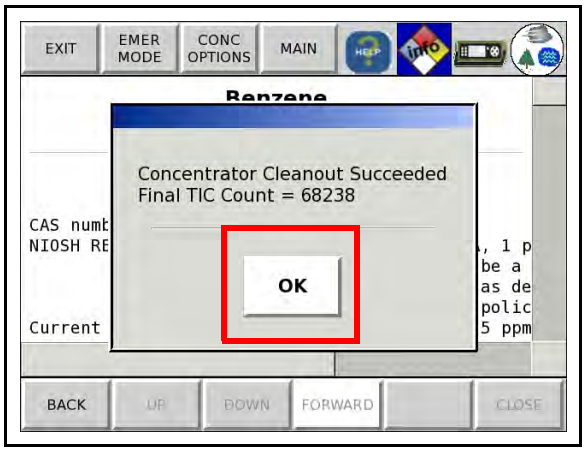
3 The HAPSITE ER will run a concentrator cleanout. (See Figure 4-16.)

Figure 4-16 Concentrator Cleanout



4 When the cleanout is successful, the **Concentrator Cleanout Succeeded** message will be displayed along with the final TIC. Push **OK** to exit the screen. (See Figure 4-17.)

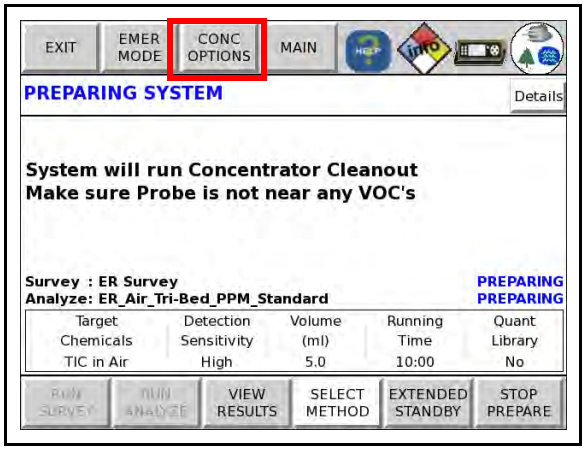
Figure 4-17 Concentrator Cleanout Succeeded



4.1.2.2 Skip Cleanout

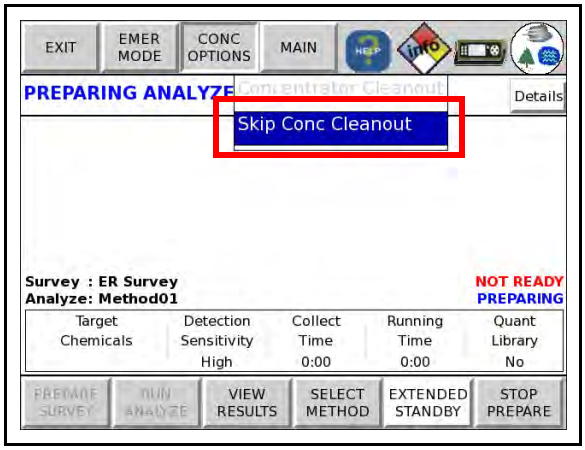
1 Touch **CONC OPTIONS** or use the **arrow keys** to highlight the **CONC OPTIONS** button and push **OK SEL**. (See Figure 4-18.)

Figure 4-18 Conc Options



2 Touch **Skip Cleanout** or highlight **Skip Cleanout** using the **arrow keys**. Push **OK SEL**. (See Figure 4-19.)

Figure 4-19 Skip Cleanout

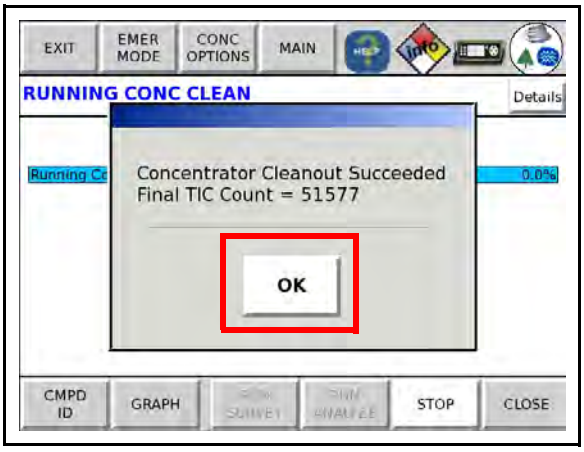


3 The system will not run a cleanout as part of its preparation.

4.1.3 Concentrator Cleanout Failure

If the concentrator cleanout is successful, the screen will display the final TIC. (See Figure 4-20.)

Figure 4-20 Cleanout Successful



If the concentrator cleanout is unsuccessful, the screen will display a concentrator cleanout failed message. See the instructions below for cleanout options.

1 Touch **Retry** to start another concentrator cleanout sequence.

2 Touch **Skip** to start running a concentrator Analyze method.

3 Touch **Abort** to return to the Main Screen.

NOTE: If **Abort** is touched, HAPSITE ER will show that the **SYSTEM IS NOT READY**.

4 HAPSITE ER will re-run the cleanout as part of its preparation.

5 If the failure box appears again, check the concentrator to verify that it is not cracked or chipped. Also, try re-installing the concentrator to ensure that it is properly seated.

4.1.4 Quick Reference SOP - Heat-up and Tune

CAUTION

Do not open the front panel in a wet or contaminated area.

1 Insert the internal standard and carrier gas canisters.

2 Insert a charged battery.

3 Connect the AC to DC power converter power supply.

4 Verify that the appropriate sample configuration (i.e., concentrator) is installed.

5 Press the **POWER** button on the front panel.

6 HAPSITE ER will heat the necessary components and perform AutoTune. A prompt to run **SURVEY** or **ANALYZE** will appear when HAPSITE ER is ready to run a sample.

7 If the default method is not the desired method, touch **STOP PREPARE**.

8 Touch **SELECT METHOD**. Highlight the desired method. Touch **Select**.

NOTE: If connecting wirelessly to the laptop, see Chapter 5, Communications and Touch Screen Options.

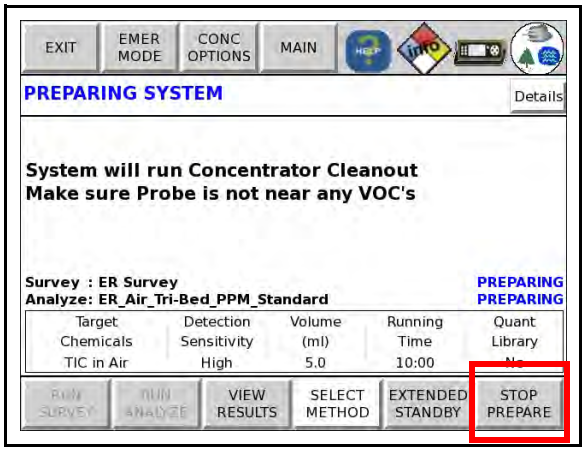
NOTE: When the **SYSTEM READY** message is displayed, touch either **RUN SURVEY** or **RUN ANALYZE**. If using the push buttons, push **SURVEY RUN** or **ANALYZE RUN**.

4.2 Selecting a Different Method Using the SELECT METHOD Icon

If the default method is not the desired method, the method can be changed. Changing the method can occur when the system is preparing or when another method has finished preparing.

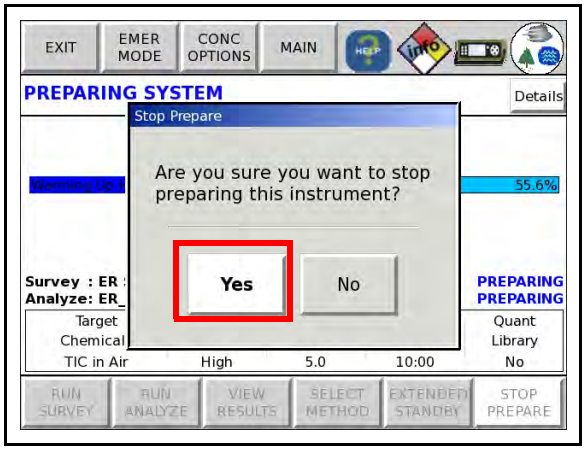
1. When the **PREPARING SYSTEM** screen is displayed, touch **STOP PREPARE**. Alternately, use the **arrow keys** to highlight **STOP PREPARE** and push **OK SEL**. (See Figure 4-21.)

Figure 4-21 Stop Prepare Screen



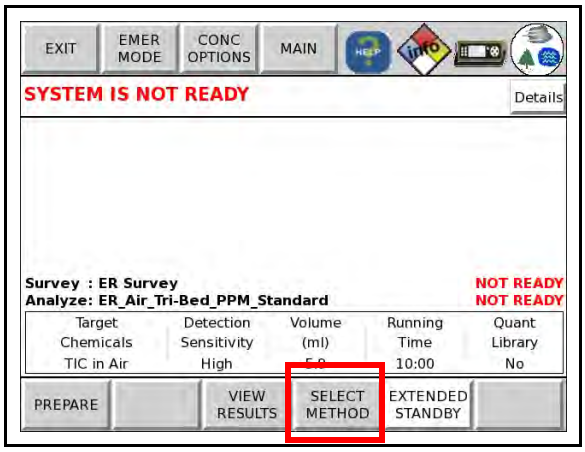
2. The screen will prompt, **Are you sure you want to stop preparing this instrument?** Touch **Yes** or using the **arrow keys**, highlight **Yes** and push **OK SEL**. (See Figure 4-22.)

Figure 4-22 Stopping Preparation



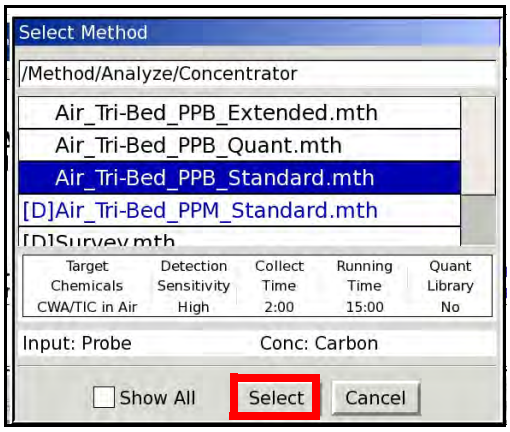
3 The **SYSTEM IS NOT READY** screen will appear. To select a new method, touch **SELECT METHOD** or using the **arrow keys**, highlight **SELECT METHOD** and push **OK SEL**. (See Figure 4-23.)

Figure 4-23 Selecting a Method Screen



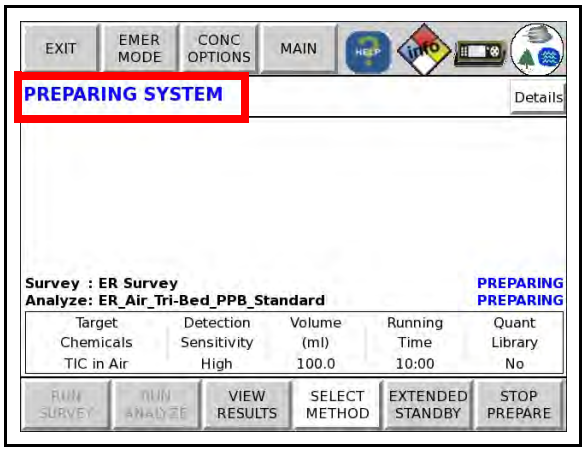
4 Scroll up or down using the scroll bar and touch the desired method to highlight it. When the desired method is highlighted, touch **Select**. Alternately, scroll up or down using the arrow keys. When the desired method is highlighted **OK SEL**. (See Figure 4-24.)

Figure 4-24 Method Selection



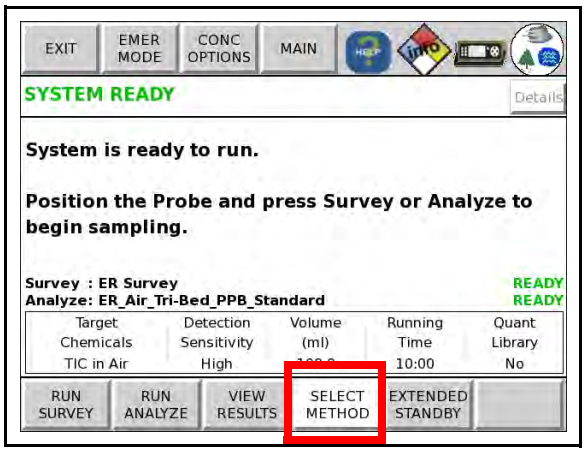
5 The **PREPARING** message will again be displayed. (See Figure 4-25.) Refer to steps 4-9 of section 4.2, Selecting a Different Method Using the SELECT METHOD Icon, on page 4-13 for further instructions on system preparation.

Figure 4-25 Preparing System



6 If the **SYSTEM READY, ANALYZE READY** or **SURVEY READY** message is already displayed and the prepared method is not the desired one, touch **SELECT METHOD**. (See Figure 4-26.)

Figure 4-26 Selecting New Method



7 Scroll up and down with the scroll bar or use the **arrow keys** to highlight the desired method, as shown in Step 4 of section 4.2. Touch **Select** or highlight **Select** using the **arrow keys** and push **OK SEL**.

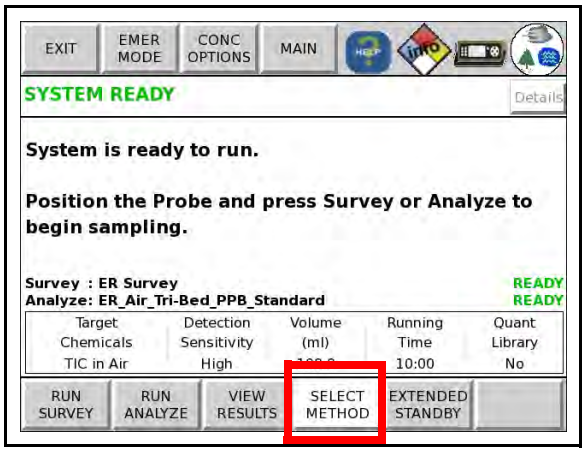
8 HAPSITE ER will begin preparing the new method. Refer to Steps 4-9 of section 4.2, Selecting a Different Method Using the SELECT METHOD Icon, on page 4-13 for further instructions on system preparation.

4.2.1 Changing the Default Method

The default method for HAPSITE ER can be changed. By changing the default method, HAPSITE ER will prepare the newly selected method upon startup.

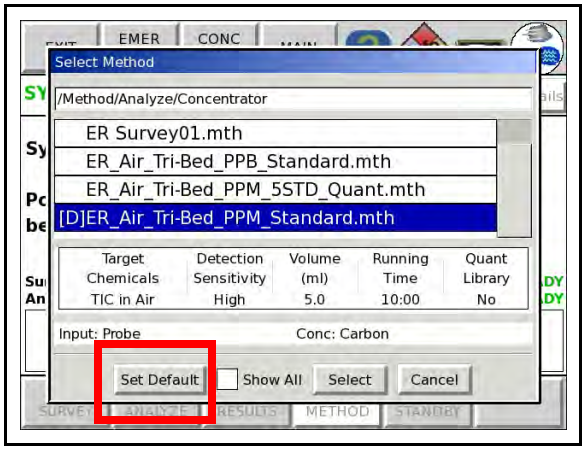
1 Touch **SELECT METHOD**. (See Figure 4-27.)

Figure 4-27 Select Method



2 Highlight the desired method. (See Figure 4-28.)

Figure 4-28 Choosing Method

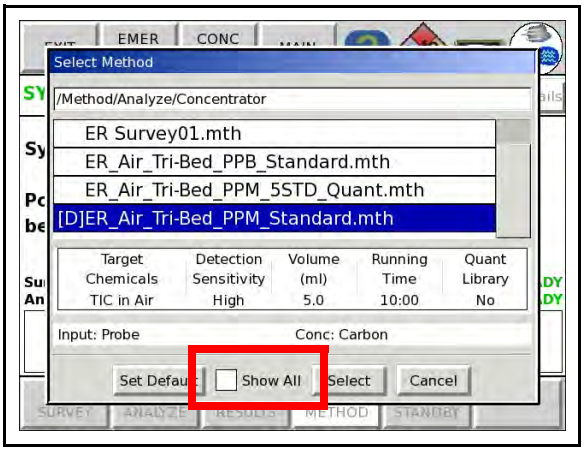


3 Touch the **Set Default** button. Upon the next startup, HAPSITE ER will begin preparing the new default method.

4.2.2 Show All

HAPSITE ER will only show methods that are compatible with the current sample and/or accessory configuration. By checking the **Show All** box, all loaded HAPSITE ER methods will appear in the text box, regardless of configuration. Non-compatible methods will be shown in a lighter gray. The non-compatible methods are for reference only and cannot be selected to run. (See Figure 4-29.)

Figure 4-29 Show All



4.3 Survey Mode

The Survey mode is used for quick analysis and tentative results. When sampling unknown compounds, it is recommended that a Survey run be completed before running Analyze.

Overview:

- Using the probe, sample the air away from the area of concern for one minute. This establishes the background of VOC's currently present in the area.

CAUTION

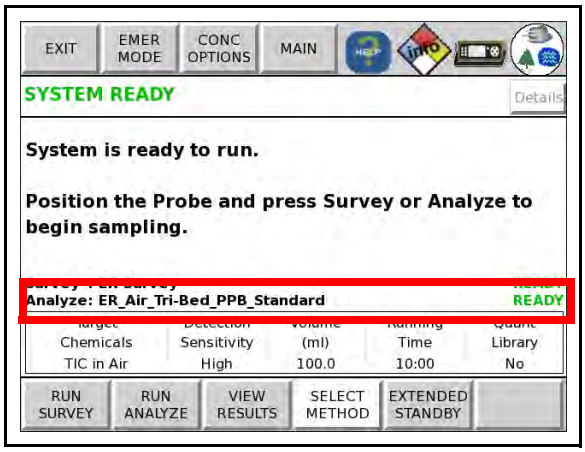
Do not touch the sample with the probe. Do not allow liquids to enter the probe.

- When a background has been established, sample directly over the point of concern. Once the TIC begins to increase, slowly move the probe away from the sample. If a compound has been identified, it will be displayed on the screen.

Procedure

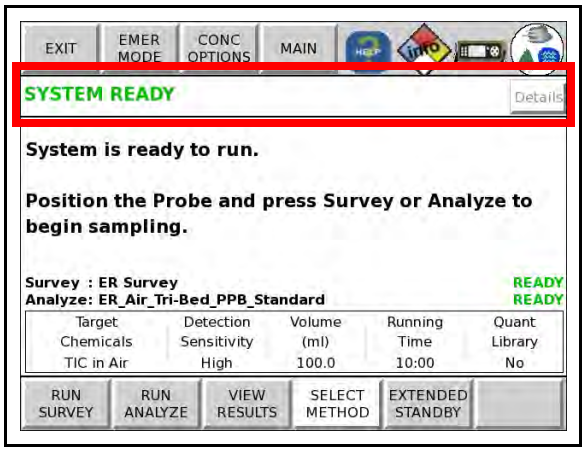
1. If an Analyze method is going to be run after Survey, verify that the appropriate sample configuration (i.e., concentrator) is installed.
2. When powered on or taken out of Extended Standby, HAPSITE ER will automatically start preparing an ER Survey and Analyze method if the probe is attached. Refer to section 4.1, Starting HAPSITE ER in Portable Mode, on page 4-1.
3. Verify that the desired Analyze method is listed under the Survey method. In Figure 4-30, the Analyze method is **ER_Air_Tri-Bed_PPB_Standard**.

Figure 4-30 Analyze Method



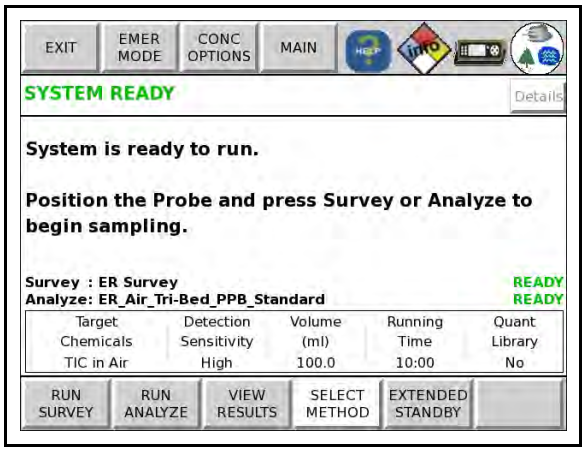
4. A **SYSTEM READY** message will be displayed with a prompt to press **Survey** or **Analyze** when HAPSITE ER is ready to sample. (See Figure 4-31.)

Figure 4-31 System Ready



5 Using the touch screen, touch **RUN SURVEY**. **(**See Figure 4-32.)

Figure 4-32 Run Survey

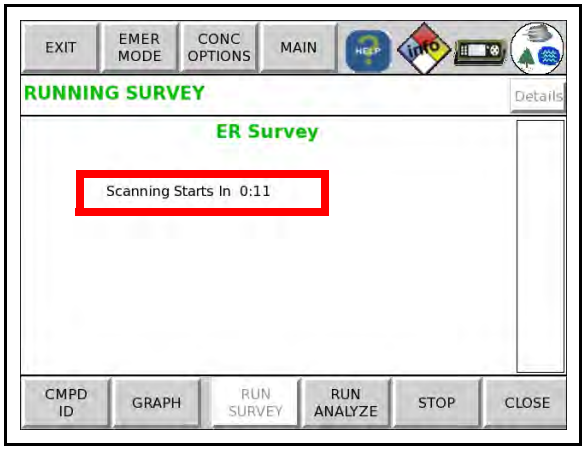


6 Alternately, push **SURVEY RUN** using the push buttons. (See Figure 4-33.)

Figure 4-33 SURVEY RUN Button

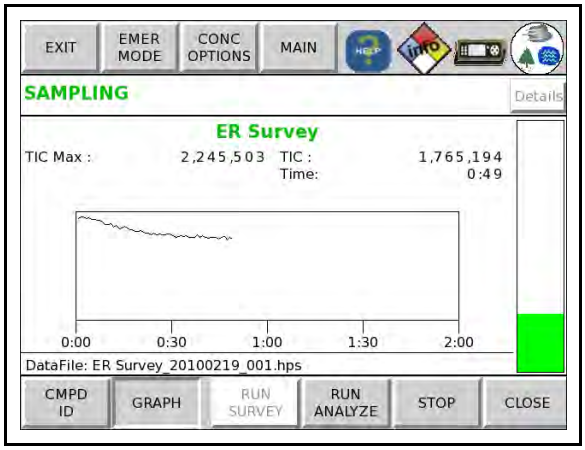
7 The front panel will momentarily display a **Start Scanning In** message before the Survey run will start. (See Figure 4-34.)

Figure 4-34 Scanning Starts Screen



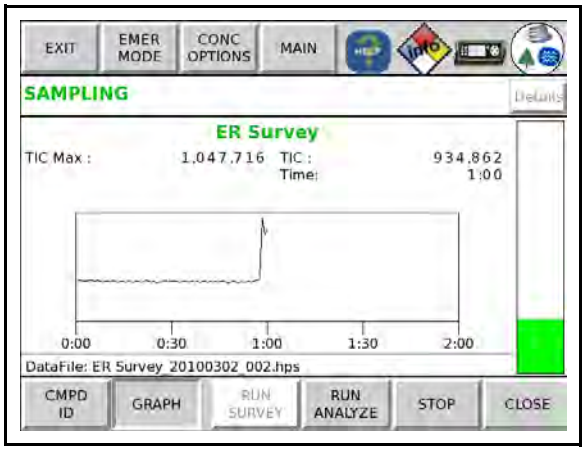
8 Sample air away from the point of concern for one minute. Remember to note the background TIC. (See Figure 4-35.)

Figure 4-35 Background Sampling



9 Hold the probe over the sample of interest for up to 1 minute. A peak may appear if the compound present is greater than 1 ppm. A compound identification may also be present on the HAPSITE ER screen. (See Figure 4-36.)

Figure 4-36 Survey



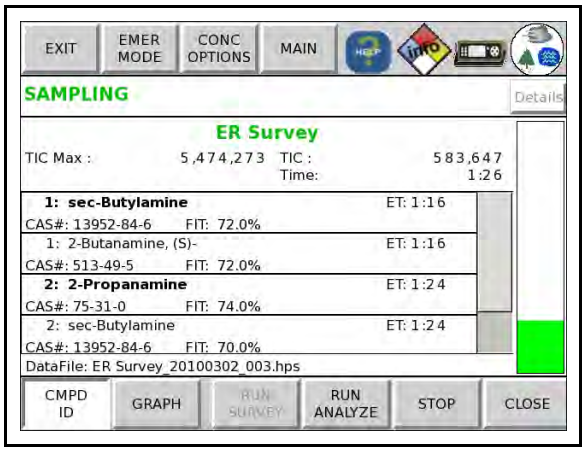
CAUTION

Do not touch the sample with the probe.
Do not allow liquids to enter the probe.

10 By touching **CMPD ID**, a list of identified compounds will appear. (See Figure 4-37.) The CAS number, the Fit and the retention time for each compound will also be displayed. This screen will also state the TIC (Total Ion Count, a measure of response) Max, the current TIC and the elapsed time of the method.

NOTE: Touching a compound on the list will display its Synonym and Exposure Limit information.

Figure 4-37 Sample Compound ID List in Survey



11 The **CMPD ID** screen can also be accessed by using the **arrow keys** to highlight **CMPD ID** and pushing **OK SEL**. (See Figure 4-38.)

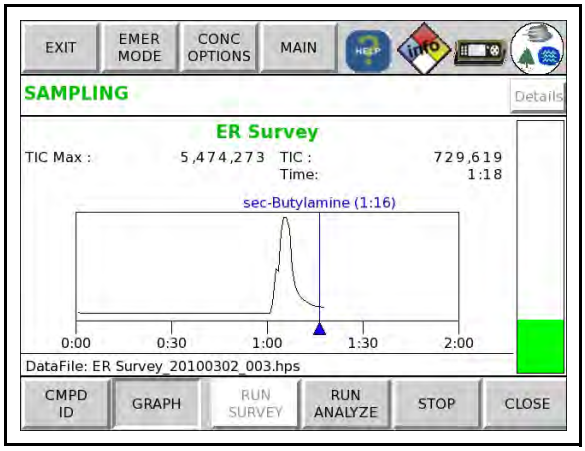
Figure 4-38 Accessing the Compound ID Screen Using the Arrow Keys

12 To view the chromatogram while the method is running, touch **GRAPH**. (See Figure 4-39.) Alternately, use the **arrow keys** to highlight **GRAPH** and push **OK SEL**.

NOTE: This screen will also state the TIC Max, the current TIC and the time the method has been running.

NOTE: Touching the blue compound identification above the chromatogram will display its Synonym and Exposure Limit information.

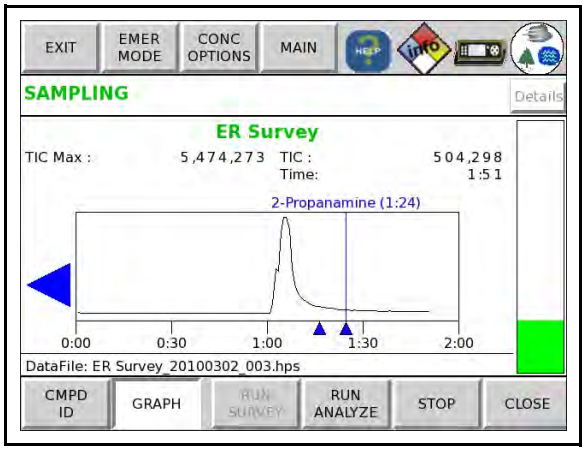
Figure 4-39 Sample GRAPH function



13 When the TIC begins to increase, move the probe away from the sample of interest. Continue the run until the TIC level returns to the initial background TIC level that was noted in Step 8 on page 4-20. (See Figure 4-40.)

NOTE: Monitor the side bar on the HAPSITE ER screen for guidance. The bar rises as the TIC increases and green signifies that the proper sampling distance is being maintained. To avoid saturation, remove the probe from the sample when the bar increases and turns yellow. If saturation occurs, the side bar will turn red and the TIC will be above 60 million.

Figure 4-40 Returning to Baseline

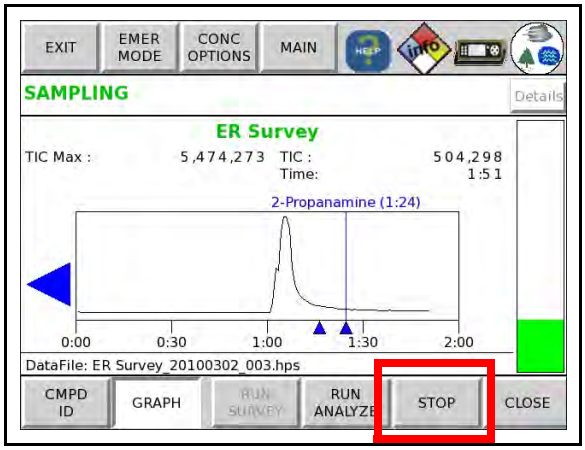


14 To confirm the Survey results with a GC/MS run, **ANALYZE** can be touched or **ANALYZE RUN** can be pushed during the Survey run. (See Figure 4-41.)

NOTE: It is advised to begin an Analyze run either after a peak has been displayed and/or Survey has been run for the full two minutes.

15 If running an Analyze method is not desired, touch **STOP** to stop the sampling process and automatically save the data. (See Figure 4-41.)

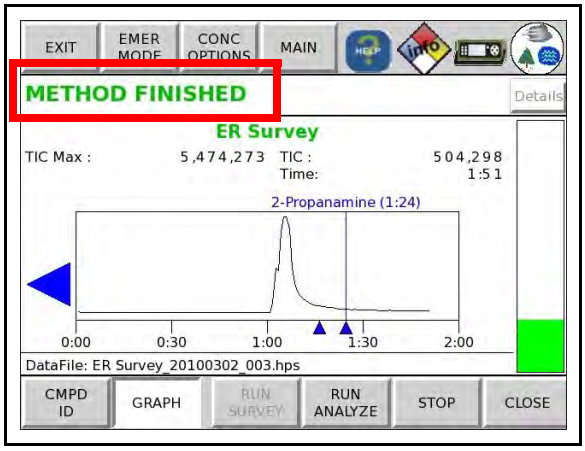
Figure 4-41 ANALYZE and STOP



16 A **METHOD FINISHED** message will appear when the Survey method has ended. (See Figure 4-42.)

NOTE: The total time required for a Survey analysis is typically less than 3 minutes. If the Survey is not stopped manually, it will automatically stop at 5 minutes.

Figure 4-42 Survey Method Finished



4.3.1 Quick Reference SOP — Survey Method

1 If an Analyze (GC/MS) method is going to be run after Survey, verify that the appropriate configuration (i.e., concentrator) is installed and the proper Analyze method is displayed on the screen.

2 If powering on HAPSITE ER or exiting Extended Standby, the HAPSITE will automatically begin preparing Survey.

2a If needed, touch **PREPARE** on the touch screen.

2b Alternately, using the **arrow keys**, highlight **PREPARE**. Push **OK SEL**.

3 When prompted by the **SYSTEM IS READY** message, touch **RUN SURVEY** or push **SURVEY RUN**.

4 Monitor background for one minute.

5 Hold the probe over the sample.

6 Move the probe away from the sample when the TIC begins to increase and a peak begins to form.

If the TIC does not increase after a full minute of sampling, move the probe away from the sample.

7 To confirm data with an Analyze (GC/MS) run, touch **RUN ANALYZE** or press **ANALYZE RUN**.

8 If an Analyze method is not desired, touch **STOP** or push **SURVEY RUN**.

9 A **METHOD FINISHED** message will be displayed when the method has ended.

4.4 ANALYZE (GC/MS) Mode with the Concentrator

4.4.1 Tri-Bed Concentrator

The Tri-Bed concentrator is used for analyzing samples with concentration levels in the low part per million to high part per trillion range. Two default qualitative methods are ER_Tri-Bed_PPM_Standard and ER_Tri-Bed_PPB Standard. Use the ER_Tri-Bed_PPM_Standard method when a response is seen in Survey. If a compound is suspected, but Survey does not show an increase in TIC (total ion count, which is a measure of response), use the ER_Tri-Bed_PPB_Standard method.

CAUTION

The concentrator feature has increased sensitivity. Use the appropriate method to avoid saturating HAPSITE ER.

4.4.2 Tenax Concentrator

This method is also used for analyzing samples with concentration levels in the low part per million to high part per trillion range. The Tenax concentrator's use is similar to that of the Tri-Bed concentrator. However, the Tenax concentrator will not effectively concentrate compounds with boiling points below 80°C.

WARNING

The Tenax concentrator will not effectively concentrate compounds with boiling points below 80°C.

4.4.3 Procedure for Running Concentrator Methods

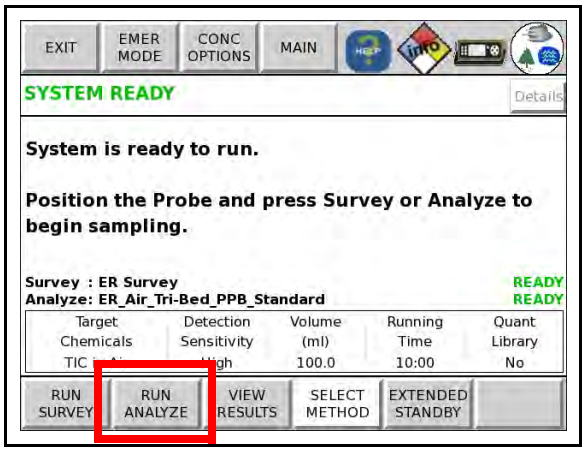
NOTE: Before an Analyze (GC/MS) concentrator method can be run, the concentrator must be installed. Refer to section 3.3.7, Replacing the Concentrator, on page 3-21 for instructions. Once installed, the concentrator will be automatically cleaned before sampling begins.

1. Verify that the appropriate concentrator is installed.
2. The HAPSITE ER will automatically start preparing a concentrator method. If HAPSITE ER does not prepare the desired concentrator method, refer to section 4.2, Selecting a Different Method Using the SELECT METHOD Icon, on page 4-13.
3. When the HAPSITE ER has finished preparing and the concentrator cleanout is successful, a **SYSTEM READY** message will be displayed with a prompt to press Survey or Analyze to begin sampling.

   NOTE: A blank run is recommended before running a sample.

4 Using the touch screen, touch **RUN ANALYZE**. (See Figure 4-43.)

Figure 4-43 Analyze Button



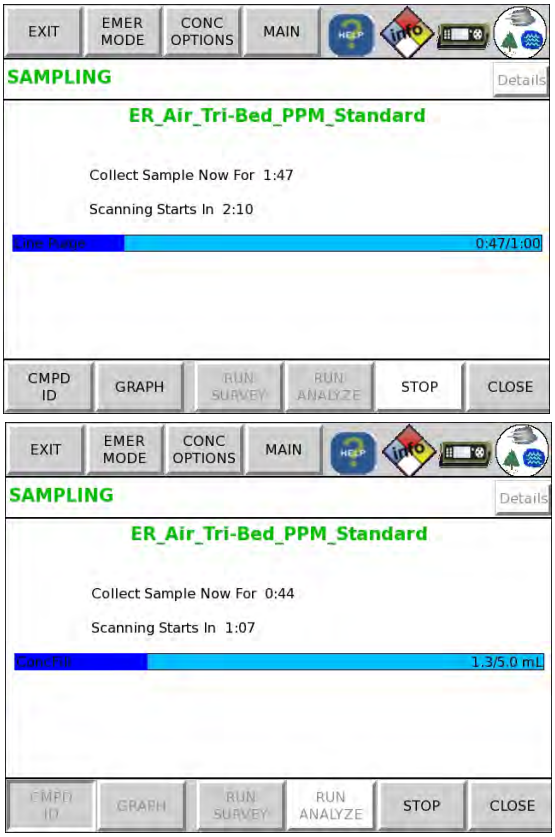
5 Alternately, if using the push buttons, push **ANALYZE RUN**. (See Figure 4-44.)

Figure 4-44 Analyze Run

6 When the screen prompts, **Collect Sample Now**, hold the probe over the sample. Continue to collect sample during both the Line Purge and Concfill screens. (See Figure 4-45.)

NOTE: The Line Purge is based on time while the ConcFill is based on volume.

Figure 4-45 Collecting Sample For Concentrator Run

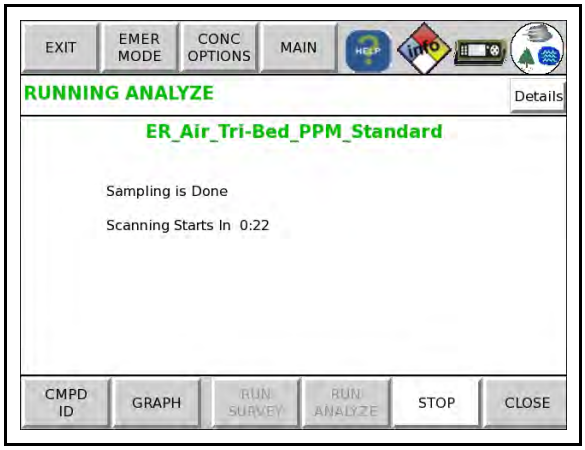


CAUTION

Do not touch the sample with the probe.
Do not allow liquids to enter the probe.

7 Move the probe away from the sample when the screen prompts, **Sampling is Done.** (See Figure 4-46.)

Figure 4-46 Sampling Done on Concentrator Run



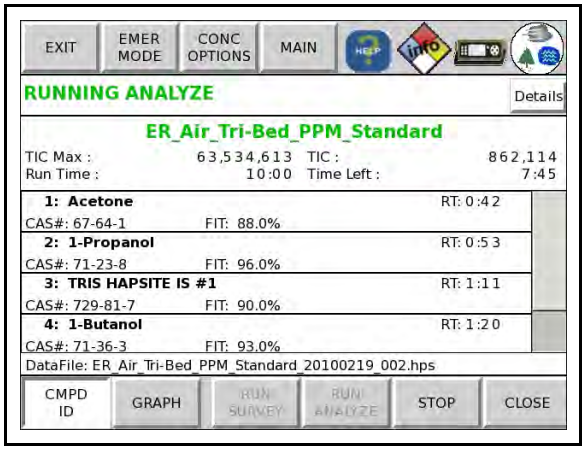
8 By touching **CMPD ID**, a list of found compounds will be displayed. (See Figure 4-47.) This page will display for each compound:

- The CAS number
- The Fit
- The retention time
- TIC (Total Ion Count) Max,
- The current TIC
- The time left until the run finishes

NOTE: Touching a compound on the list will display its Synonym and Exposure Limit information if it is contained in the NIOSH database.

8a The **CMPD ID** screen can also be accessed by using the **arrow keys** to highlight **CMPD ID** and pushing **OK SEL**.

Figure 4-47 Sample Compound Identification For Concentrator

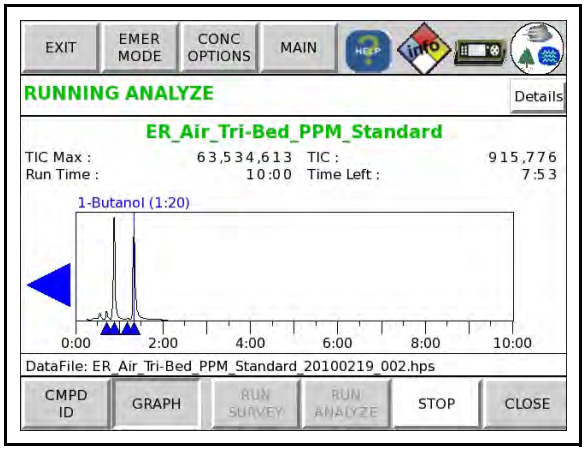


9 To view the chromatogram while the method is running, touch **GRAPH**. (See Figure 4-48.) Alternately, use the **arrow keys** to highlight **GRAPH**. Push **OK SEL**. This screen will display:

- The TIC Max
- The current TIC
- The time left until the run finishes

NOTE: Touching the blue compound identification above the chromatogram will display its Synonym and Exposure Limit information.

Figure 4-48 Sample Chromatogram View For Concentrator

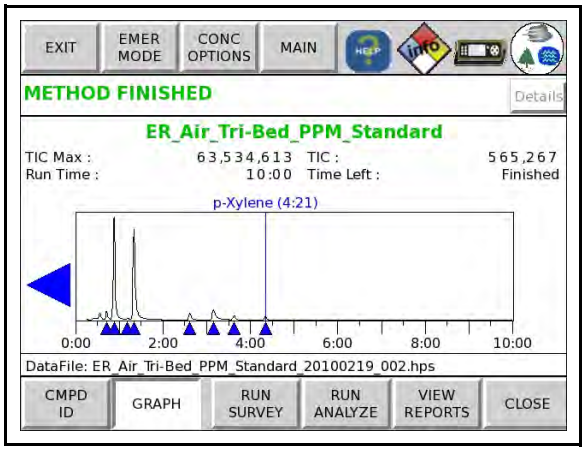


10 A **METHOD FINISHED** message will be displayed when the Analyze method has ended. (See Figure 4-49.)

NOTE: Another Analyze (GC/MS) run can be started immediately after one has finished. Depending upon the temperature profile, the column may need to cool before another run may begin.

NOTE: Refer to section 4.5.1, View Results/View Reports, on page 4-31 for more information on reviewing the data.

Figure 4-49 Sample Concentrator Method Finished



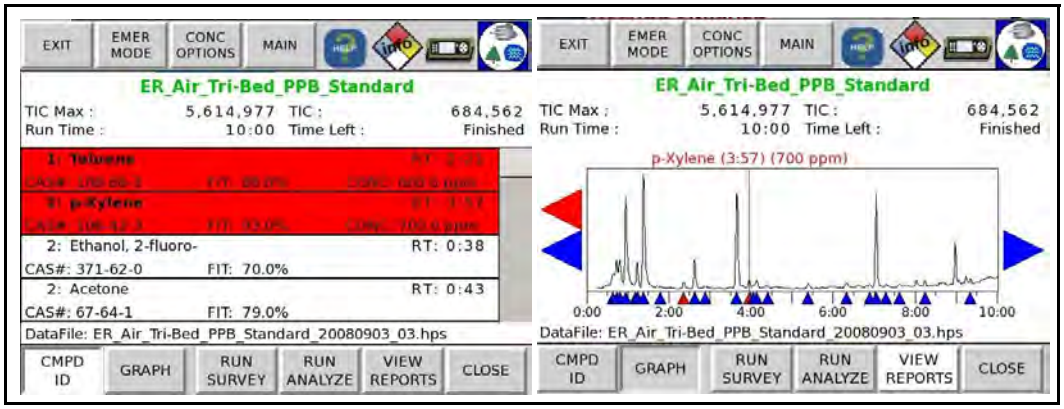
4.4.4 Quick Reference SOP — Concentrator Methods

1. Verify that the concentrator is installed.
2. Refer to section 4.1.4, Quick Reference SOP - Heat-up and Tune, on page 4-12 for startup instructions.
3. Verify that the desired method is displayed on the Analyze line.
4. Touch **RUN ANALYZE** or push **ANALYZE RUN** when the **SYSTEM IS READY** screen is displayed.
5. When the screen prompts, **Collect Sample Now**, hold the probe over the sample until the screen prompts, **Sampling Is Done**.
6. When the run is complete, a **Method Finished** prompt will be displayed.
7. Refer to section 4.5.1, View Results/View Reports, on page 4-31 for information on data review.

4.5 Detecting Hazardous Chemicals

If the HAPSITE ER Analyze message turns red, the chemical's concentration is either approaching the IDLH limit or the chemical is a Chemical Warfare Agent. In CMPD ID mode, the compound will be highlighted in red and in GRAPH mode, the name of the compound will be written in red. Red arrows on the side of the screen will be displayed in GRAPH mode if there is more than one red compound. (See Figure 4-50.)

Figure 4-50 IDLH Warnings

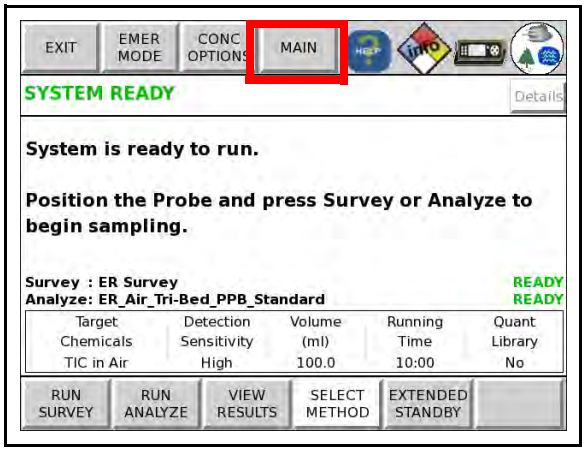


4.5.1 View Results/View Reports

Data files and reports can be viewed from the main front panel screen or from the sample analysis screen. Follow the instructions below to view results and reports.

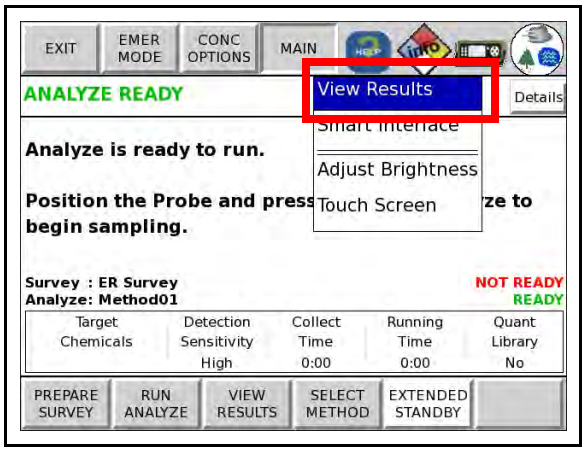
1 To access data files and reports from the main screen, touch **MAIN**. (See Figure 4-51.)

Figure 4-51 MAIN



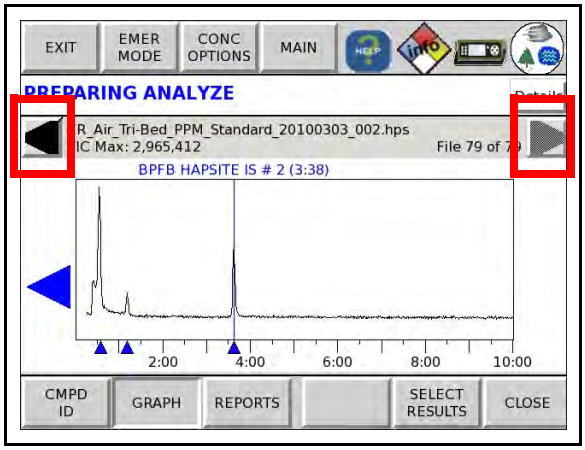
2 Touch **View Results**. (See Figure 4-52.)

Figure 4-52 View Results



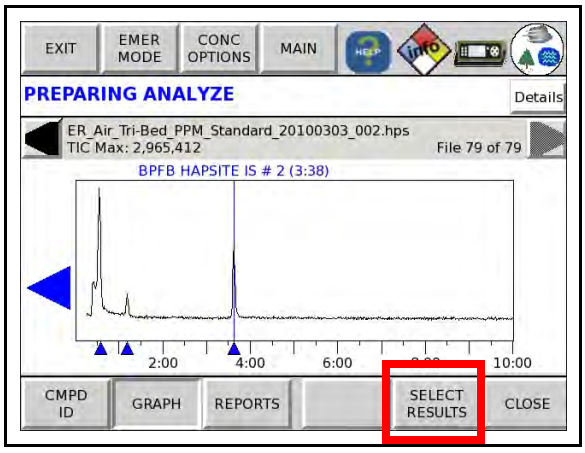
3 The most recent file for the selected method will be displayed on the screen. Use the black, touch screen **arrow keys** to access other data files from the same method. (See Figure 4-55.) If using the push buttons, use the front panel **arrow keys**. The left **arrow key** will access earlier files. The right arrow will access later ones. (See Figure 4-53.)

Figure 4-53 Arrow Keys



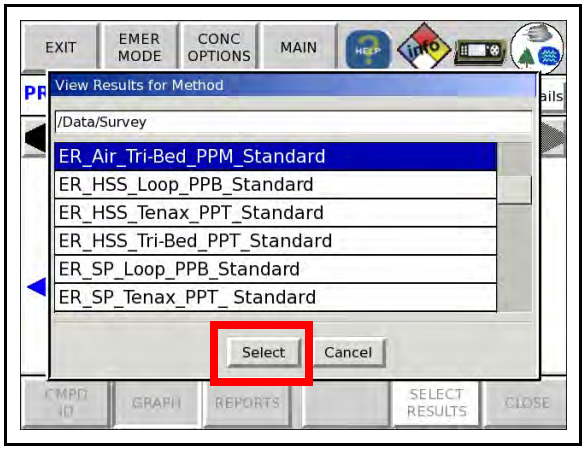
4 To view files from another method, use the **SELECT RESULTS** button. (See Figure 4-54.)

Figure 4-54 Select Results



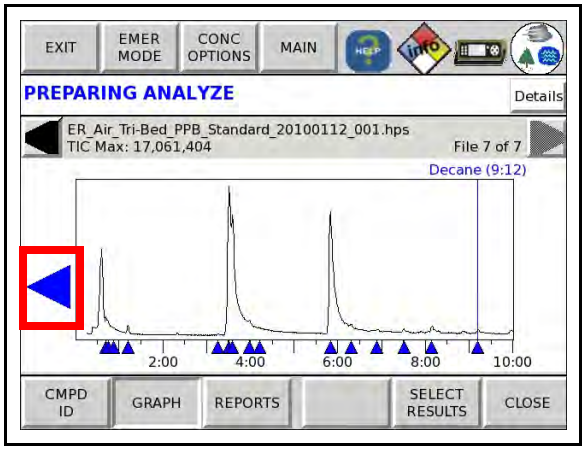
5 Scroll through the method files until the desired method is highlighted. Either touch **Select** or push **OK SEL**. (See Figure 4-55.)

Figure 4-55 Review Results Highlighting Black Arrows



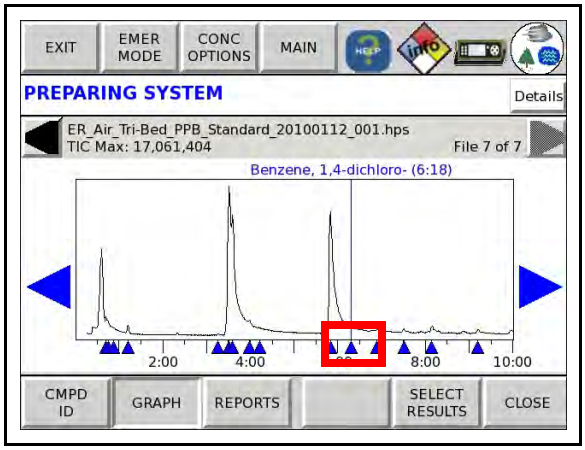
6 The big blue arrows are used to scroll through the peaks in the chromatogram. The identified compound and its retention time will appear in the area below the file name. (See Figure 4-56.)

Figure 4-56 Blue Arrows



7 Touch the small blue triangles to display the compound identification and retention time for the compound directly above it. (See Figure 4-57.)

Figure 4-57 Small Blue Triangles



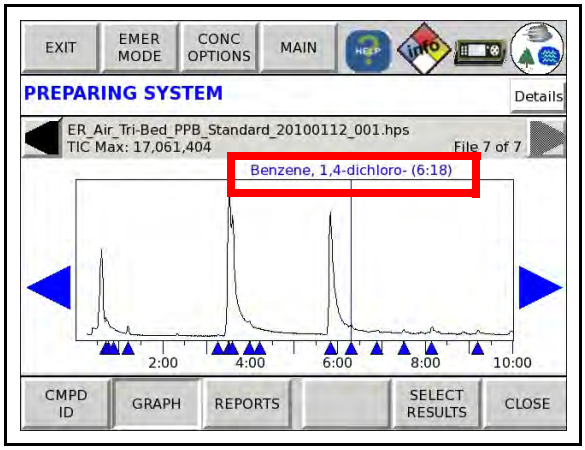
NOTE: Most functions can be accessed using the push buttons. However, accessing the blue triangles and blue arrows are only available on the touch screen.

DANGER

If a RED TRIANGLE is displayed, HAPSITE ER has detected a compound with a concentration that is approaching or has reached the IDLH level or it has detected a Chemical Warfare Agent. Refer to section 4.5, Detecting Hazardous Chemicals, on page 4-30.

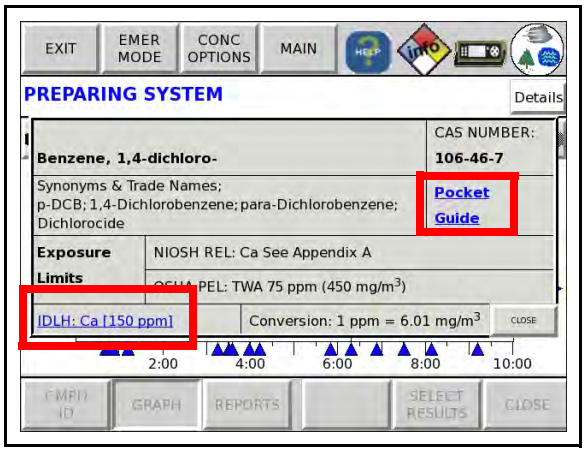
8 Touching a specific compound in the list will display that compound's Synonym and Exposure Limits. (See Figure 4-58.)

Figure 4-58 Displaying the Synonyms and Exposure Limits



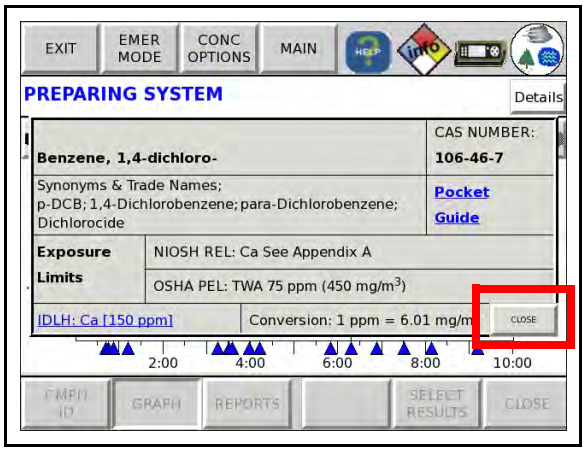
9 A link to the *NIOSH Pocket Guide to Chemical Hazards (NPG)* will also be displayed in blue. The link is entitled Pocket Guide. In the bottom left corner, there is a link to the *Immediately Dangerous to Life and Health Concentrations (IDLH).* The link is blue and entitled IDLH. (See Figure 4-59.) For further instructions on using NIOSH and other info databases, see section 4.7, Info Icon, on page 4-41.

Figure 4-59 Links to NPG and IDLH



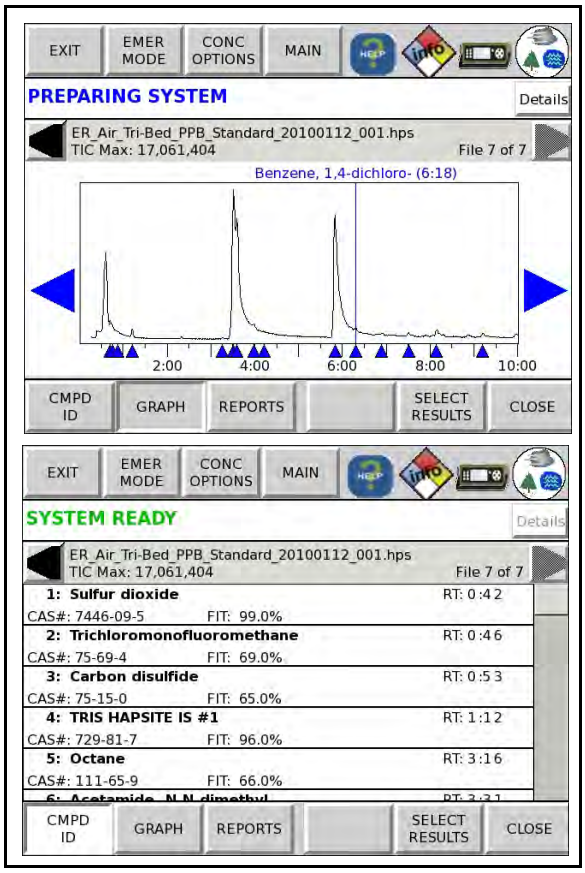
10 Touch **CLOSE** to return to the data screen. (See Figure 4-60.)

Figure 4-60 CLOSE



11 Touching the **CMPD ID** (Compound Identification) button while in **Review Results**, will show a list of the compounds found on the selected run. The CAS number, the Net Fit and the retention time for each compound will also be shown. (See Figure 4-61.)

Figure 4-61 CMPD ID

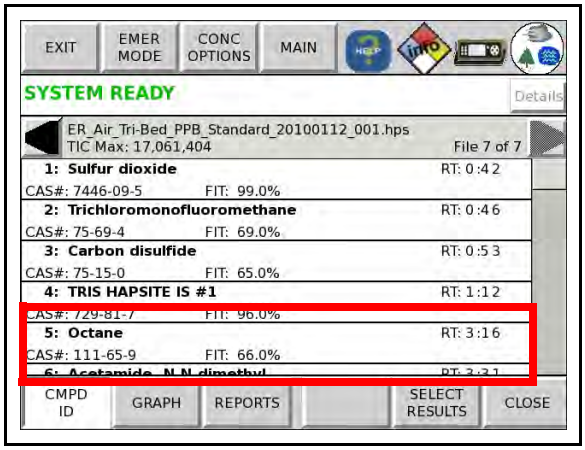


DANGER

If a RED TRIANGLE is displayed, HAPSITE ER has detected a compound with a concentration that is 10% of the IDLH level or it has detected a Chemical Warfare Agent.

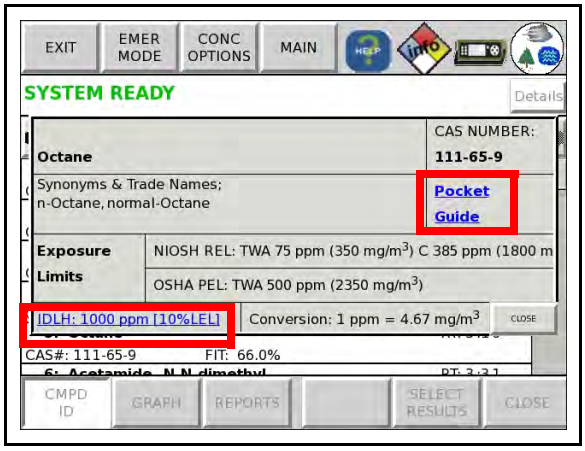
12 Touching a specific compound in the list will display that compound's Synonym and Exposure Limits. (See Figure 4-62.)

Figure 4-62 Synonym and Exposure Limits



13 A link to the *NIOSH Pocket Guide to Chemical Hazards (NPG)* will also be displayed in blue. The link is entitled *Pocket Guide*. In the bottom left hand corner, there is a link to the *Immediately Dangerous to Life and Health Concentrations (IDLH).* The link is blue and entitled IDLH. (See Figure 4-63.) For further instructions on using NIOSH and other *info* databases, see section 4.7, Info Icon, on page 4-41.

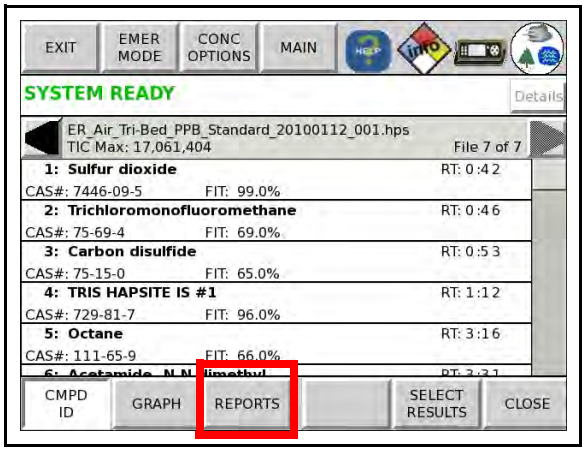
Figure 4-63 NIOSH Link



NOTE: HAPSITE ER can detect more compounds than those contained in these databases. Therefore, if the screen displays N/A and does not have links available, the compound is not included in these databases.

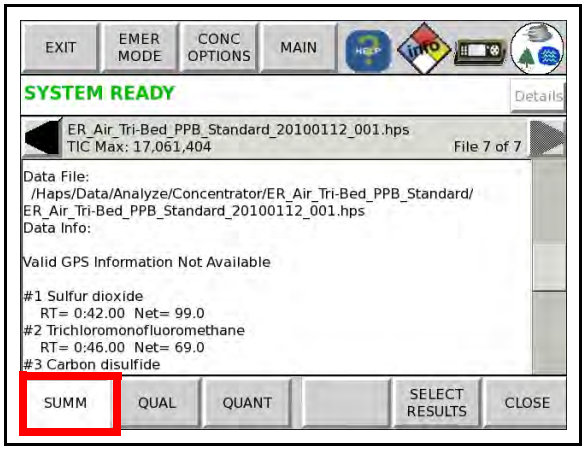
14 To view the run's **Summary**, **Qualitative** and **Quantitative Reports**, touch the **REPORTS** button. Alternately, use the **arrow keys** to highlight the **REPORTS** button and push **OK SEL**. (See Figure 4-64.) This can be accessed from the **GRAPH** page or the **CMPD ID** from **View Results**.

Figure 4-64 Viewing REPORTS



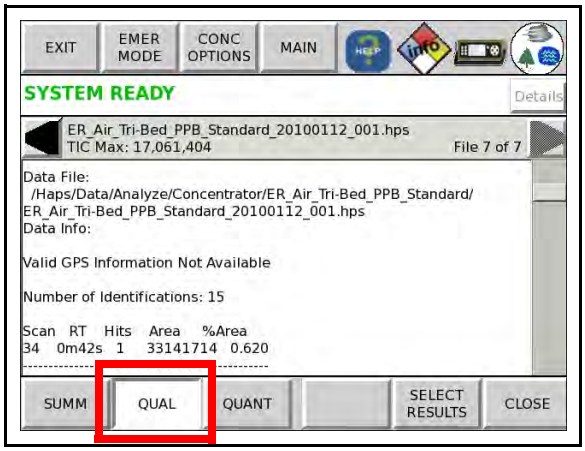
15 The Summary Report can be found by touching the **SUMM** key. (See Figure 4-65.) Alternately, highlight the **SUMM** key and push **OK SEL**. For each compound found, information regarding the Net Fit and the retention time will be displayed.

Figure 4-65 Summary Report



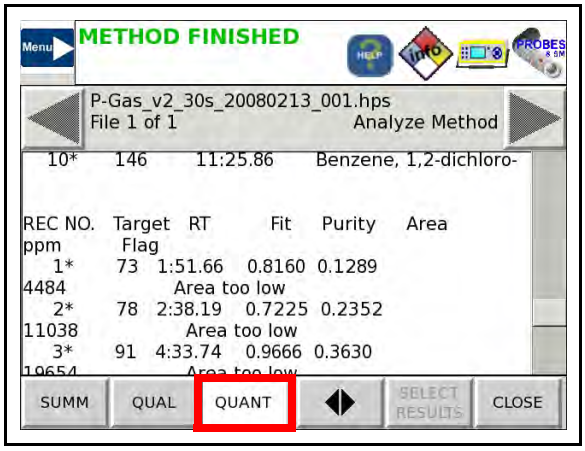
16 The Qualitative Report can be found by touching the **QUAL** key. (See Figure 4-66.) Alternately, highlight the **QUAL** key and push **OK SEL**. For each compound found, information regarding the Net Fit, the retention time, the CAS number, the area and the number of hits will be displayed.

Figure 4-66 Qualitative Report



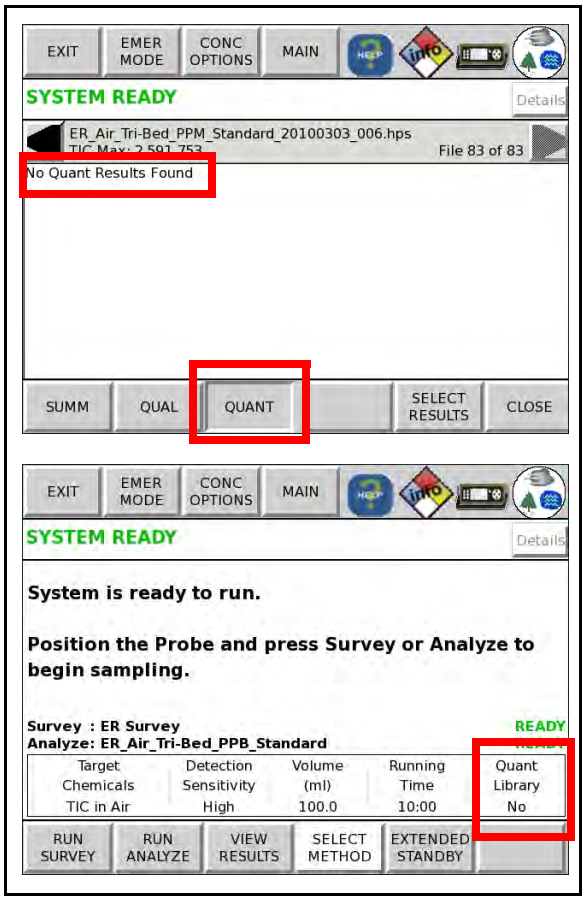
17 The Quantitative Report can be found be touching the **QUANT** key. (See Figure 4-67.) Alternately, highlight the **QUANT** key and push **OK SEL**. For each compound found, information regarding the target ion, the retention time, the Net Fit, the purity, the area and the concentration will be displayed.

Figure 4-67 Quantitative Reports



NOTE: If the method is not quantitative, the message "**No quant reports found"** will be displayed on the **QUANT** report screen. To determine if the method is quantitative, see the box in the bottom right hand corner of the main screen. (See Figure 4-68.)

Figure 4-68 Type of Method



4.6 Help Icon

The **Help** icon is located on the front panel in the top right hand corner. (See Figure 4-69.)

Figure 4-69 Help Icon

Help can be accessed by touching the Help icon or pushing the **HELP** button that is located on the front panel. (See Figure 4-70.)

Figure 4-70 Help Push Button

The main Help screen displayed will display a **Survey** link, an **Analyze** link, a **View Results** link, a **Select Method** link and a **Go To Standby** link. Touching a link will provide instructions for performing the specified function. Touching **Simple Steps** at the bottom of the page will give a step-by-step outline of how to perform the desired function. The **Book** icon will give a more detailed summary of the function.

4.7 Info Icon

The **Info** icon is located next to the **Help** icon in the right hand corner of the HAPSITE ER screen. (See Figure 4-71.) **Info** can be accessed by touching this button or pushing the **STAT** key until the NIOSH database is displayed. When the **Info** page is displayed, the **Info** icon will be highlighted in blue.

Figure 4-71 Info Icon

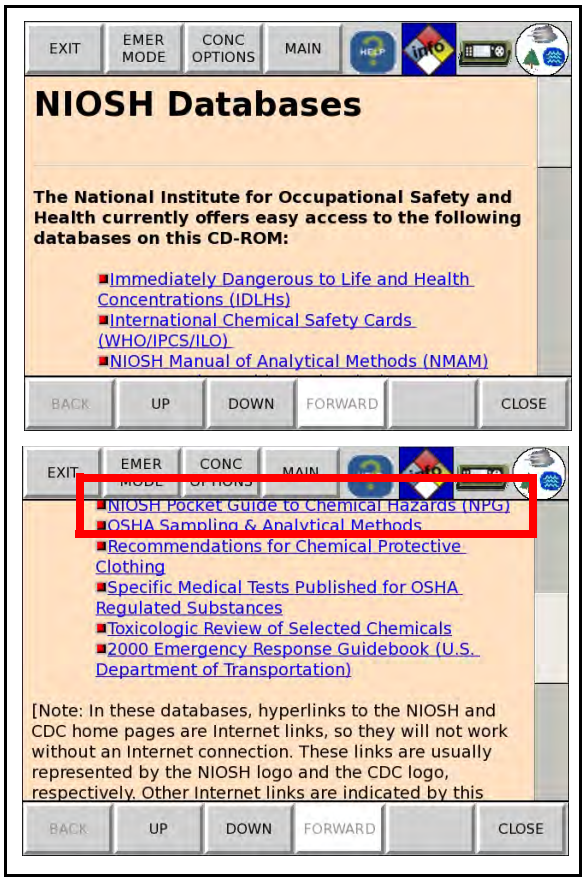
The NIOSH Database screen will be displayed. (See Figure 4-72.) This screen provides links to *Immediately Dangerous to Life and Health Concentrations* (*IDLHS), International Chemical Safety Cards, NMAM, The NIOSH Pocket Guide to Chemical Hazards (NPG), OSHA Sampling and Analytical Methods, Recommendations for Chemical Protective Clothing, Specific Medical Tests Published for OSHA Regulated Substances,* and *Toxicologic Review of Selected Chemicals.* These publications provide information on Exposure Limits, Synonyms and Detection Limitations.

Scrolling to the bottom of the page will access additional links.

- The **Conversion Calculator** converts concentration units
- **Hazard ID's** accesses specific NIOSH studies about hazardous conditions
- **PPE** recommends the proper equipment needed to withstand exposure to hazardous conditions
- **Respiratory Protection** provides information on selecting the proper respirator
- **Hazard Controls** accesses specific studies that have identified ways to reduce hazardous exposures
- **Indoor Air Quality** includes selected publications from the EPA about improving air quality
- The **Periodic Table**
- **RTECS User Guide** was designed by NIOSH to provide synonyms, skin and eye irritation data, mutation data, and respiratory effects data for certain compounds. It stands for *The Registry of Toxic Effects of Chemical Substances*

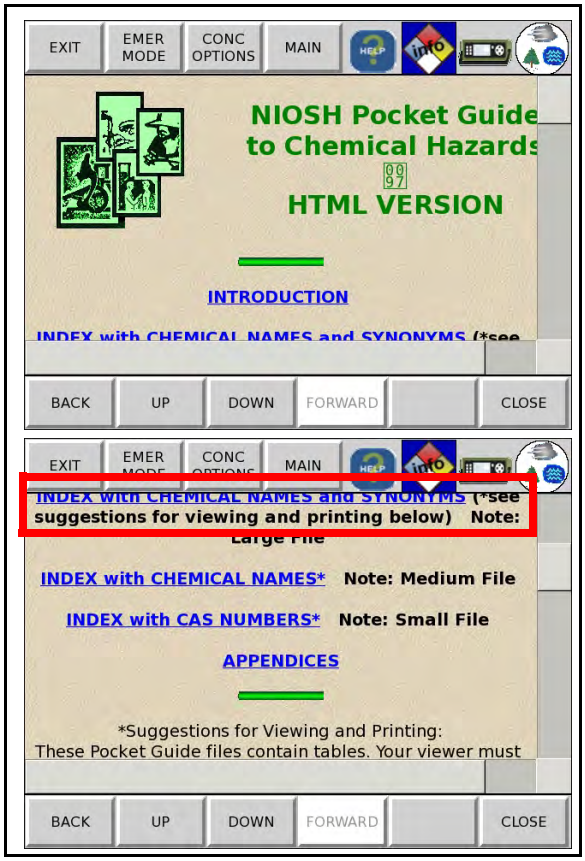
1 An important resource in this database is *The NIOSH Pocket Guide to Chemical Hazards (NPG). (*See Figure 4-72.) To access, scroll to the fourth option on the list and touch the *The NIOSH Pocket Guide to Chemical Hazards (NPG)* link.

Figure 4-72 NIOSH Pocket Guide to Chemical Hazards



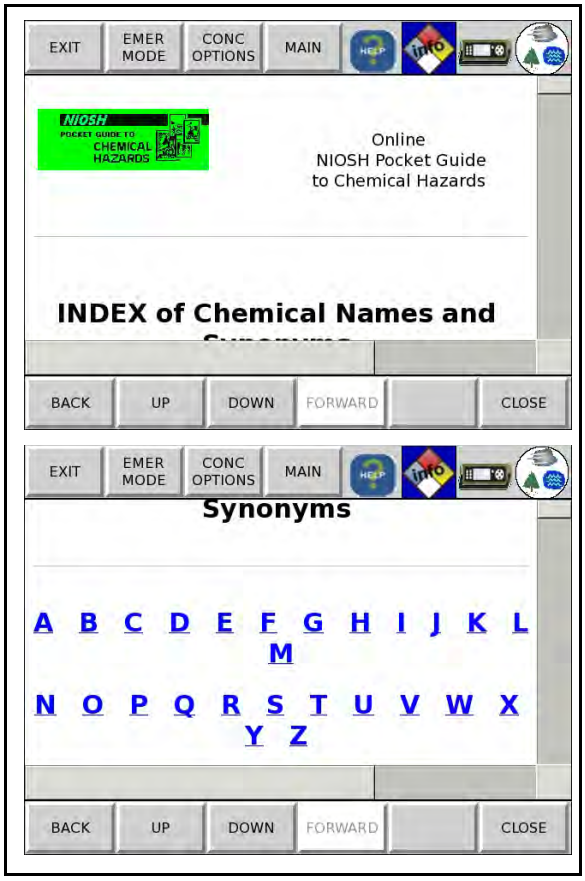
2 When the publication appears, touch **INDEX with CHEMICAL NAMES and SYNONYMS**. (See Figure 4-73.)

Figure 4-73 NIOSH Pocket Guide



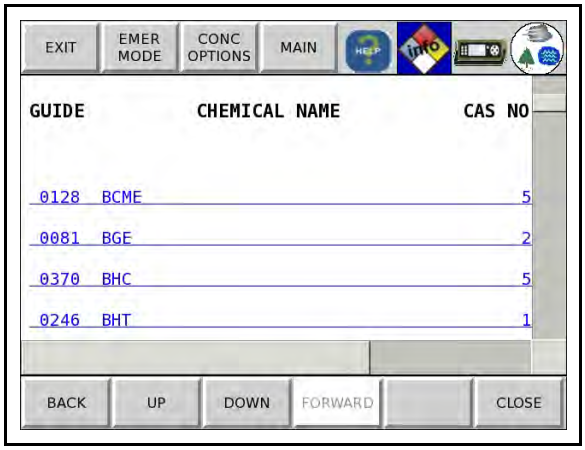
3 Scroll down to display an alphabet. Touch the first letter of the desired compound. (See Figure 4-74.)

Figure 4-74 Pocket Guide Index



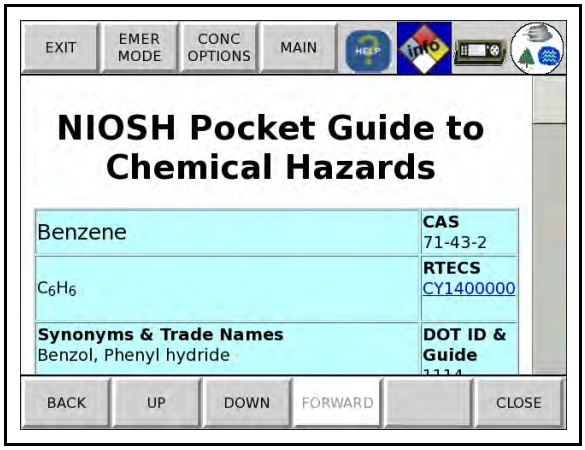
4 A list of the chemicals that start with the selected letter will be displayed. (See Figure 4-75.)

Figure 4-75 Index of Chemicals By Name



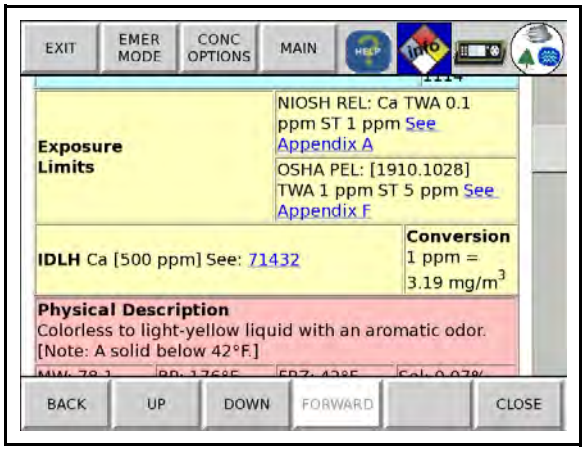
5 Touch the desired chemical. The Pocket Guide for this specific chemical will be displayed. (See Figure 4-76.)

Figure 4-76 NIOSH Pocket Guide for a Specific Chemical



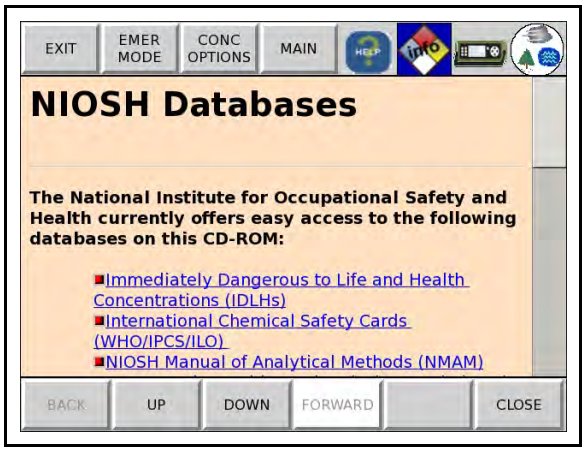
6 Scrolling down will display information about the exposure limit and the boiling point of the chemical. The boiling point will determine if the chemical can be detected by the HAPSITE ER. See section 2.2 for boiling point recommendations. (See Figure 4-77.)

Figure 4-77 NIOSH Pocket Guide Exposure Limit and IDLH Information



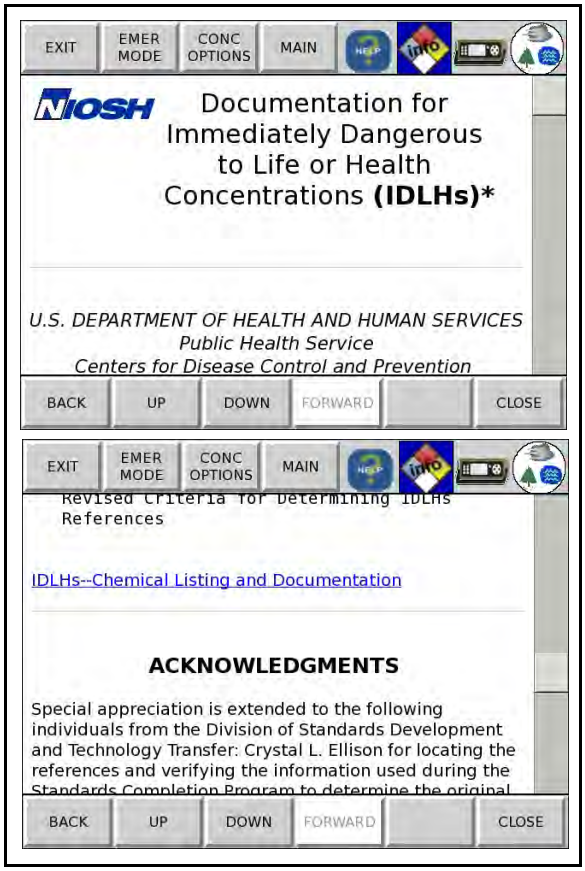
7 To access information regarding *Immediately Dangerous to Life and Health Concentrations* (IDLHs), touch the first hyperlink on the info screen. (See Figure 4-78.)

Figure 4-78 IDLHs



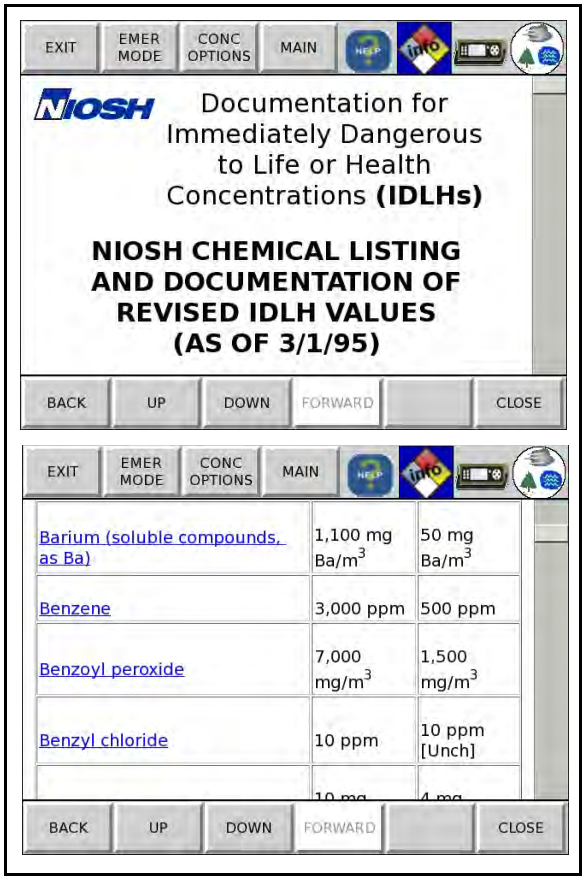
8 Scroll down or touch **DOWN** until the **IDLHs-Chemical Listing and Documentation** link is displayed. Touch this link. (See Figure 4-79.)

Figure 4-79 Chemical Listing and Documentation Link



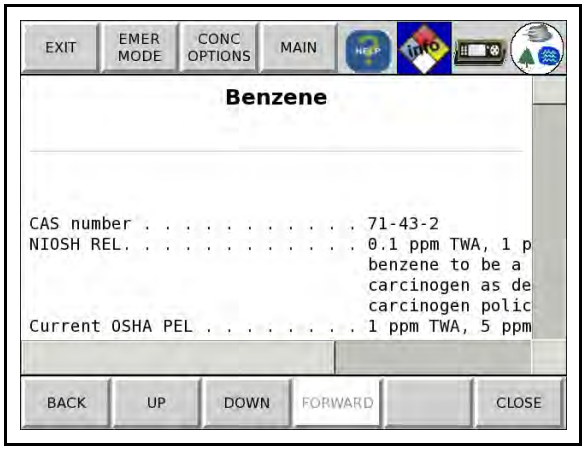
9 Scroll down, press **DOWN** or use the down arrow to find the desired compound. Press the link to view the compound's information. (See Figure 4-80.)

Figure 4-80 Selecting IDLH of Compound



10 Information regarding the compound's NIOSH REL, OSHA PEL and toxicity data will be displayed. (See Figure 4-81.)

Figure 4-81 IDLH Screen

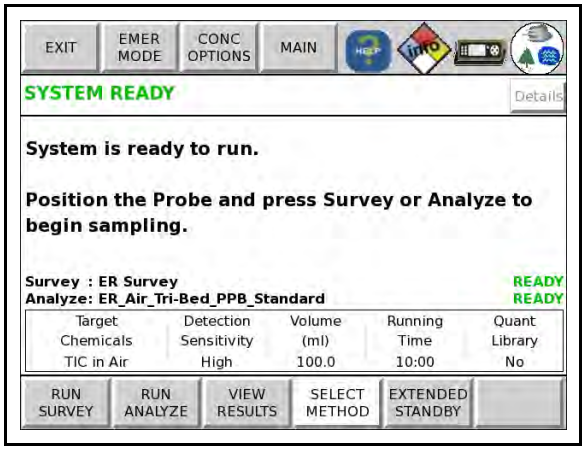


4.7.1 HAPSITE ER Icon

The **HAPSITE ER** icon provides information the status of the ER and its consumables. Information regarding battery power, gas consumption, heaters, tune status, and GPS can be accessed through this screen.

1 The **System Parameters** screen can also be displayed by touching the **HAPSITE ER** icon. (See Figure 4-82.)

Figure 4-82 HAPSITE Icon



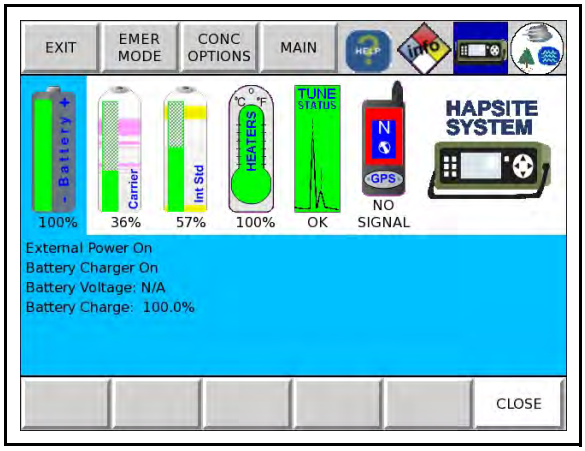
2 Alternately, push the **SYSTEM STAT** button until the **HAPSITE ER** icon is highlighted. (See Figure 4-83.)

Figure 4-83 SYSTEM STAT Push Button

4.7.1.1 Battery Icon

If a battery is installed, the **Battery** icon will display information about the battery's charge level. The charge level is found as a vertical bar graph inside the battery icon. If a battery is not installed, **EXTPWR** will be displayed under the icon and the icon's charge level bar graph will turn red. (See Figure 4-84.)

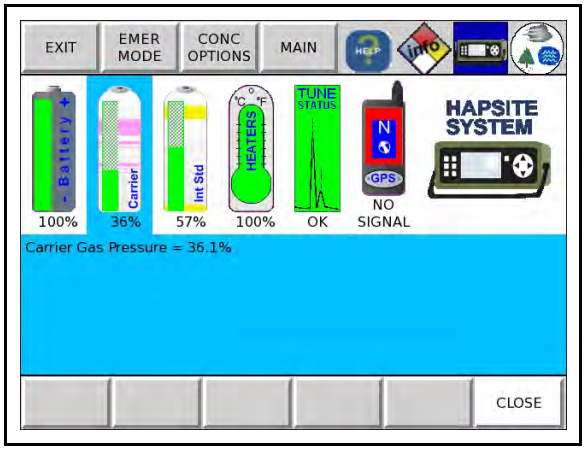
Figure 4-84 Battery Icon



4.7.1.2 Carrier Gas Icon

The carrier gas is also known as the nitrogen gas. Touching the **Carrier Gas** icon, will provide information about the pressure of the gas in the can. A vertical bar graph in the icon will provide a percentage of gas remaining in the canister. (See Figure 4-85.)

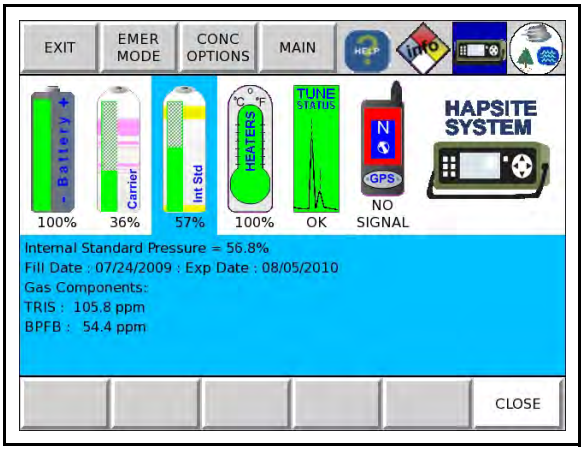
Figure 4-85 Carrier Gas Icon



4.7.1.3 Internal Standard Icon

The **Internal Standard** icon uses a vertical bar graph to provide a percentage of gas remaining in the canister. Touching the icon will display the canister's fill date, the canister's expiration date, and the actual PPM of BPFB and TRIS concentrations in the canister. (See Figure 4-86.)

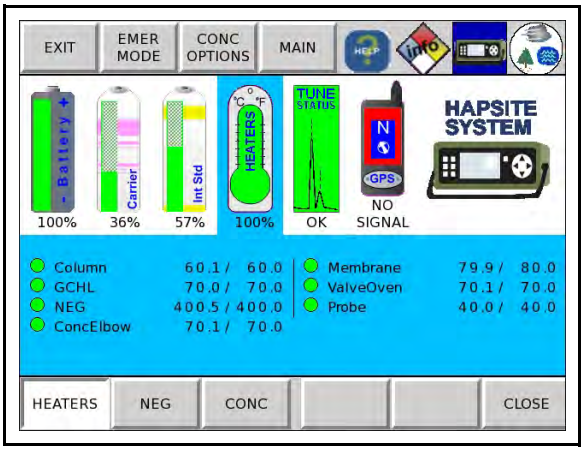
Figure 4-86 Internal Standard Icon



4.7.1.4 HEATERS Icon

The **HEATERS** icon also has the following options at the bottom of the touch screen: **HEATERS**, **NEG** and **CONC**. The bar graph located on the **HEATERS** icon represents the progress of the Heaters. (See Figure 4-87.)

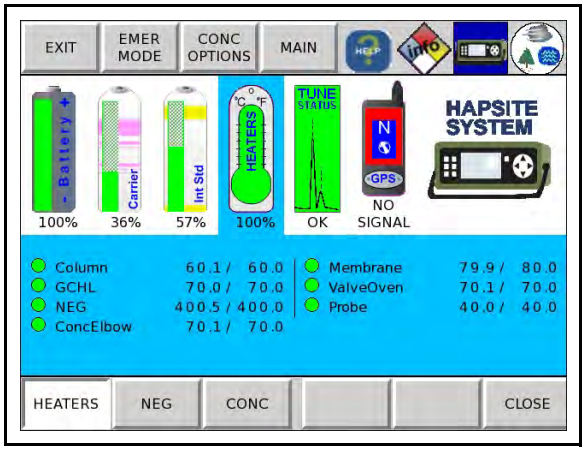
Figure 4-87 Heaters Icon



4.7.1.4.1 HEATERS Button

Touching the **HEATERS** icon provides the current temperatures of the column, the membrane, the valve oven, the probe, the GCHL, the Concentrator Elbow, and the NEG Heater as HAPSITE ER is heating. See Figure 4-87. The number after the actual temperature is the setpoint temperature. For example, if the temperatures read 55/70, 55 °C is the component's current temperature and 70 °C is the setpoint temperature. (See Figure 4-88.)

Figure 4-88 Temperatures of Heaters

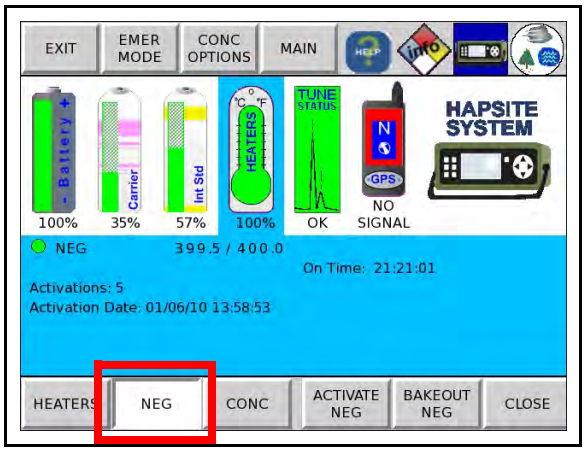


4.7.1.4.2 NEG Button

The **NEG** button provides information about the NEG. This includes the NEG's current and setpoint temperatures, the hours of NEG use, and the date the NEG was activated. The number of times the NEG has been activated and the date(s) of reactivation are displayed on this screen.

From this screen, there is a button to activate the NEG and also a button for NEG bakeout. (See Figure 4-89.) For more information, see Chapter 12, Maintenance.

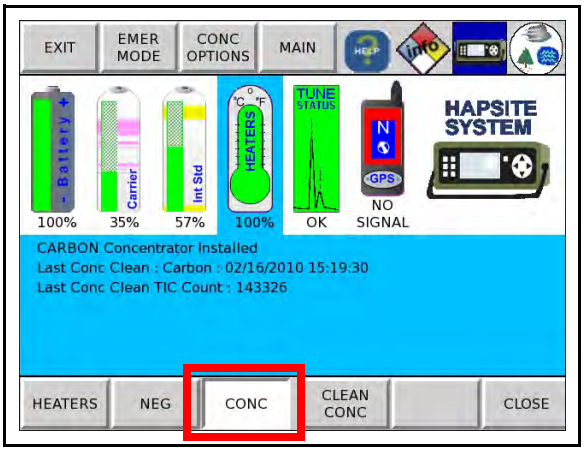
Figure 4-89 NEG Button



4.7.1.4.3 CONC Button

Information about the concentrator can be found through this button. After touching the **CONC** button, another key, **CONC CLEAN**, will be displayed. If this button is active (black lettering), a concentrator cleanout can be started. Touch the **CONC CLEAN** button if a concentrator cleanout is desired. If the **CONC CLEAN** button is grayed out, a concentrator cleanout is in the process of running or a sample loop is installed. Above the buttons, the progress of the cleanout will be displayed by a blue bar graph. (See Figure 4-90.)

Figure 4-90 CONC Button

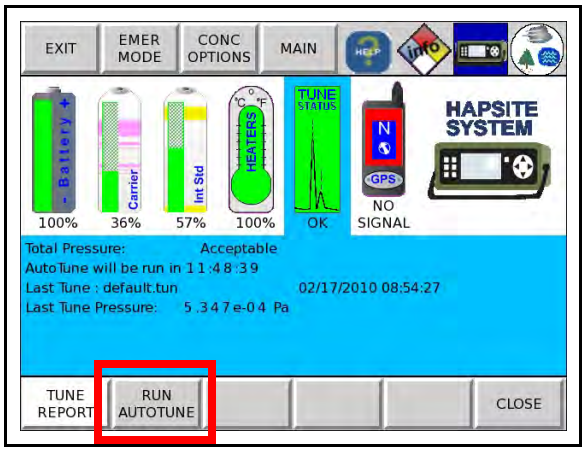


4.7.1.5 TUNE STATUS Icon

This icon provides information about the state of the HAPSITE's tune. If the **TUNE** icon is green, the tune status is acceptable. The **TUNE** icon will turn yellow when an AutoTune has been manually aborted or skipped. The icon will turn blue when HAPSITE ER is in the process of tuning. If the **TUNE** icon is red, the AutoTune has failed or the system is preparing to run an AutoTune.

To run an AutoTune, either touch **PREPARE** and HAPSITE ER will run a tune check as part of its preparation, or press the **RUN AUTOTUNE** button, which is shown at the bottom of the screen. This button allows for an AutoTune to be run from the front panel. (See Figure 4-91.)

Figure 4-91 Run AutoTune



Touching the **TUNE STATUS** icon will also provide the file name of the last tune report, the time the instrument tuned, and the date the instrument tuned. It will also show a countdown of the time to the next tune check.

The pressure of the MS at the last AutoTune will be displayed. If a method is being run or manual tune is open, the current MS pressure will also be displayed. If a method is not running and the last tune pressure was within range, an Acceptable message will be displayed.

4.7.1.5.1 TUNE REPORTS

After the **TUNE STATUS** icon has been touched, see Figure 4-92, a new button, **TUNE REPORTS**, will be shown at the bottom of the screen. This button accesses data from past Tune Reports. (See Figure 4-93.) For more information on **Tune Reports**, see Chapter 9, Tune.

Figure 4-92 Tune Status Icon

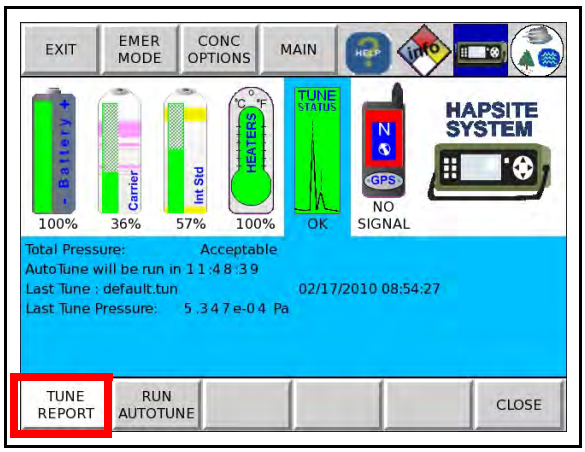
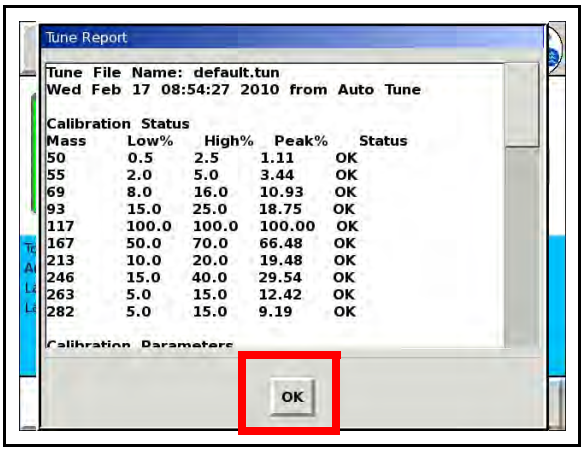


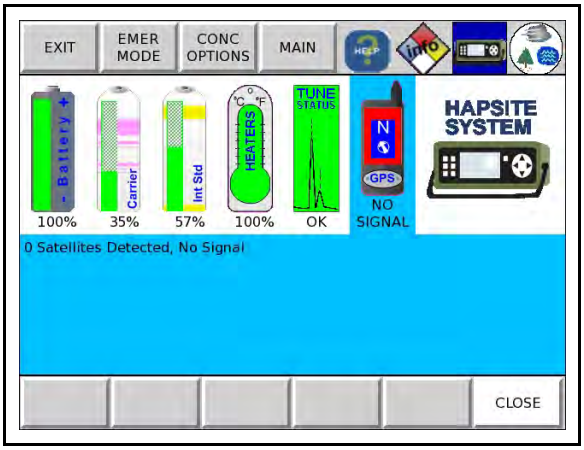
Figure 4-93 Tune Report



4.7.1.6 GPS Icon

The **GPS** icon will give the latitude and longitude coordinates of the HAPSITE ER position. It also provides the number of satellites found on the GPS System. (See Figure 4-94.)

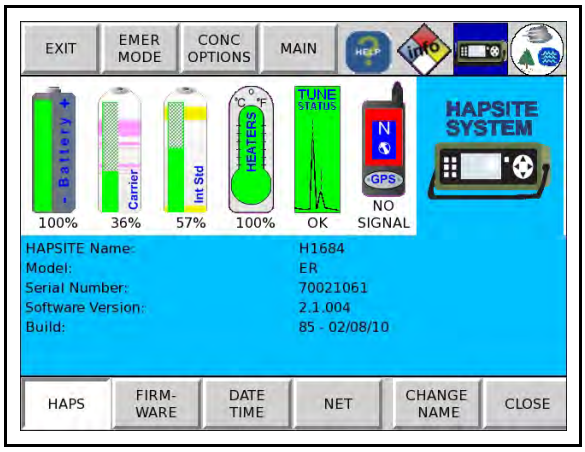
Figure 4-94 GPS Icon



4.7.1.7 HAPSITE SYSTEM Icon

This icon provides additional system information. This information includes the version number of the software and firmware, the date and time, and the IP address. It also provides the HAPSITE ER's serial number. (See Figure 4-95.)

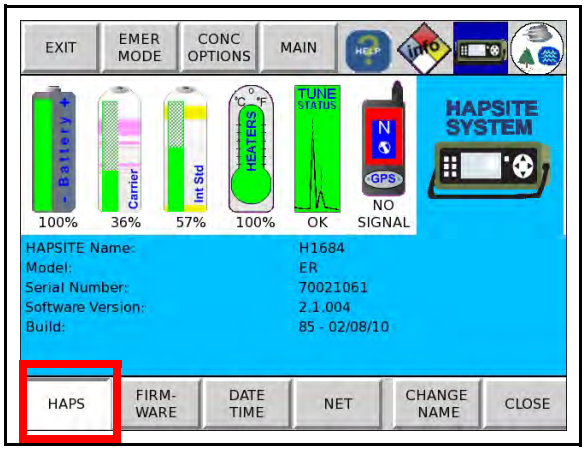
Figure 4-95 HAPSITE SYSTEM Icon



4.7.1.7.1 HAPS Button

The **HAPS** button provides the HAPSITE name, the HAPSITE ER's Serial Number, and the current version number of the software. It also provides the software build date. (See Figure 4-96.)

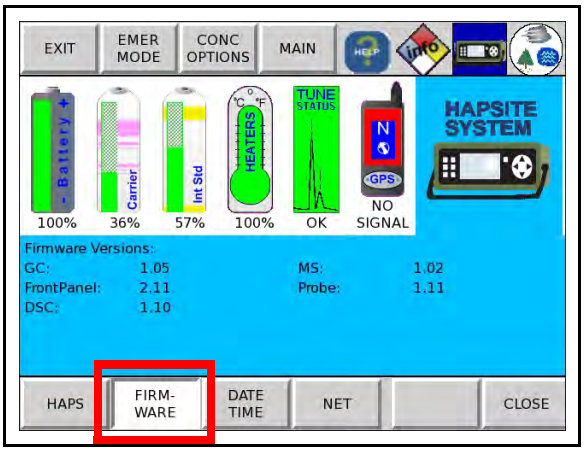
Figure 4-96 HAPS Button



4.7.1.7.2 FIRMWARE Button

The **FIRMWARE** button gives the version number of the G.C., the front panel board, the mass spectrometer and the probe. (See Figure 4-97.)

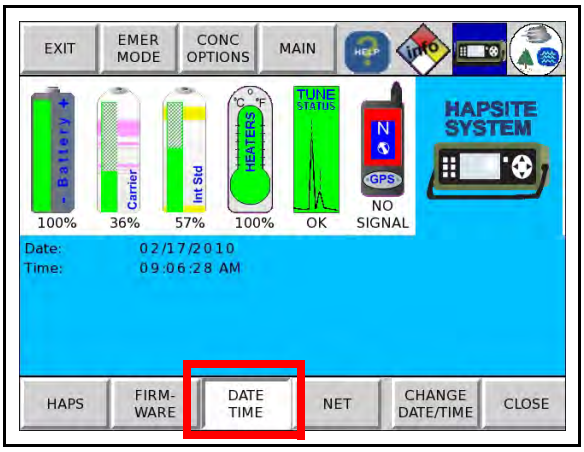
Figure 4-97 FIRMWARE Button



4.7.1.7.3 DATE TIME Button

This button gives the present date and time. (See Figure 4-98.)

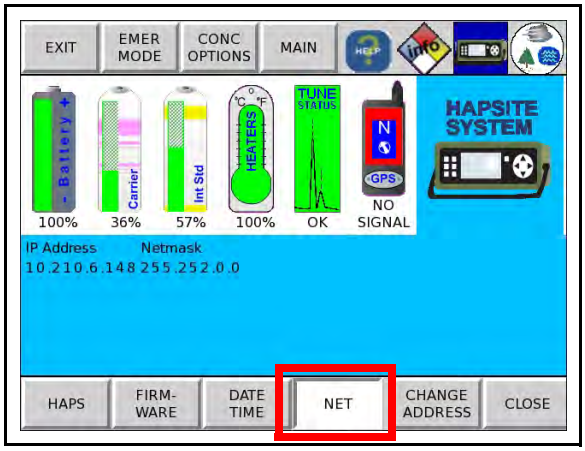
Figure 4-98 DATE TIME



4.7.1.7.4 NET Button

The **NET** button provides the IP address for HAPSITE ER and the Subnet mask. This will be used when using the wireless connection on the Laptop. See Chapter 5, Communications and Touch Screen Options. (See Figure 4-99.)

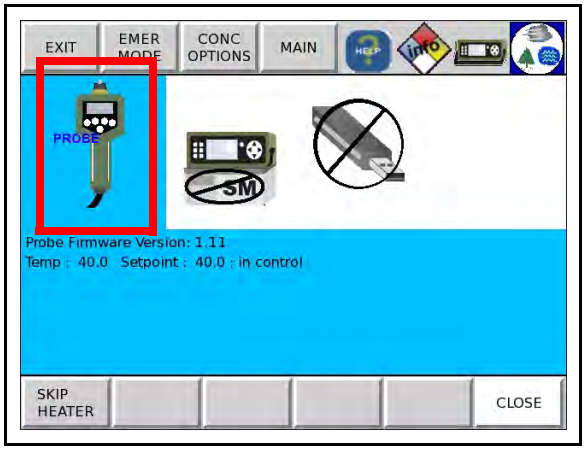
Figure 4-99 NET Button



4.7.2 Attachments

The **Attachments** option on the **STATUS** Menu displays information regarding the current sampling configuration of the HAPSITE ER (Air Probe, Headspace, etc.). If the Air Probe is installed, an icon of the probe will be displayed. Touching the **PROBE** icon will display the installed version of the probe's firmware. (See Figure 4-100.)

Figure 4-100 Probe Icon



If the Service Module is installed, the Service Module icon will be shown. Touching the **Service Module** icon will display the installed version of the service module's firmware and the turbo speed of the service module's pump. Options for attaching and detaching the service module can be found through this screen. For more information on the service module, see the Service Module Manual.

The Headspace Sampling System icon will appear when it is attached to the HAPSITE ER. Touching the HSS or SituProbe icon will display the information regarding the firmware version and accessory's heaters. See the Headspace Sampling System and SituProbe Purge and/or Trap Sampling Systems' manuals for further information.

4.7.3 Info

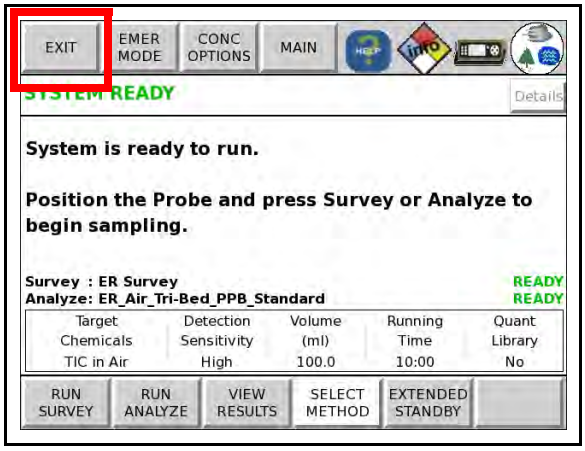
The info option on the **STATUS** Menu will access the NIOSH Database screen. It is equivalent to touching the **info** icon.

4.8 EXIT Menu

The **EXIT** menu is located on the top row of the front panel. (See Figure 4-101.) This option will access **Turn Off**, **Reboot** or **Standby**. **Turn off** will shut down the HAPSITE ER's power. **Reboot** will reset the microprocessor in HAPSITE ER and reload the drivers. It will also restart the operating system, HAPSITE ER program and the front panel program. The **Standby** option will put the system into Extended Standby. Refer to section 4.8.1 on page 4-61 for Extended Standby instructions.

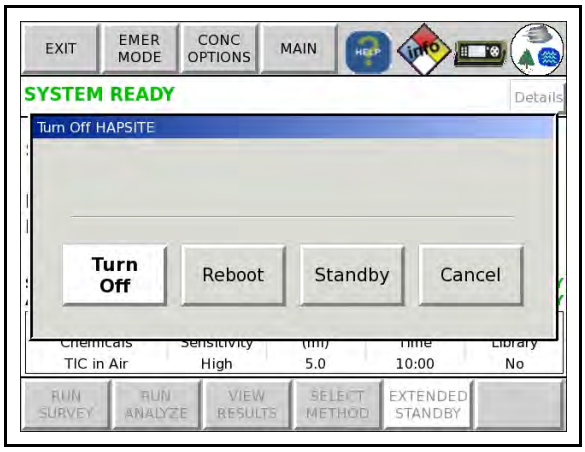
1 Touch **EXIT**. Alternately, use the arrow keys to highlight **EXIT** and push **OK SEL**. (See Figure 4-101.)

Figure 4-101 Exit Menu



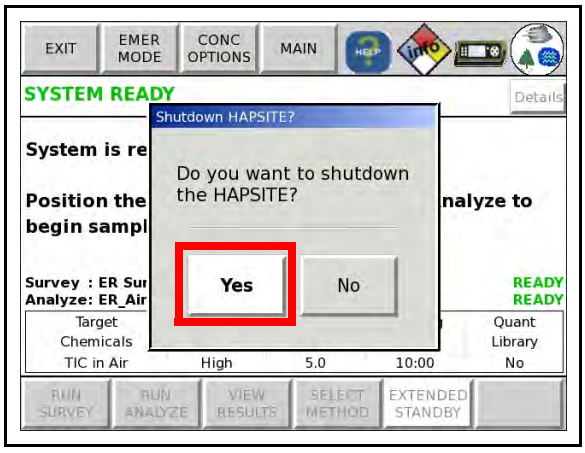
2 The three exit options will be displayed on the screen. There will also be a **Cancel** button. Either touch or use the **arrow keys** to highlight the desired choice on the screen. If using the push buttons, push **OK SEL**. (See Figure 4-102.)

Figure 4-102 EXIT Selections



3 A prompt will be displayed to confirm the selection. For example, if **Turn Off** is selected, a prompt **Are you sure you want to shutdown the HAPSITE?** will appear on the screen. Touch **Yes** or select **Yes** and push **OK SEL** to continue. (See Figure 4-103.)

Figure 4-103 Confirming Shutdown



4 For **Turn Off**, the HAPSITE will turn off the power.

4a For **Reboot**, the screen will turn off and in approximately one minute, the screen will become active again. The preparation sequence will be restarted.

4b For **Standby**, the Extended Standby screen will be displayed. See section 4.8.1, Extended Standby, on page 4-61.

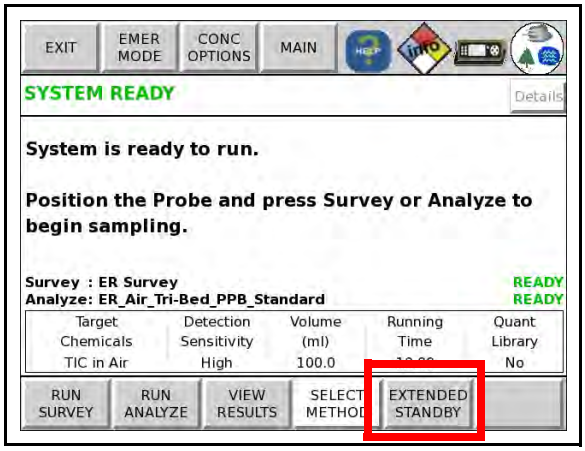
4.8.1 Extended Standby

Extended Standby is the preferred storage mode. In this state, the NEG remains heated at 400°C and the ion pump continues pumping to maintain a vacuum in the Mass Spectrometer. HAPSITE ER turns of the heaters for all other components. When in Extended Standby, remove the gas canisters to avoid consumption.

Extended Standby extends NEG pump life and allows the system to prepare faster. Proceed as follows to place the system into Extended Standby.

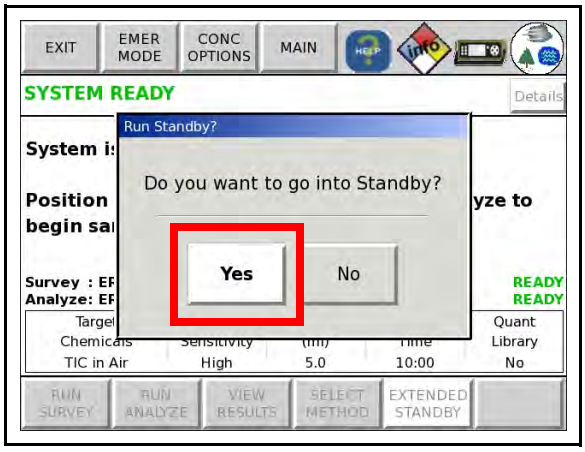
1 Touch **EXTENDED STANDBY**. Alternately, use the arrow keys to highlight **EXTENDED STANDBY** and push **OK SEL**. (See Figure 4-104.)

Figure 4-104 Extended Standby



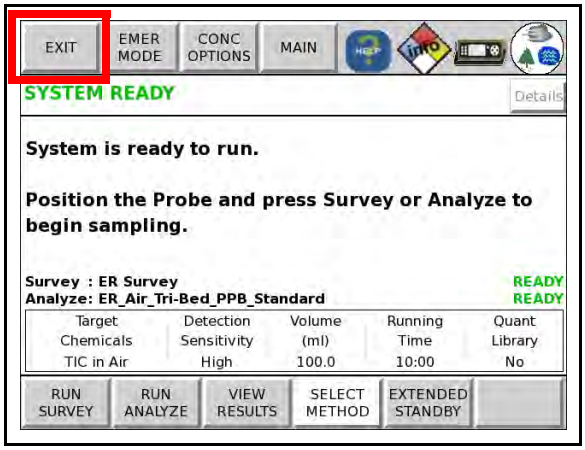
2 When the screen prompts, **Do you want to go into Standby?,** touch **Yes**. Alternately, using the **arrow keys**, highlight **Yes** and push **OK SEL**. (See Figure 4-105.)

Figure 4-105 Confirming Standby Option



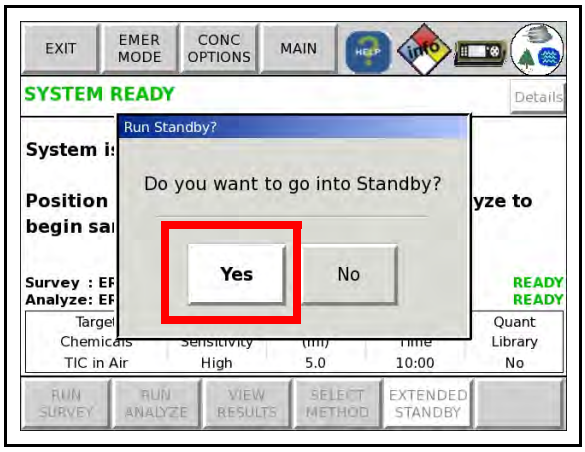
3 Alternately, touch **EXIT** or use the **arrow keys** to highlight **EXIT**. Push **OK SEL**. (See Figure 4-106.)

Figure 4-106 EXIT Button



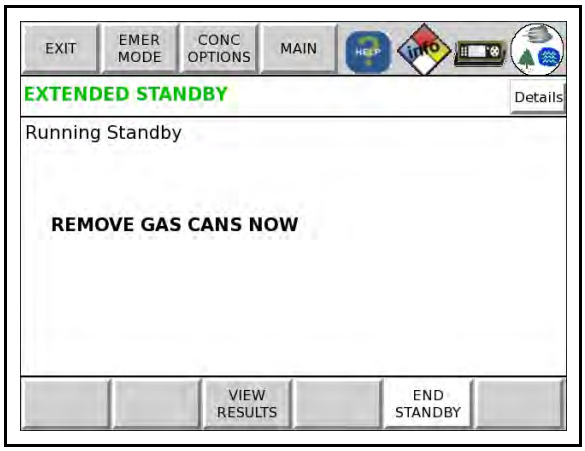
4 When the screen prompts, **Do you want to go into Standby?,** touch **Yes**. Alternately, using the **arrow keys**, highlight **Yes** and push **OK SEL**. (See Figure 4-107.)

Figure 4-107 Confirming Standby Option



5 The HAPSITE will go into Extended Standby. Remove the gas canisters. (See Figure 4-108.)

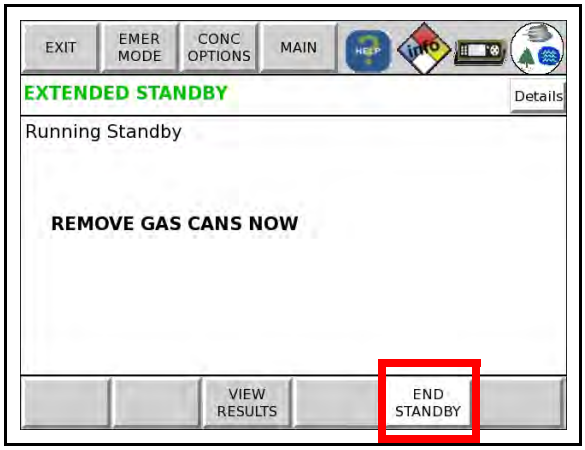
Figure 4-108 Extended Standby



4.8.1.1 End Standby

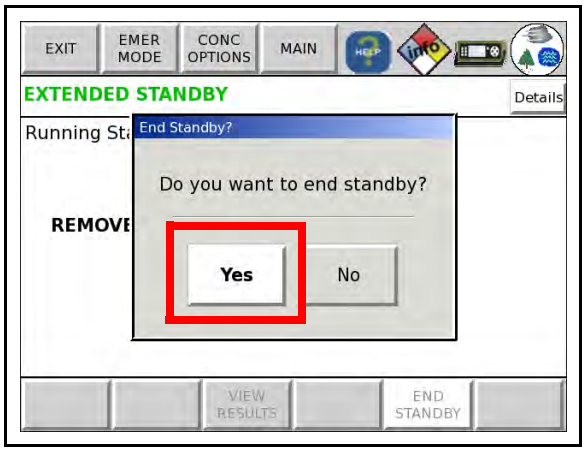
1 To End Standby, touch **END STANDBY** or using the **arrow keys**, highlight **END STANDBY** and push **OK SEL**. (See Figure 4-109.)

Figure 4-109 END STANDBY



2 When the system prompts, **Are you sure you want to end standby?,** touch **Yes**. Alternately, highlight **Yes** using the **arrow keys** and push **OK SEL**. (See Figure 4-110.)

Figure 4-110 Confirming End Standby



Chapter 5
Communications and Touch Screen Options

5.1 Communications

HAPSITE ER has two communication options: the cross-over cable and the wireless connection. The wireless settings will be configured with the laptop at the factory. Before connecting wirelessly, the wireless radio on HAPSITE ER and the wireless button on the laptop will have to be enabled. Follow the instructions below to turn on the radio. Refer to section 3.2.4, Connecting the Laptop, on page 3-14 for instructions on attaching the laptop.

5.1.1 Wireless Range

HAPSITE is equipped with an 802.11b/g wireless adapter. The typical range for a signal is 300 feet (100 meters) with no obstructions. The following may degrade the signal:

- Metal buildings
- Concrete structures
- Electric devices in the area

5.1.2 Turning On the Radio

This procedure gives instructions for turning on the radio, which is necessary for wireless communication.

DANGER

When the HAPSITE ER radio is on, even if wireless communication is not being used, a radio signal is being transmitted. The only way to eliminate the radio signal is to turn the radio off.

1 Open the front panel of HAPSITE ER.

2 Remove the cover from the power switch (for the wireless radio). It is located on the far left side. To remove, unscrew the cover by turning it counter-clockwise. See Figure 5-1.

Figure 5-1 Unscrewing wireless cap

DANGER

HAPSITE contains a wireless transmitter/receiver that emits electromagnetic radiation (EMR). This radiation in a tactical or operational environment may potentially be used to locate HAPSITE and its operators. This radiation also has the potential to detonate some types of unexploded ordnance (UXO), or improvised explosive devices (IEDs), or both, if HAPSITE is transmitting in the safety exclusion area around the device(s). There is a hardware switch to turn off the wireless radio so that HAPSITE may still be used in areas where these hazards are a concern. Consult applicable regulations and policies when using HAPSITE with the wireless device active in such environments.

3 Press the power button until a click is heard. The green lights adjacent to **Radio** and **WLAN** should illuminate. When the green lights are illuminated, the wireless radio is being powered. See Figure 5-2.

Figure 5-2 Pushing wireless button

4 Replace the switch cover by placing it over the switch. Turn it clock-wise until finger tight.

5.1.3 Wireless Module Indicator Lights

Located on the Wireless Module inside the HAPSITE front cover are four indicator lights:

RADIO . . . . . When illuminated, the radio is enabled.

WLAN. . . . . When illuminated, the wireless connection is linked to the laptop. The LED blinks when transmitting or receiving data.

LAN . . . . . When illuminated, the HAPSITE is connected via a crossover cable to the laptop. The LED blinks when transmitting or receiving data. The LED will be extinguished if the crossover cable is disconnected.

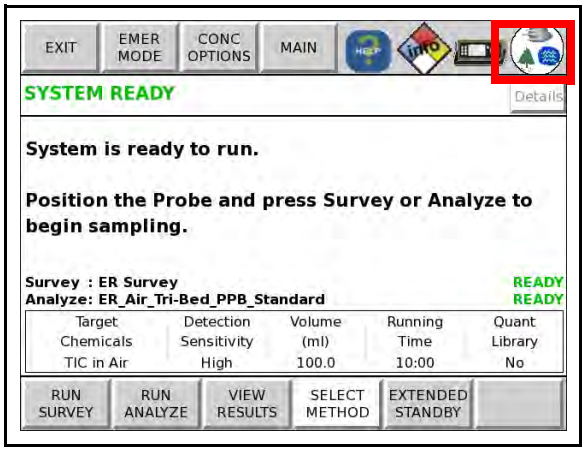
586 . . . . . When illuminated, the HAPSITE 586 processor is linked to a wired or wireless connection.

5.2 Setting Up Communications

NOTE: Setting up communications is an **Advanced** user function.

1 To locate the **HAPSITE H** number on the front panel, touch the **HAPSITE** icon. (See Figure 5-3.)

Figure 5-3 HAPSITE icon

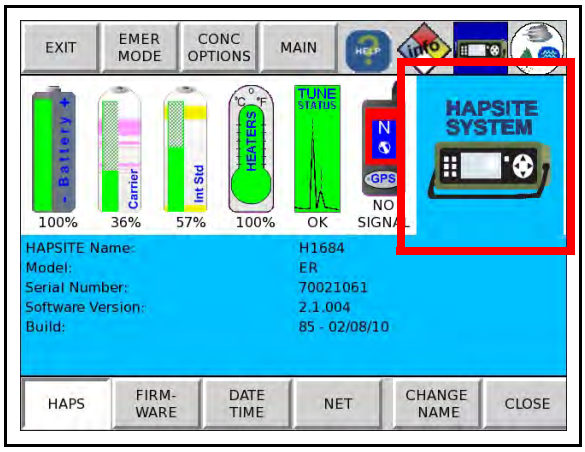


2 Alternately, push the **STAT** button until the **HAPSITE** icon is highlighted. (See Figure 5-4.)

Figure 5-4 STAT button

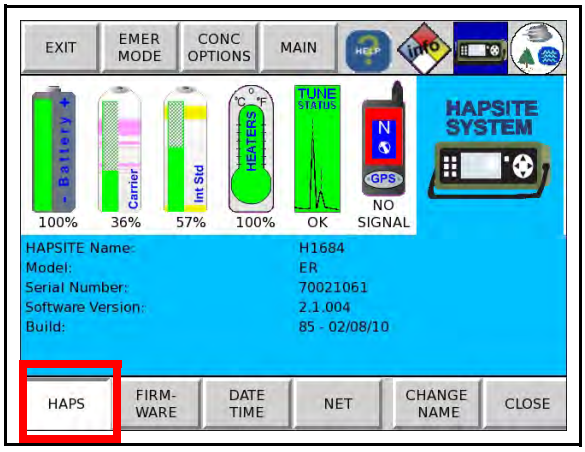
3 Touch the **HAPSITE System** icon. (See Figure 5-5.)

Figure 5-5 HAPSITE System



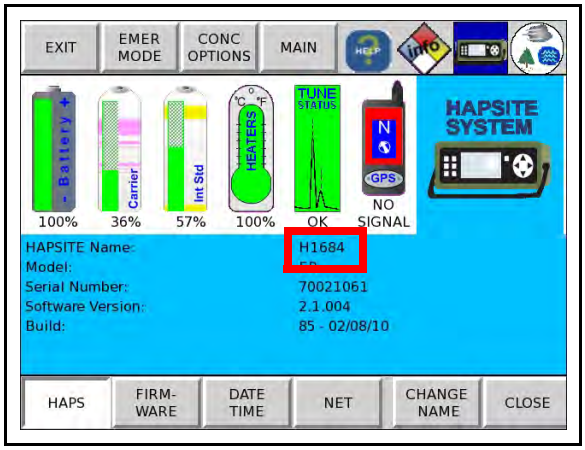
4 Touch the **HAPS** button or use the **arrow keys** to highlight the **HAPS** button and push **OK SEL**. (See Figure 5-6.)

Figure 5-6 HAPS button



5 Locate and note the **HAPSITE Name**. (See Figure 5-7.)

Figure 5-7 HAPSITE name

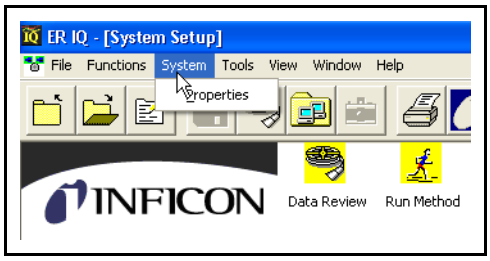


6 Open **ER IQ** Software. (See Figure 5-8.)

Figure 5-8 ER IQ Software

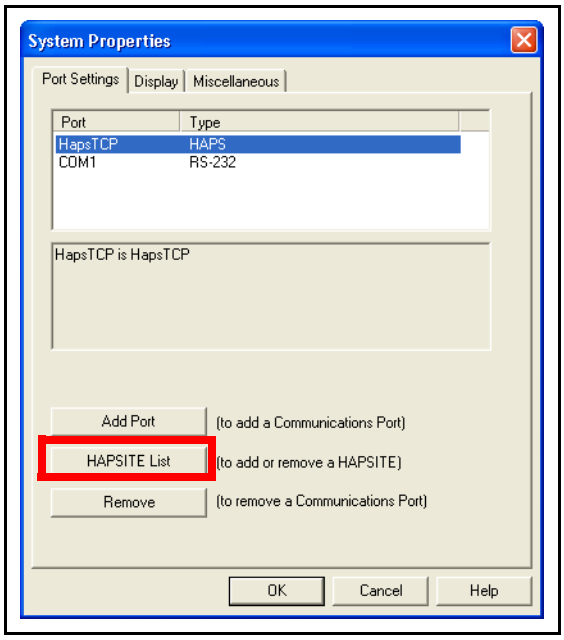
7 From the **System** drop-down menu, select **Properties**. (See Figure 5-9.)

Figure 5-9 Selecting Properties from the System Drop-down Menu



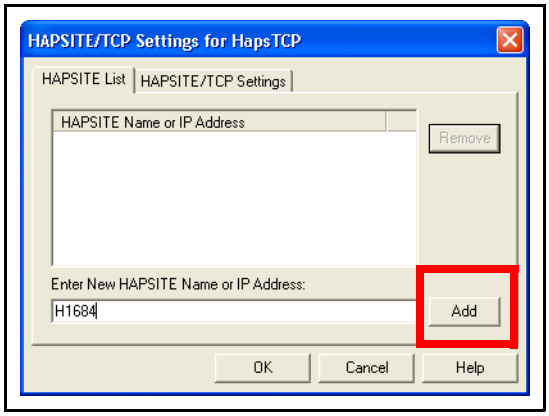
8 Click the **HAPSITE List** button. (See Figure 5-10.)

Figure 5-10 HAPSITE List Button



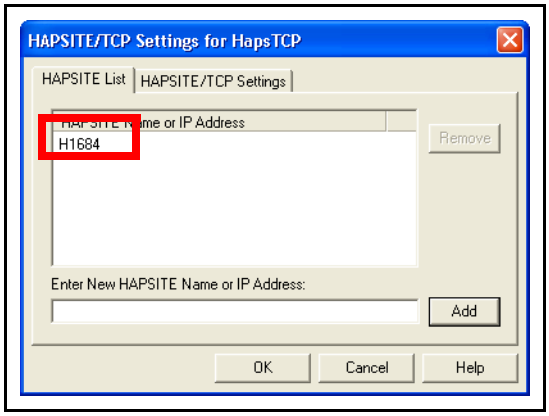
9 Enter the **H number** into the **Enter HAPSITE Name or IP Address**. Click **Add**. (See Figure 5-11.)

Figure 5-11 Add HAPSITE



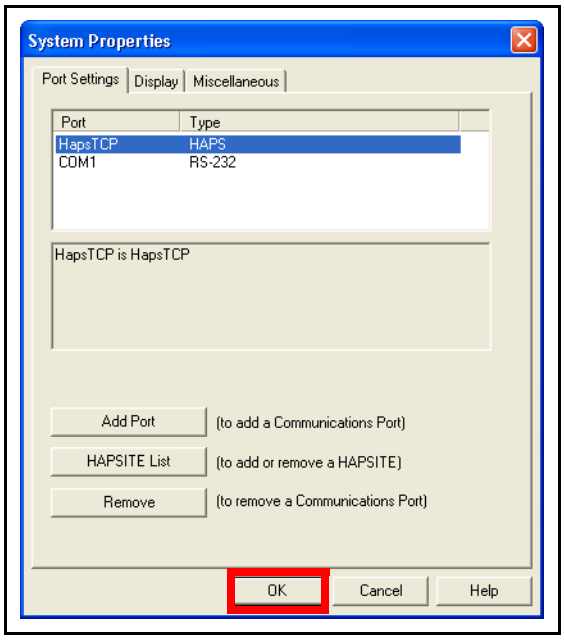
10 The newly added HAPSITE will appear in the HAPSITE List. (See Figure 5-12.) Press **OK**.

Figure 5-12 Adding the HAPSITE



11 Press **OK** on the **System Properties** window. (See Figure 5-13.)

Figure 5-13 System Properties



12 The newly added **HAPSITE** icon will now appear at the bottom of the **System Setup** screen. If HAPSITE is displayed, as seen in Figure 5-14, then communications have been established.

Figure 5-14 Newly added HAPSITE

12a If the HAPSITE icon is overlaid with a gray “X”, HAPSITE is not trying to communicate with the computer.

Figure 5-15 Gray X

12b If the **HAPSITE** icon is overlaid with a red “X”, HAPSITE is not properly communicating with the laptop. (See Figure 5-16.) For example, the cross-over cable is disconnected.

Figure 5-16 Red X

12c If the **HAPSITE** icon is overlaid with a blue “X”, communication has not been fully established. (See Figure 5-17.) Continue with Configuring HAPSITE for Communications, see section 5.3.

Figure 5-17 Blue X

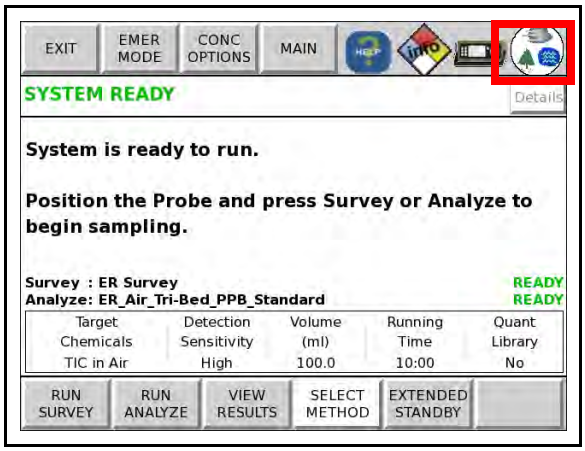
13 If a communication error has occurred, which is indicated by an “X”, follow the instructions in Configuring HAPSITE for Communications, see section 5.3 below.

5.3 Configuring HAPSITE for Communications

If communication between HAPSITE and the laptop could not be established using section 5.2, Setting Up Communications, on page 5-4, continue as follows.

1 To locate the **HAPSITE H** number on the front panel, touch the **HAPSITE** icon. (See Figure 5-18.)

Figure 5-18 HAPSITE Icon

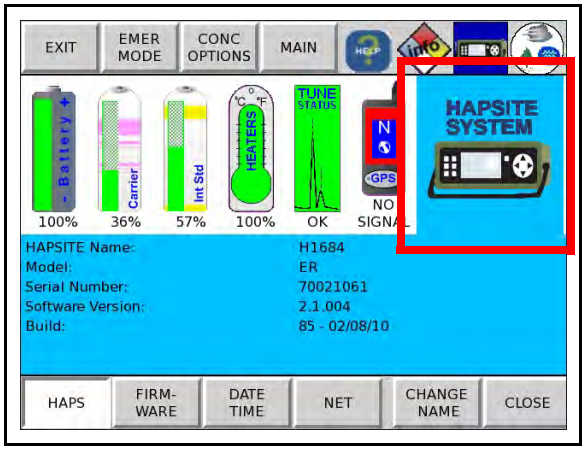


2 Alternately, push the **STAT** button until the **HAPSITE** icon is highlighted. (See Figure 5-19.)

Figure 5-19 STAT Button

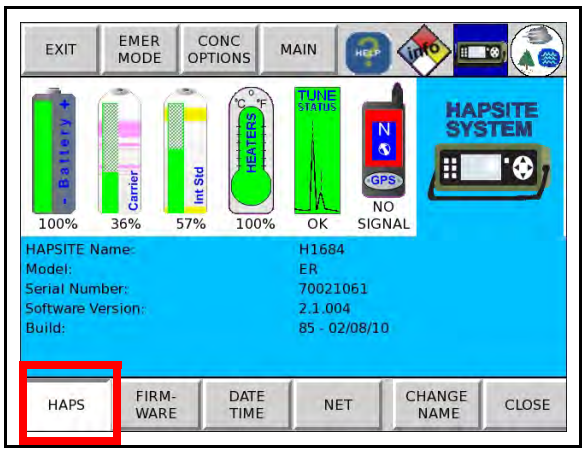
3 Touch the **HAPSITE System** icon. (See Figure 5-20.)

Figure 5-20 HAPSITE System



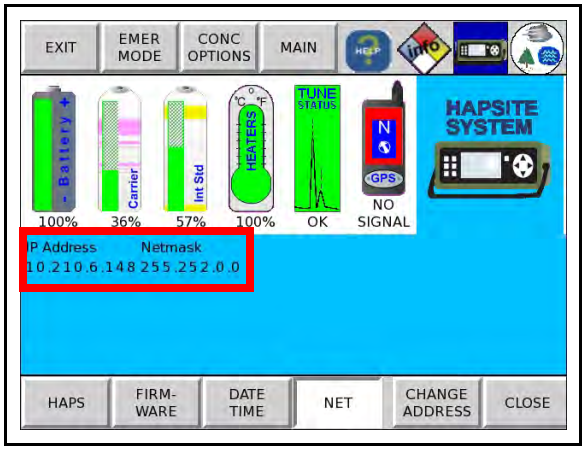
4 Touch the **HAPS** button or use the **arrow keys** to highlight the **HAPS** button and push **OK SEL**. (See Figure 5-21.)

Figure 5-21 HAPS Button



5 Touch the **NET** button or use the arrow keys to highlight the **NET** button and push **OK SEL**. (See Figure 5-22.)

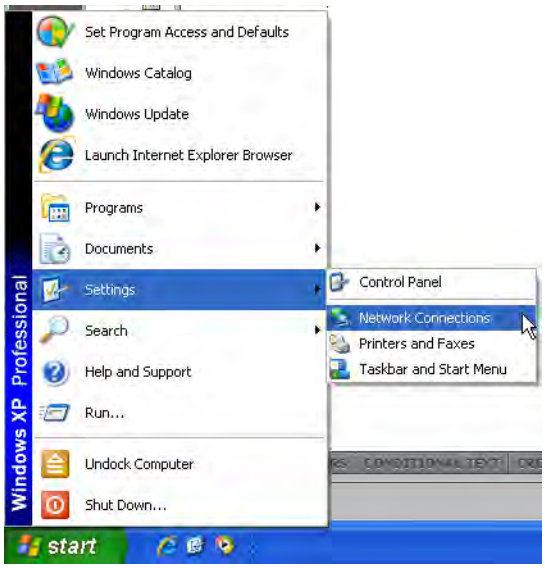
Figure 5-22 Locating the IP Address



6 The **IP Address** and the **Netmask** of HAPSITE will be displayed. For example: 10.210.6.148/255.252.0.0. Each HAPSITE will have a unique **IP Address**.

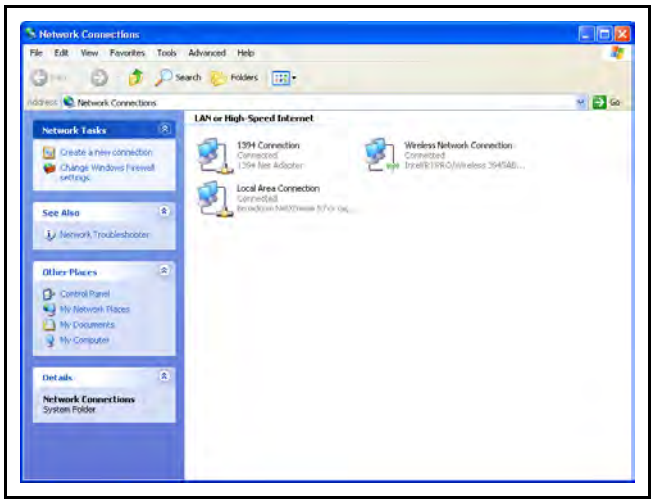
7 On the laptop, click the **start** button on Microsoft Windows. Mouse over the **Settings** option and click **Network Connections**. (See Figure 5-23.)

Figure 5-23 Network Connections



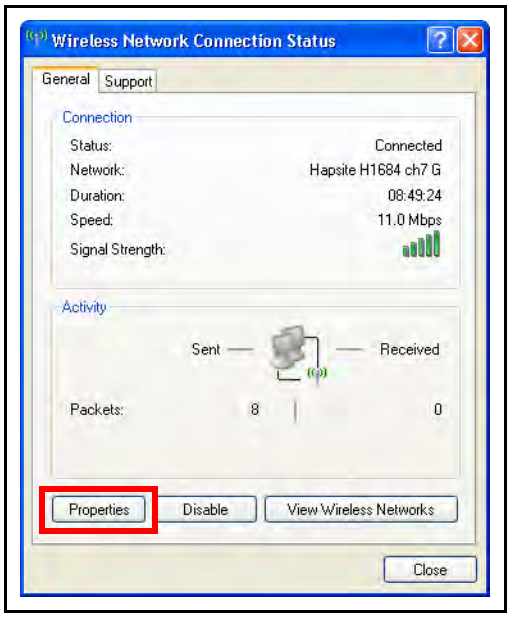
8 The following window will be displayed. Double-click on the desired connection. Choose local area connection to troubleshoot a crossover cable. Choose **Wireless Connection** to connect wirelessly. (See Figure 5-24.)

Figure 5-24 Wireless Connection



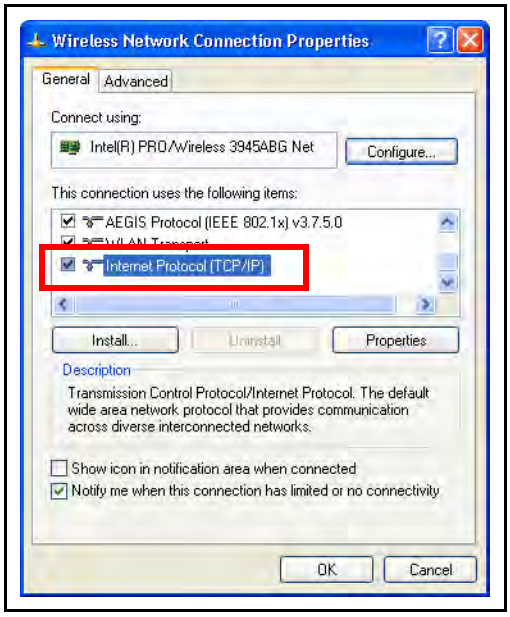
9 The **Connection Status** window will open. Click **Properties**. (See Figure 5-25.)

Figure 5-25 Connection Status



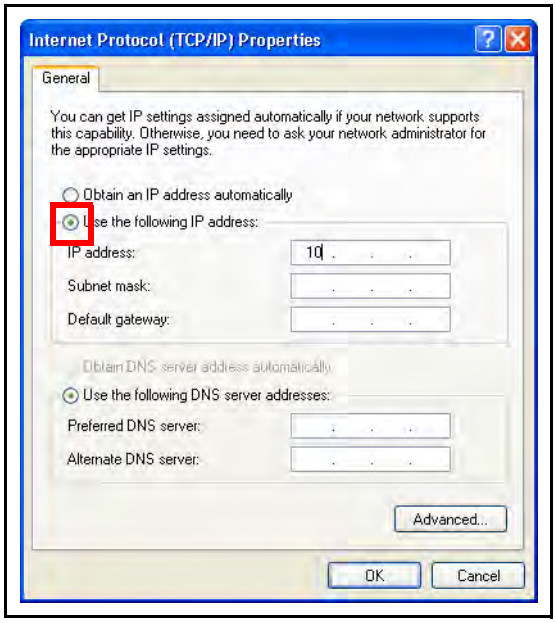
10 In the **General** tab, scroll down and highlight **Internet Protocol (TCP/IP)**, click **Properties**. (See Figure 5-26.)

Figure 5-26 Internet Protocol (TCP/IP)



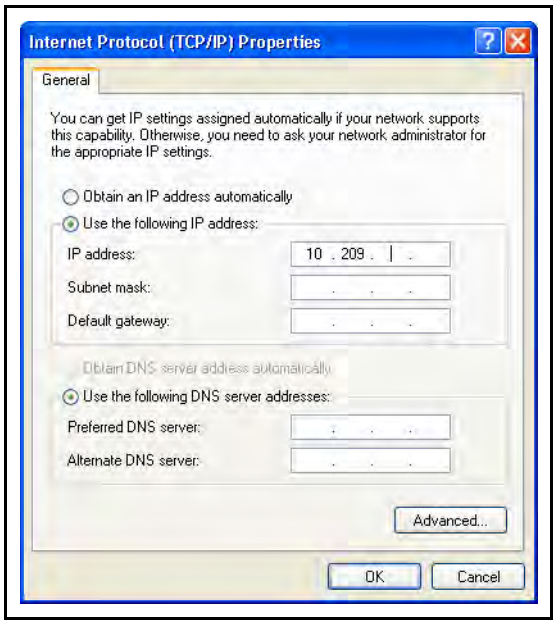
11 Select **Use the following IP address**. Enter the first number of the IP address into the first slot. For example, if the IP Address is **10.210.6.148**, enter **10** into the first slot. (See Figure 5-27.)

Figure 5-27 Use the Following IP Address



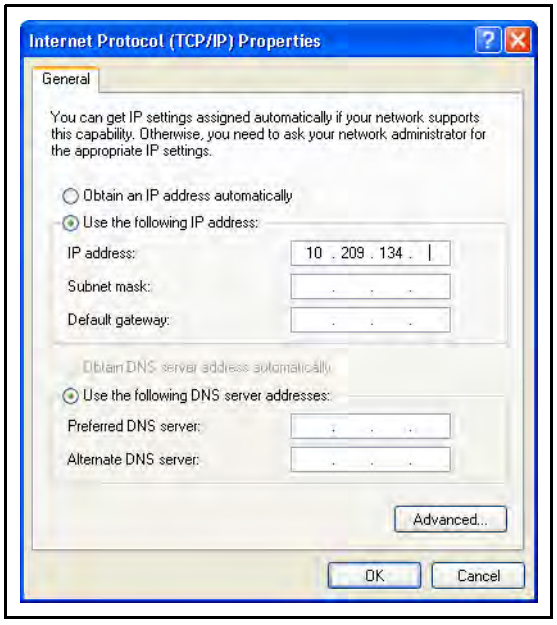
12 For the second number of the **IP Address**, enter **210** if connecting with the cable and **209** if connecting with the wireless radio into the second slot. (See Figure 5-28.)

Figure 5-28 Second Number of IP Address



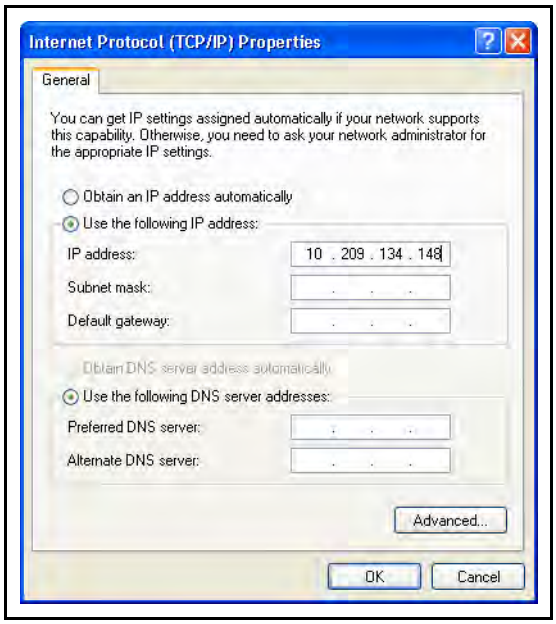
13 For the third number of the **IP Address**, add **128** to the number in the IP address. In this example, adding **128** to **6** equals **134,** so **134** is entered into the third slot. (See Figure 5-29.)

Figure 5-29 Third Number of IP Address



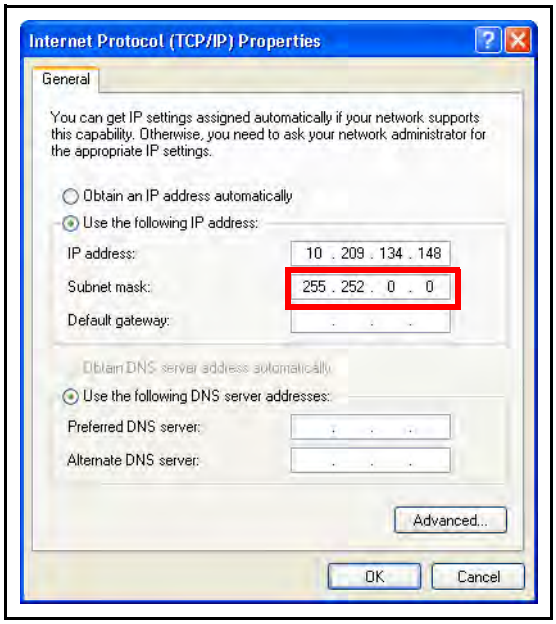
14 The fourth number of the **IP Address** is entered into the fourth slot without modification. Therefore, in this example, **148** would be entered into the fourth slot. (See Figure 5-30.)

Figure 5-30 Fourth Number of IP Address



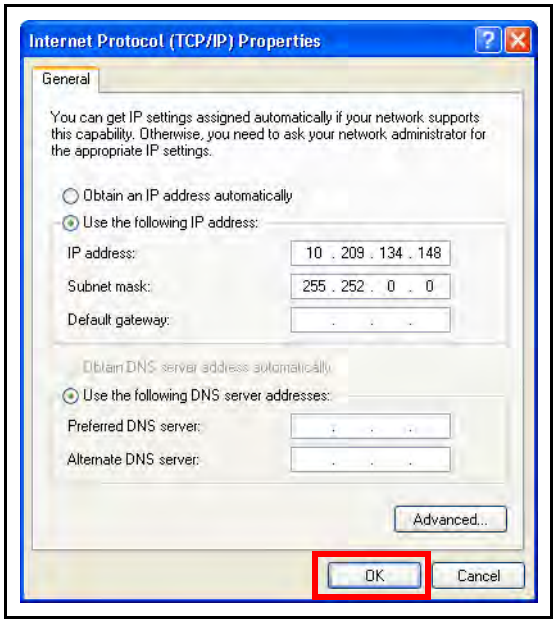
15 Enter in the Subnet mask exactly as displayed. (See Figure 5-31.)

Figure 5-31 Subnet Mask



16 Click **OK** in the **Internet Protocol Properties** window to close. (See Figure 5-32.)

Figure 5-32 Clicking OK



17 Communication between the HAPSITE ER and laptop is now established as indicated by the absence of an “X” over the **HAPSITE ER Sensor icon** in the **System Setup** screen. (See Figure 5-33.)

Figure 5-33 System Setup

5.3.1 Turning Off the Radio

See the following procedure for instructions for turning off the radio when wireless communication is not desired.

NOTE: When the HAPSITE radio is on, even if the wireless communication is not being used, a radio signal is being transmitted. The only way to eliminate the radio signal is to turn off the radio.

DANGER

HAPSITE contains a wireless transmitter/receiver that emits electromagnetic radiation (EMR). This radiation in a tactical or operational environment may potentially be used to locate the HAPSITE and its operators. This radiation also has the potential to detonate some types of unexploded ordnance (UXO), or improvised explosive devices (IEDs), or both, if HAPSITE is transmitting in the safety exclusion area around the device(s). Discussed below is a hardware switch to turn off the wireless radio so that HAPSITE may still be used in areas where these hazards are a concern. Consult applicable regulations and policies when using HAPSITE with the wireless device active in such environments.

1. Open the front panel of HAPSITE.
2. Remove the cover from the power switch (for the wireless radio). It is located on the far left hand side. To remove, unscrew the cover by turning it counter-clockwise. (See Figure 5-34.)

Figure 5-34 Unscrewing wireless cap

3 Press the button until a click is heard. The green lights adjacent to **Radio** and **WLAN** should extinguish. When the green lights are extinguished, the power to the wireless radio is off. (See Figure 5-35.)

Figure 5-35 Pushing wireless button

4 Replace the switch cover by placing it over the switch. Turn it clock-wise until finger tight.

5.4 Wireless Information

DANGER

HAPSITE contains a wireless transmitter/receiver that emits electromagnetic radiation (EMR). This radiation in a tactical or operational environment may potentially be used to locate HAPSITE and its operators. This radiation also has the potential to detonate some types of unexploded ordnance (UXO), or improvised explosive devices (IEDs), or both, if HAPSITE is transmitting in the safety exclusion area around the device(s). There is a hardware switch to turn off the wireless radio so that HAPSITE may still be used in areas where these hazards are a concern. Consult applicable regulations and policies when using HAPSITE with the wireless device active in such environments.

5.4.1 Regulatory Compliance Information for UNITED STATES Users

This section of the Operating Manual lists FCC compliance information for the HAPSITE system that contains the wireless communication option.

NOTE: This equipment contains an OEM Embedded Wireless Bridge (Ethernet to Wireless LAN) Module from Quatech Inc.

FCC ID: F4AWLNG1

This device compiles with Part15 of the FCC rules and 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 undesired operation.

CAUTION

To maintain compliance with FCC standards and regulations and to ensure the proper operation of the wireless communication system used within the HAPSITE ER instrument, ONLY use the antenna that was originally supplied with the instrument. If damage occurs to the original antenna please contact the INFICON service department for a replacement antenna (see Chapter 1 for contact information).

5.4.1.1 FCC Statement

This equipment has been tested and found to comply with the limits for a Class B digital device, pursuant to Part 15 of the FCC Rules. These limits are designed to provide reasonable protection against harmful interference in a residential installation. This equipment generates, uses and can radiate radio frequency energy and if not installed and used in accordance with the instructions, may cause harmful interference to radio communications. However, there is no guarantee that interference will not occur in a particular installation. If this equipment does cause harmful interference to radio or television reception, which can be determined by turning the equipment off and on, the user is encouraged to try to correct the interference by one or more of the following measures:

- Reorient or relocate the receiving antenna
- Increase the separation between the equipment and receiver
- Connect the equipment into an outlet on a circuit different from that to which the receiver is connected
- Consult the dealer or an experienced radio/TV technician for assistance

5.4.1.2 FCC RF Exposure Statement

WARNING

To satisfy RF exposure requirements, this device and its antenna must operate with a separation distance of at least 20 cm from all persons and must not be co-located or operating in conjunction with any other antenna or transmitter.

5.4.2 Regulatory Compliance Information for CANADIAN Users

This section of the Operating Manual lists Industry Canada (IC) compliance information for the HAPSITE system that contains the wireless communication option.

NOTE: This equipment contains an OEM Embedded Wireless Bridge (Ethernet to Wireless LAN) Module from Quatech Inc.

IC: 3913A-WLNG1

This device compiles with RSS-210 of Industry Canada (IC) and 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 undesired operation.

5.4.2.1 Industry Canada (IC) Notices

This equipment complies with Canadian RSS-210.

CAUTION

This device has been designed to operate with an antenna having a maximum gain of 5.0 dB. An antenna having a higher gain is strictly prohibited per regulations of Industry Canada (IC). The required antenna impedance is 50 ohms.

To reduce potential radio interference to other users, the antenna type and gain should be so chosen that the equivalent isotropically radiated power (EIRP) is not more than required for successful communications.

5.4.3 Regulatory Compliance Information for EUROPEAN Users

This section of the Operating Manual lists CE and R&TTE compliance information for the HAPSITE system that contains the wireless communication option.

HAPSITE ER is marked with the following symbol:

This symbol indicates compliance with the essential requirements of Directive 73/23/EEC and the essential requirements of articles 3.1(b), 3.2 and 3.3 of Directive 1999/5/EC. Such marking is indicative that this equipment meets or exceeds the following technical standards:

- EN 300 328-2 — Electromagnetic compatibility and Radio spectrum Matters (ERM); Wideband Transmission systems; data transmission equipment operating in the 2.4 GHz ISM band and using spread spectrum modulations techniques.
- EN 301 489-17 — Electromagnetic compatibility and Radio Spectrum Matters (ERM); Electromagnetic Compatibility (EMC) standard for radio equipment and services; Part 17: Specific conditions for 2.4 GHz wideband transmission systems and 5 GHz high performance RLAN equipment.
- EN 61010-1 — Safety requirements for electrical equipment for measurement, control and laboratory use.

5.4.3.1 European Usage Restrictions

CAUTION

European usage restrictions apply to this equipment. The end user must comply with the usage restrictions noted in the table below when operating this equipment in the counties that have restrictions.

HAPSITE ER is marked with the following symbol:

This symbol indicates that usage restrictions apply to this equipment. Such marking indicates that the end user must comply with the following statements about usage restrictions:

- To ensure compliance with local regulations, be sure to select the country in which the access point is installed.
- This instrument can be used as shown in Table 5-1:

Table 5-1 Country - Restriction

Countries	Restrictions
France	Outdoor use limited to 10mW e.i.r.p. within the band 2454 to 2483.5 MHz.
Italy	If used outside of own premises, general authorization is required.
Luxembourg	General authorization is required for public service.
Romania	On a secondary basis. Individual license required.
Austria, Denmark, Finland, Germany, Greece, Iceland, Ireland, Liechtenstein, Luxembourg, Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, United Kingdom	None

5.4.3.2 European EMC Compliance Statement

Table 5-2 European EMC Compliance Statements

English	Hereby, INFICON Inc. declares that this HAPSITE ER Portable GC/MS is in compliance with the essential requirements and other relevant provisions of Directive 1999/5/EC.
Finnish	INFICON Inc. vakuuttaa täten että HAPSITE ER Portable GC/MS tyyppinen laite on direktiivin 1999/5/EY oleellisten vaatimusten ja sitä koskevien direktiivin muiden ehtojen mukainen.
Dutch	Hierbij verklaart INFICON Inc. dat het toestel HAPSITE ER Portable GC/MS in overeenstemming is met de essentiële eisen en de andere relevante bepalingen van richtlijn 1999/5/EG.
	Bij deze verklaart INFICON Inc. dat deze HAPSITE ER Portable GC/MS voldoet aan de essentiële eisen en aan de overige relevante bepalingen van Richtlijn 1999/5/EC.

Table 5-2 European EMC Compliance Statements (continued)

French	Par la présente INFICON Inc. déclare que l'appareil HAPSITE ER Portable GC/MS est conforme aux exigences essentielles et aux autres dispositions pertinentes de la directive 1999/5/CE.
Danish	Undertegnede INFICON Inc. erklærer herved, at følgende udstyr HAPSITE ER Portable GC/MS overholder de væsentlige krav og øvrige relevante krav i direktiv 1999/5/EF.
German	Hiermit erklärt INFICON Inc. dass sich dieser HAPSITE ER Portable GC/MS in Übereinstimmung mit den grundlegenden Anforderungen und den anderen relevanten Vorschriften der Richtlinie 1999/5/EG befindet". (BMWi)
	Hiermit erklärt INFICON Inc. die Übereinstimmung des Gerätes HAPSITE ER Portable GC/MS mit den grundlegenden Anforderungen und den anderen relevanten Festlegungen der Richtlinie 1999/5/EG. (Wien)
Swedish	Härmed intygar INFICON Inc. att denna HAPSITE ER Portable GC/MS står I överensstämmelse med de väsentliga egenskapskrav och övriga relevanta bestämmelser som framgår av direktiv 1999/5/EG.
Greek	ΜΕ ΤΗΝ ΠΑΡΟΥΣΑ INFICON Inc. ΔΗΛΩΝΕΙ ΟΤΙ HAPSITE ER Portable GC/MS ΣΥΜΜΟΡΦΩΝΕΤΑΙ ΠΡΟΣ ΤΙΣ ΟΥΣΙΩΔΕΙΣ ΑΠΑΙΤΗΣΕΙΣ ΚΑΙ ΤΙΣ ΛΟΙΠΕΣ ΣΧΕΤΙΚΕΣ ΔΙΑΤΑΞΕΙΣ ΤΗΣ ΟΔΗΓΙΑΣ 1999/5/ΕΚ
Italian	Con la presente INFICON Inc. dichiara che questo HAPSITE ER Portable GC/MS è conforme ai requisiti essenziali ed alle altre disposizioni pertinenti stabilite dalla direttiva 1999/5/CE.
Spanish	Por medio de la presente INFICON Inc. declara que el HAPSITE ER Portable GC/MS cumple con los requisitos esenciales y cualesquiera otras disposiciones aplicables o exigibles de la Directiva 1999/5/CE.
Portuguese	INFICON Inc. declara que este HAPSITE ER Portable GC/MS está conforme com os requisitos essenciais e outras disposições da Directiva 1999/5/CE.

5.4.3.3 European Safety Compliance Statement

This device has been tested and certified according to the safety standard EN 61010-1: 2001 and is intended to be used in accordance with the information provided in this manual. For additional information concerning the directives and standards that this instrument complies with, please refer to the Declaration of Conformity that is located in the front of this manual.

Chapter 6
Laptop Operation

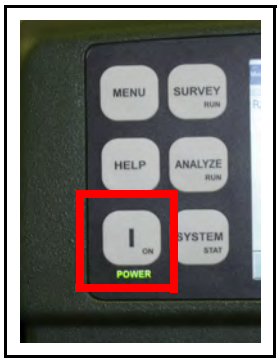
6.1 Laptop Operation

NOTE: See Chapter 7, ER IQ Software for additional information on the **ER IQ** software installed on the laptop computer.

6.1.1 Sampling Procedure

1. For assembly instructions, refer to section 3.2, Basic Assembly, on page 3-5.
2. Press the **POWER** button on the front panel to turn on HAPSITE ER. HAPSITE takes 1-2 minutes to boot. (See Figure 6-1.)

Figure 6-1 POWER Button



NOTE: If desired and equipped, HAPSITE can be used with the laptop computer via the wireless connection. Refer to Chapter 5, Communications and Touch Screen Options for additional information on set-up and usage.

3. Locate the power cord and mouse (optional). Plug them into the appropriate ports on the computer. Open the laptop and press the power button.

6.2 Survey Mode

Survey mode is used for quick analysis and tentative results. It is generally two minutes long and detects compounds with a concentration greater than 1 ppm.

CAUTION

Do not touch the sample with the probe. Do not allow liquids to enter the probe.

6.2.1 Sampling Procedure

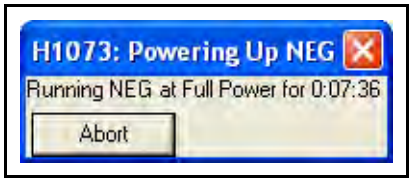
1. Open the **ER IQ** software by double-clicking on the ER IQ icon. (See Figure 6-2.)

Figure 6-2 ER IQ Icon

2. If the probe is attached, HAPSITE will begin preparing a Survey method. If this method is not the desired one, see section 6.4, Selecting a New Method, on page 6-11.

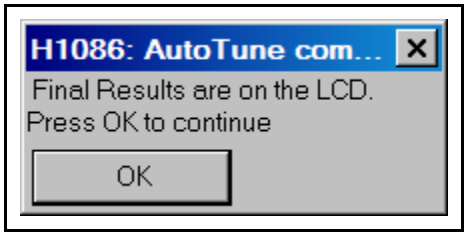
NOTE: The following message will be displayed while HAPSITE prepares for sampling. No action is required from the user. (See Figure 6-3.)

Figure 6-3 NEG Full Power



3. As part of the preparation, an AutoTune will run. If the AutoTune is successful, the following message will display. Click **OK**. (See Figure 6-4.) If AutoTune fails, see section 9.4, Performing Manual Tune, on page 9-7.

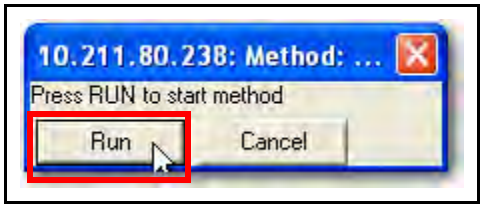
Figure 6-4 AutoTune Complete



4 HAPSITE will check pressures and automatically heat all necessary components to the setpoint temperatures. Progress will be indicated by a bar graph. Once all components have reached their setpoint temperatures, a prompt will be displayed to **Press RUN to start method**.

5 Click the **RUN** button on the pop-up window or from the **Control Panel** on the screen. (See Figure 6-5.)

Figure 6-5 Run Button

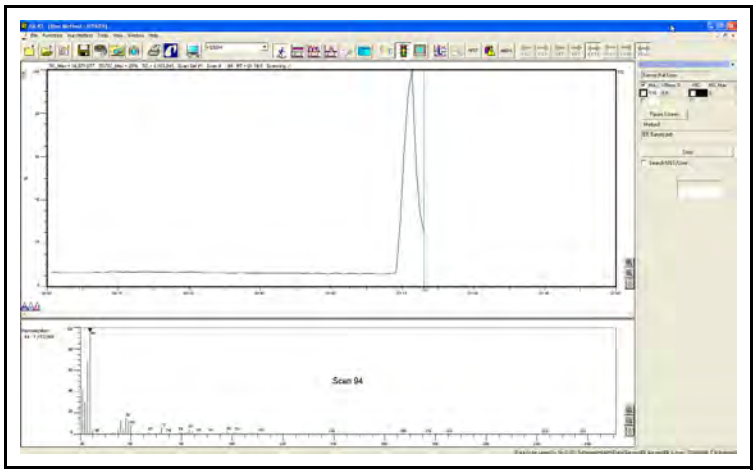


6 Sample the background for one minute and note the TIC (the total ion count, which is a measure of response.) (See Figure 6-6.)

Figure 6-6 Sample Background

7 When the TIC increases 2 to 3 times the baseline level, move the probe away from the sample. A peak may appear if the compound concentration is greater than 1 ppm. A compound identification may also be present on the HAPSITE screen. (See Figure 6-7.)

Figure 6-7 Peak in Survey



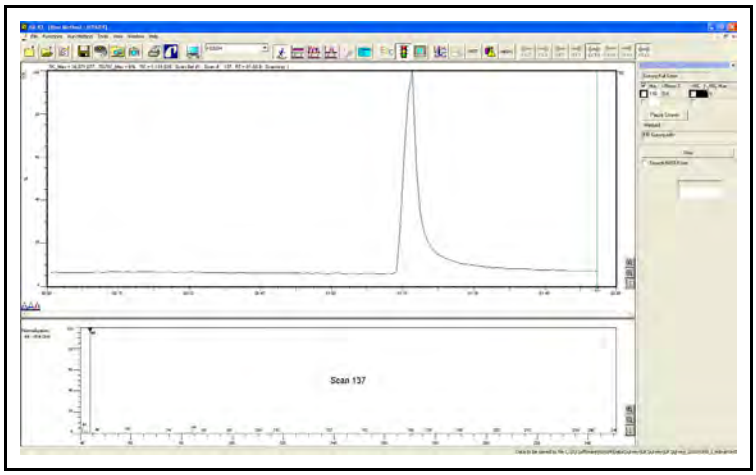
NOTE: No response may indicate either the compound present is less than the detection limit, or that no detectable compound is present.

8 Monitor the TIC for guidance. If the TIC approaches 60 million, move the probe away from the sample to avoid saturation. If the system is saturated, there will also be red lines in the peak on the laptop.

9 If the TIC does not increase, hold the probe over the sample of interest for up to a minute. If the TIC does not increase after a full minute, move the probe away from the sample.

10 Monitor the TIC until it decreases to the initial background level that was noted in Step 6. (See Figure 6-8.)

Figure 6-8 TIC Decreasing



11 Click the **Stop** button, in the center of the **Control Panel** on the right side of the screen, to stop the sampling process. If it has not already been stopped manually, the Survey run will stop automatically when the run time has reached five minutes. (See Figure 6-9 to Figure 6-11.)

Figure 6-9 Stop button on laptop screen

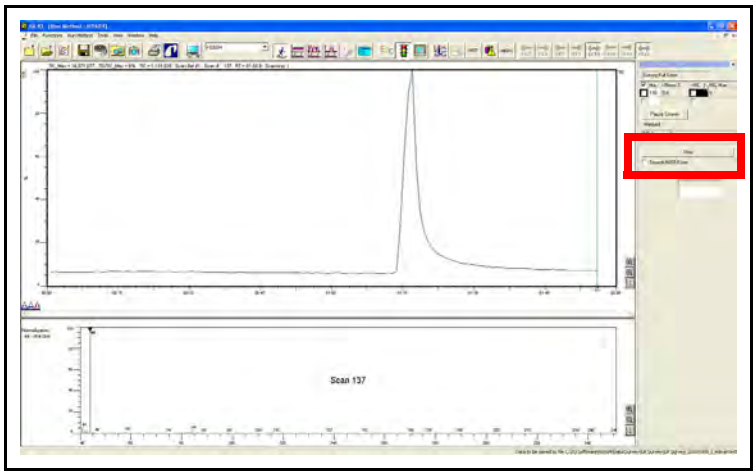
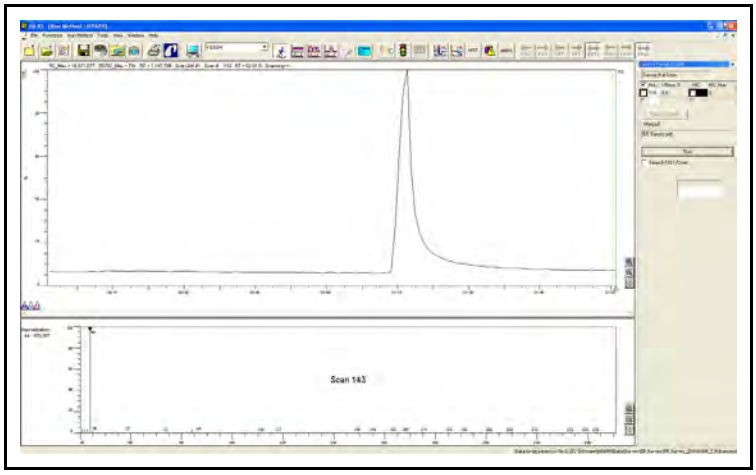


Figure 6-10 Stop button

NOTE: Survey is a tentative identification. To confirm results, run an **Analyze** (GC/MS) method.

Figure 6-11 Survey Run Complete



12 Record the data file name to reference for later review. See Chapter 8, Data Review for instructions on recalling data.

6.2.2 Quick Reference SOP — Running Survey Mode

1. Double-click the **ER IQ** software icon.
2. Double-click the **Run Method** icon.
3. Wait for heaters to reach the setpoint temperatures.
4. Click the **RUN** button in the pop-up window.
5. Sample background for one minute and note the TIC.
6. Hold the probe over the sample until a response that is 2 to 3 times the baseline is observed. If the TIC does not increase, sample for a full minute.
7. Press **Stop** to stop the method.

NOTE: This is a tentative identification. To confirm results, run an **Analyze** (GC/MS) method.

CAUTION

Do not touch the sample with the probe. Do not allow liquids to enter the probe.

6.3 ANALYZE (GC/MS) Mode with the Concentrator

6.3.1 Tri- Bed Concentrator

The Tri-Bed concentrator is used for analyzing samples with concentrations in the part per million to high part per trillion range. Two default qualitative methods are **ER_Tri-Bed_PPM_Standard** and **ER_Tri-Bed_PPB Standard**. Use the **ER_Tri-Bed_PPM_Standard** method when a response is seen in Survey. If a compound is suspected, but Survey does not show an increase in TIC (total ion count, which is a measure of response), use the **ER_Tri-Bed_PPB_Standard** method.

CAUTION

The concentrator feature has increased sensitivity. Use the appropriate method to avoid saturating HAPSITE ER.

6.3.2 Tenax Concentrator

The Tenax concentrator is also used for analyzing samples with concentration levels in the low part per million to high part per trillion range. The Tenax concentrator will not effectively concentrate compounds with boiling points below 80°C, but may be more effective at concentrating compounds with higher boiling points.

WARNING

The Tenax concentrator will not effectively concentrate compounds with boiling points below 80°C.

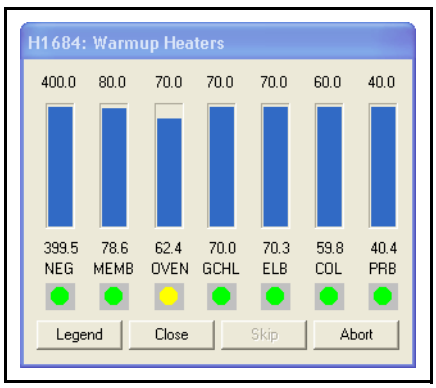
For concentrator installation instructions, refer to section 3.3.7, Replacing the Concentrator, on page 3-21 for instructions. Once installed, the concentrator must be cleaned before sampling begins.

1. Verify that the concentrator is installed.
2. When powered on (refer to section Chapter 4 on page 4-1) or taken out of **Extended Standby** (refer to section 4.8.1 on page 4-61), HAPSITE will automatically start preparing a concentrator method. If the method that HAPSITE begins preparing is not the desired one, refer to section 6.4, Selecting a New Method, on page 6-11.
3. Power on the laptop by pushing the **POWER** button. Open **ER IQ** Software by double-clicking on the **ER IQ** icon. (See Figure 6-12.)

Figure 6-12 ER IQ Software icon

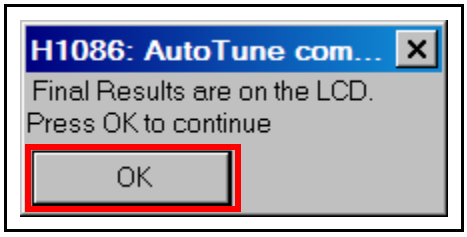
4. HAPSITE will begin preparing to run the default concentrator method. It will heat all necessary components, check pressures and run an AutoTune, if necessary. Progress of the heaters indicated by a bar graph on the laptop screen.

Figure 6-13 Heater progress



5 When the AutoTune is finished, the following message will be displayed. Click **OK**. (See Figure 6-14.)

Figure 6-14 AutoTune Complete



NOTE: If AutoTune fails, refer to section 9.4, Performing Manual Tune, on page 9-7.

6 A concentrator cleanout will also be run as part of the preparation of HAPSITE. Hold the probe in a clean environment for the duration of the cleanout. If the cleanout is successful, a **SYSTEM IS READY** message will be displayed on the front panel. The TIC on the chromatogram will be less than 5 million.

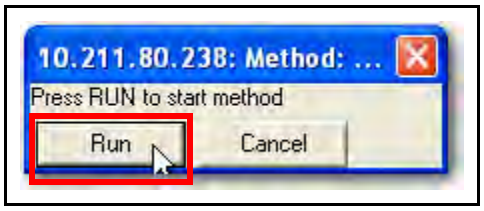
NOTE: If the cleanout is unsuccessful, refer to section 4.1.3, Concentrator Cleanout Failure, on page 4-11.

NOTE: If this method is not the desired method, refer to section 4.2, Selecting a Different Method Using the SELECT METHOD Icon, on page 4-13.

7 Once all temperature zones have reached their setpoints, a prompt will be displayed to **Press RUN to start method**.

8 Click **RUN** button on the pop-up window or from the Control Panel on the screen. (See Figure 6-15.)

Figure 6-15 Run Button



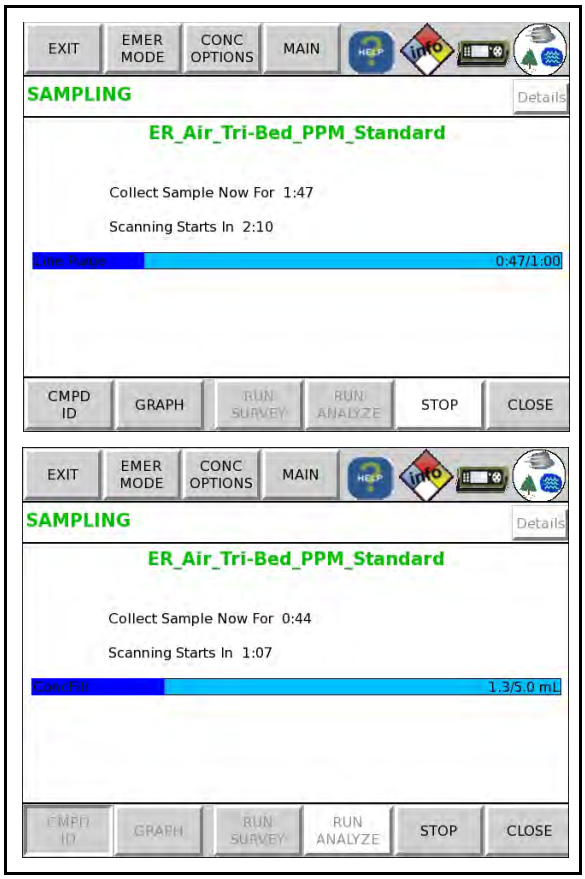
9 When the HAPSITE screen prompts **Collect Sample Now**, place the probe over sample for the entire specified sampling time. Be sure to keep the probe over the sample for both the Line Purge and Concfill events. (See Figure 6-16.)

NOTE: The Line Purge event is collected by time and the Concfill is collected by volume.

CAUTION

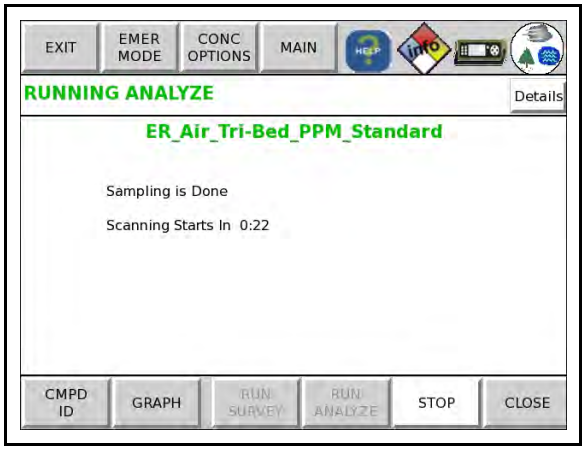
Do not place the sample probe in liquids while sampling.

Figure 6-16 Collecting Sample for Concentrator



10 When prompted **Sampling is Done** on the HAPSITE screen, remove the probe from the sample source. (See Figure 6-17.)

Figure 6-17 Sampling is Done For Concentrator



11 As the method runs, the chromatogram will begin to appear on the Laptop screen.

12 The message **METHOD FINISHED** will appear on the HAPSITE screen when the run is complete. (See Figure 6-18.) An example of a completed chromatogram on the laptop is shown in Figure 6-19.

Figure 6-18 Method Finished for Concentrator

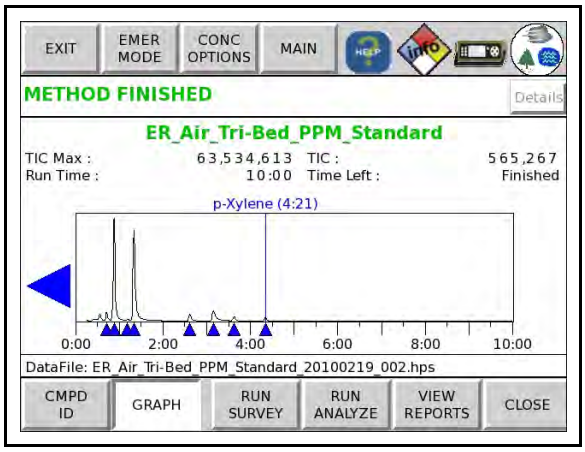
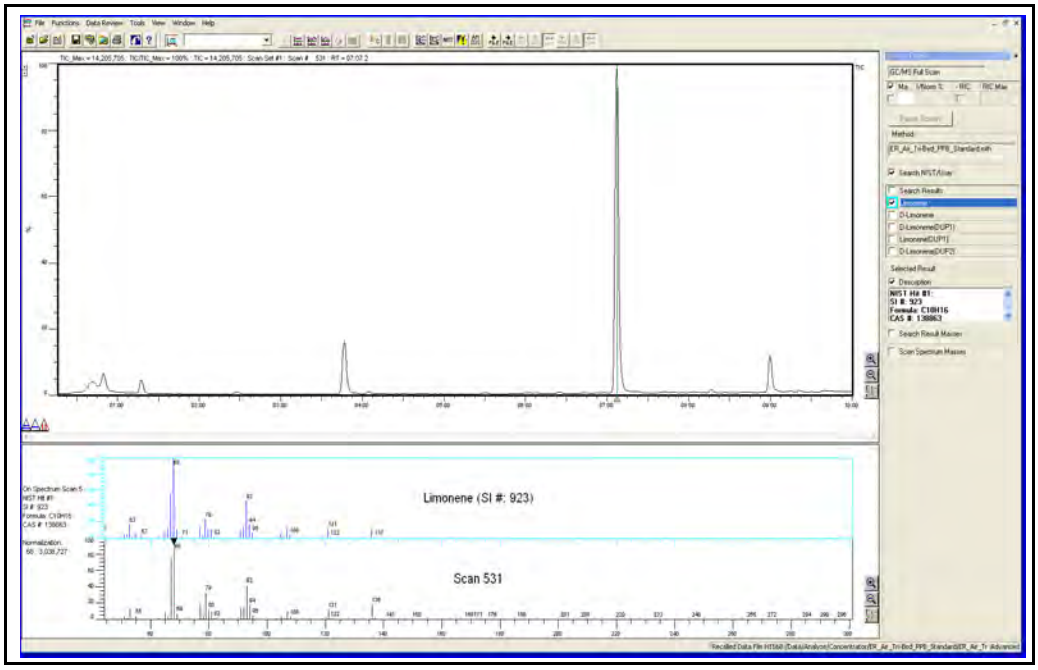


Figure 6-19 Concentrator Run Finished



13 Review results at the end of the run. If red lines appear on the chromatogram, saturation has occurred. To clear saturation, run blank runs until the saturation has cleared.

CAUTION

The concentrator feature has increased sensitivity. Take care to avoid saturating HAPSITE.

6.3.3 Quick Reference SOP — Tri-Bed Concentrator Method

1. Verify that the concentrator is installed.
2. If the system is shutdown or in **Extended Standby**, either power on HAPSITE or take the system out of **Extended Standby**. HAPSITE will begin preparing a concentrator method.
3. When HAPSITE has finished preparing, a prompt to press **Run** will be displayed on the laptop screen.
4. When the screen prompts, **Collect Sample Now For**, hold the probe over the sample until the screen prompts, **Sampling is Done**.
5. When the run is complete, a **Method Finished** prompt will be displayed.
6. See section 4.5.1, View Results/View Reports, on page 4-31 or Chapter 8, Data Review for information on data review.

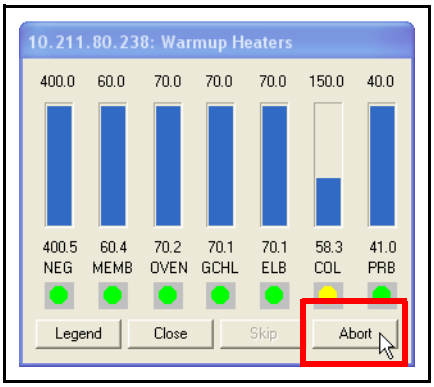
CAUTION

Do not place the sample probe in liquids while sampling.

6.4 Selecting a New Method

1. Click the **Abort** button. (See Figure 6-20.)

Figure 6-20 Aborting method

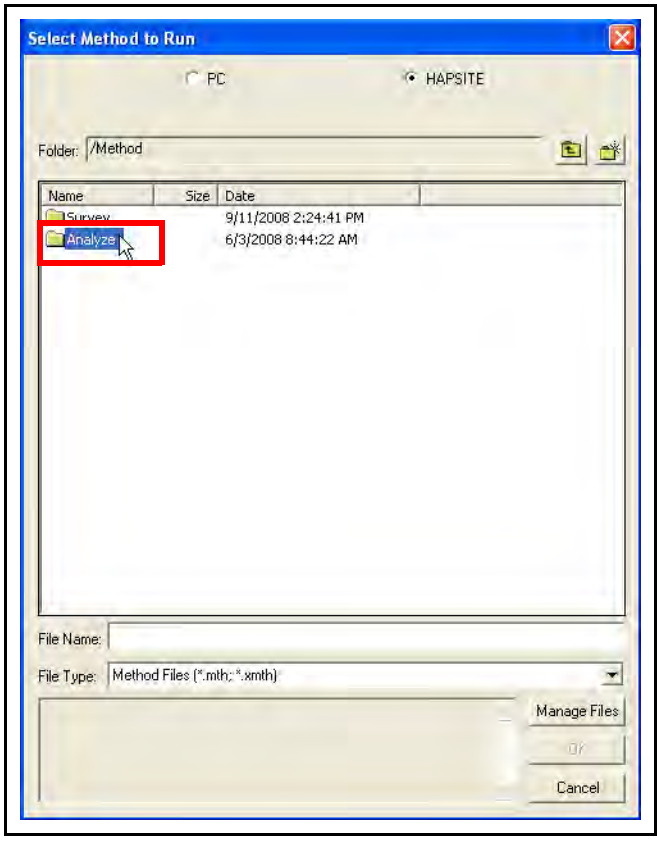


2. Double-click on the **Run Method** icon. A dialog is displayed for selecting the desired method. In the example below, **ER_Air_Tri-Bed_PPB_Standard** will be selected.

3 Double-click the **Analyze** folder. (See Figure 6-21.)

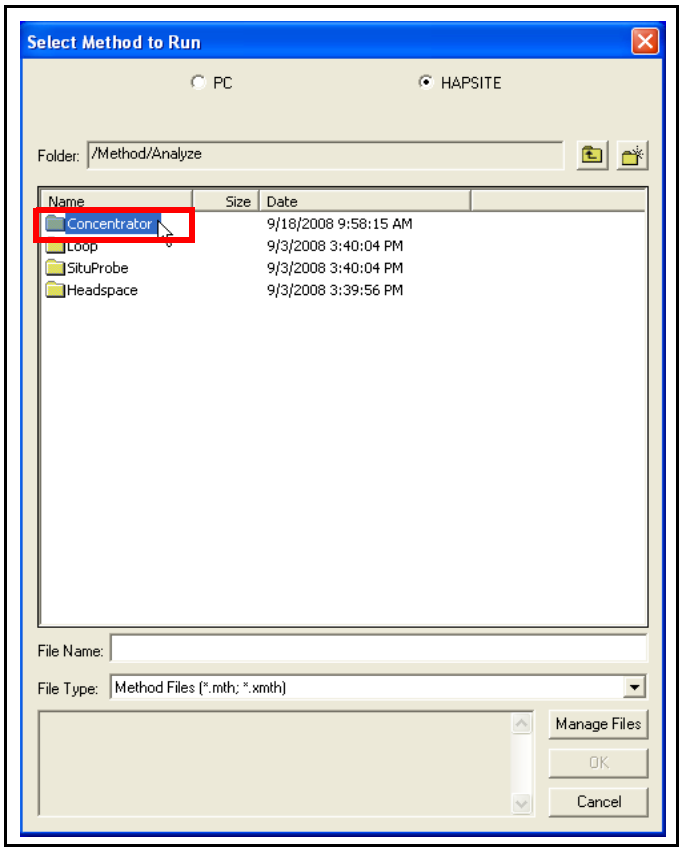
NOTE: Use the buttons at the top of the dialog to choose the methods on HAPSITE ER.

Figure 6-21 Choosing the Mode of Operation



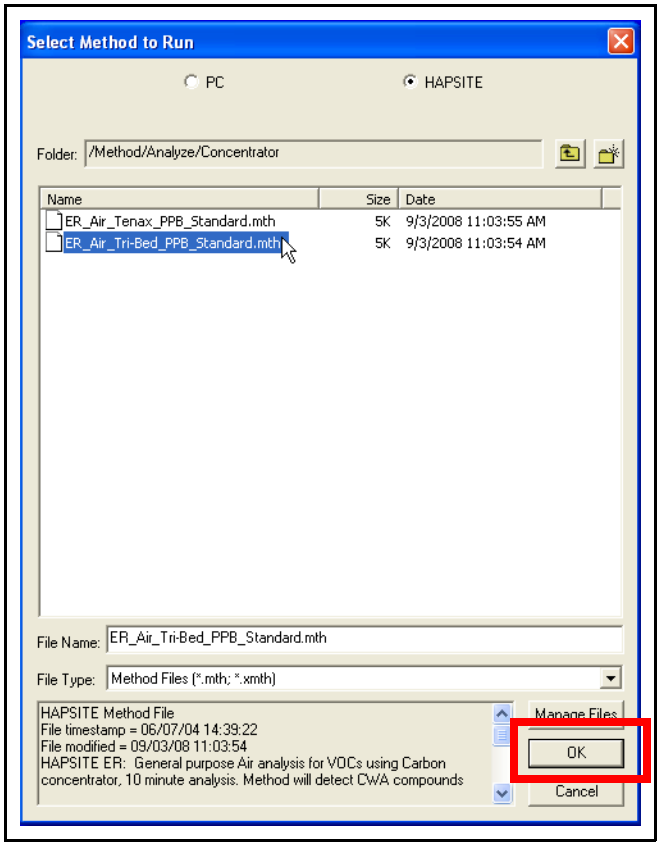
4 Choose a folder that matches the sampling configuration of HAPSITE. The concentrator folder refers to the Probe accessory. In this example, the probe is installed. Double-click the **Concentrator** folder. (See Figure 6-22.)

Figure 6-22 Selecting the Sampling Configuration



5 Click the desired method and then, click **OK**. This example shows the **ER_Air_Tri-Bed_PPB_Standard.mth** method. (See Figure 6-23.)

Figure 6-23 Selecting the Method



6 The software will check the pressure in the gas canisters, heat up all necessary components and run an AutoTune (if required). A concentrator cleanout will also be run if needed.

7 When it is finished heating, a prompt will appear to indicate HAPSITE ER is ready to run a sample. Click **RUN**. For detailed instructions, refer to section 6.3, ANALYZE (GC/MS) Mode with the Concentrator, on page 6-6.

CAUTION

Do not place the sample probe in liquids while sampling.

Chapter 7
ER IQ Software

7.1 HAPSITE Software - ER IQ

ER IQ software is the laptop software that controls instrument operation, runs analyses, manages files and creates reports. Data collected with HAPSITE ER is viewed and interpreted using **ER IQ**. This software allows for use of the entire NIST mass spectral library. This section provides instructions on **Data Review** and analysis. The **Data Review** section of the **ER IQ** laptop software allows access to previously acquired data for review and analysis, or to view data that is being acquired in real time. **ER IQ** software operates with Microsoft® Windows® on the laptop.

7.1.1 Computer System Requirements

The following is the minimum recommended laptop computer system for communication with one HAPSITE:

Processor . . . . . Pentium III 550 MHz or greater

RAM . . . . . 512 MB or greater

Hard Disk Space
to load ER IQ . . . . . 20 Mb

Hard Disk Space for storage . . . . . 10 GB

Monitor . . . . . 15 inch, SVGA or greater

Monitor Resolution . . . . . 1024 x 768 or greater

Communications . . . . . Ethernet port

Operating System . . . . . Windows XP or 7

7.2 Software Installation

The software is loaded onto the laptop at the factory. If reinstallation is necessary, the software installation instructions are located on the **ER IQ** software CD or can be downloaded off the INFICON website.

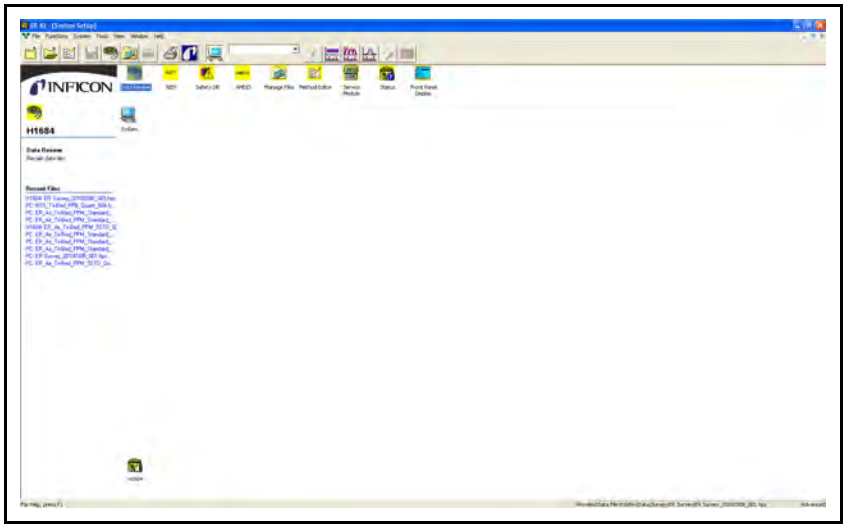
7.2.1 System Setup Screen

1 Double-click the **ER IQ** icon to open the **ER IQ** software.

*Figure 7-1 **ER IQ** icon*

2 To connect to a HAPSITE, see section 5.2. When opening **ER IQ**, the main window of the software is the **System Setup** screen. See Figure 7-2.

Figure 7-2 System Setup View in ER IQ software



7.3 Introduction

Upon opening **ER IQ**, the first screen displayed is the **System Setup Screen**, which controls instrument operation. This screen is used to run analyses, access data files, create or edit methods, and set parameters of various HAPSITE ER components.

7.3.1 System Setup Menu

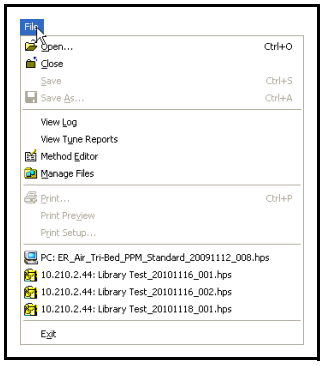
The main menu toolbar includes **File**, **Functions**, **System**, **Tools**, **View**, **Window** and **Help** options. (See Figure 7-3.)

Figure 7-3 Main Menu toolbar

7.3.1.1 File Menu

The **File** menu is shown in Figure 7-4.

Figure 7-4 File menu



Open opens a data file from either **ER IQ** or the laptop.

Close closes the data file.

Save is grayed out when in the **System Setup Screen**. However, when a data file is opened, a new screen, the **Data Review Screen**, will be displayed. The **Save** option will be activated in the Data Review Screen and changes to the data file can be saved.

Save As is grayed out in the **System Setup** screen. However, when a data file is opened, a new screen, the **Data Review** screen, will be displayed. The **Data Review** screen will have the **Save As** option activated. The data file can be saved with a different name and/or to a different location.

View Log allows for event log files (.evt) to be opened. Examples of files logged are warnings, errors and run history.

View Tune Reports allows for tune reports (.tun) to be opened. For more information on tune reports, see section 9.3 on page 9-3.

Method Editor opens the **Method Editor** function. It performs the same function as the **Method Editor icon**. See Chapter 10, Method Editor for further instructions.

Manage Files opens the **Manage Files** function. It performs the same function as the Manage Files icon. See section 7.4 on page 7-18.

Print will print files and is active on the **Data Review** screen.

Print Preview will display an example of the final printing layout and is active on the **Data Review** screen.

Print Setup accesses the printer setup options.

Recently Accessed Files are displayed below **Print Setup**. Double-click on a file name to open it in the **Data Review** screen.

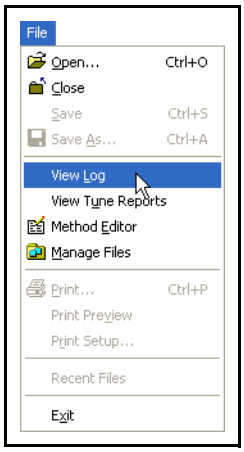
Exit closes **ER IQ**.

7.3.1.1.1 View Log

HAPSITE will log errors, warnings and events if desired. See Parameters on page 7-36 for information on enabling this function. A warning signifies there is a problem with the unit, such as high pressure. If the warning is ignored, it will become an error. An example of an event is the system coming online or going offline.

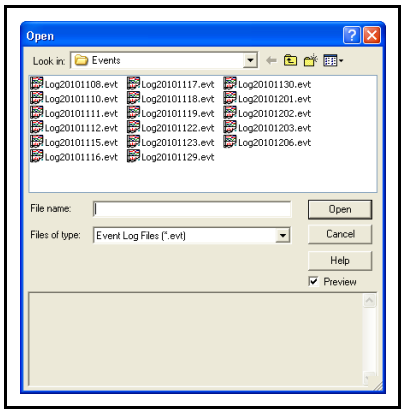
1 Select **View Log** from the **File** menu. (See Figure 7-5.)

Figure 7-5 View Log



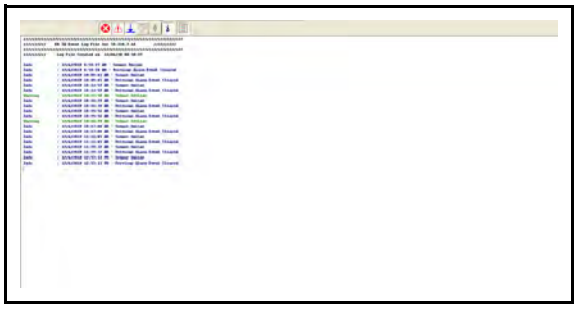
2 Double-click the desired log file. (See Figure 7-6.)

Figure 7-6 Desired Log file



3 The log file will be displayed. (See Figure 7-7.)

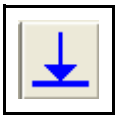
Figure 7-7 Displaying the Log file



7.3.1.1.2 Log File Toolbar

The following icons will be displayed on the **Log File Toolbar**.

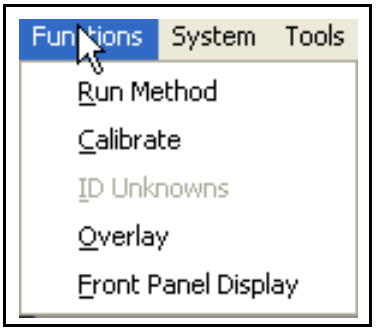
Table 7-1 Log File Toolbar

Icon	Function
	Displays the logged warnings
	Displays the logged errors
	Displays the logged events
	Displays all logged files
	Color codes the warnings, errors and events

7.3.2 Functions Menu

The **Functions** menu is shown in Figure 7-8.

Figure 7-8 Functions menu



The **Run Method**, **Calibrate**, **Overlay** and **Front Panel Display** options function identically to the icons of the same name. For further instructions, see Chapter 7, ER IQ Software, Chapter 7, ER IQ Software for the Calibrate icon, section 8.9, Chromatogram Overlay, on page 8-49 and/or section 7.7, Front Panel Display Icon, on page 7-37.

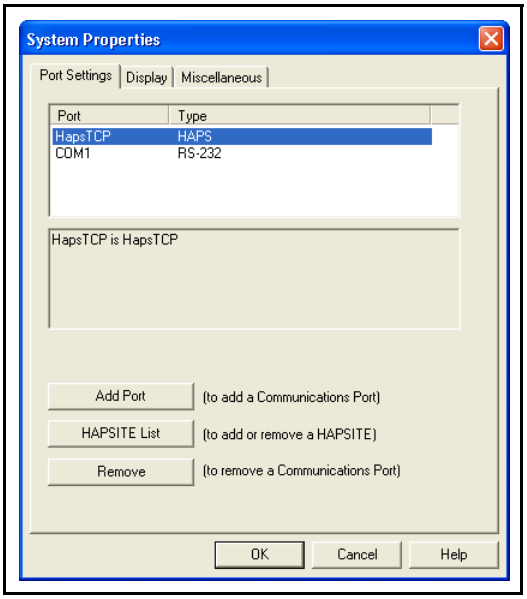
7.3.3 System

The **System** menu is shown in Figure 7-9.

Figure 7-9 System menu

Clicking **Properties** will open the **System Properties** window. (See Figure 7-10.)

Figure 7-10 System Properties

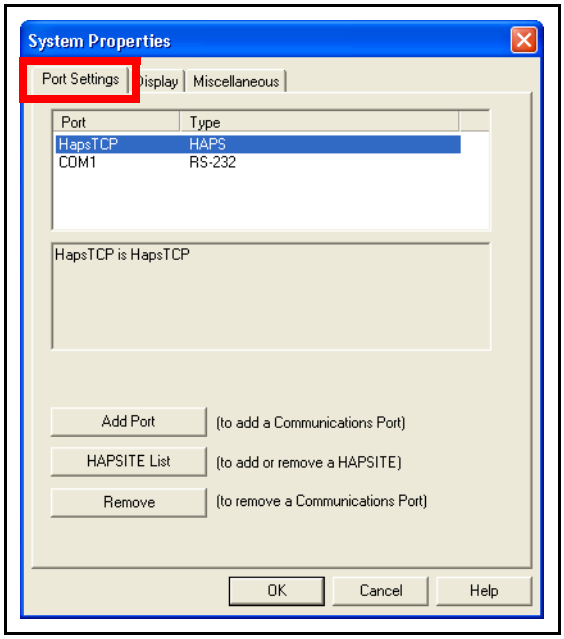


7.3.3.1 Port Settings Tab

Port Settings is the default tab in the **System Properties** window. (See Figure 7-11.)

HAPSITE ER is configured at the factory to connect to the laptop. However, the **HAPSITE List** option allows the user to add a different **HAPSITE ER** to the laptop or connect a **HAPSITE ER** to a new laptop.

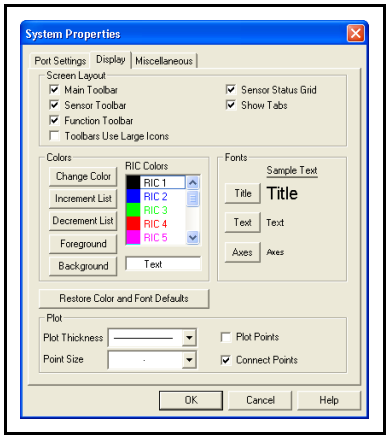
Figure 7-11 System Properties



7.3.3.2 Display Tab

The **Display** tab is used to change the appearance of **ER IQ** settings, including the thickness of the chromatogram line, the fonts used and the screen layout. (See Figure 7-12.)

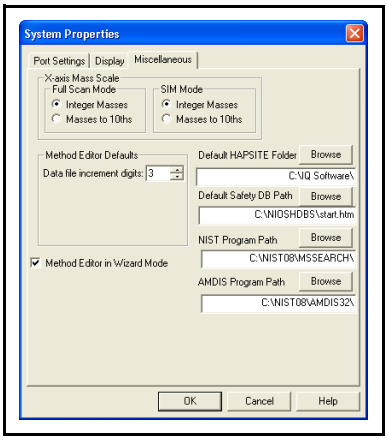
Figure 7-12 Display tab



7.3.3.3 Miscellaneous Tab

The **Miscellaneous** tab displays the default pathways, the data file increment digits, the software, safety and library pathways, the scaling preferences for the chromatogram and option to select **Wizard Mode** for **Method Editor**. (See Figure 7-13.)

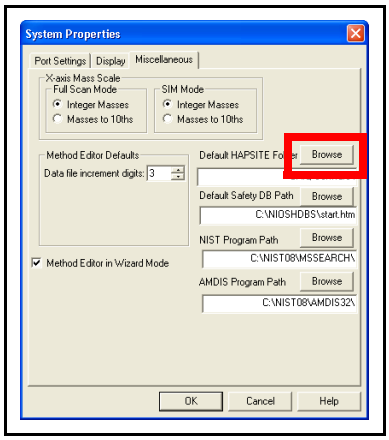
Figure 7-13 Miscellaneous tab



Four default software pathways are displayed. The **Browse** buttons access folders to reset the pathways, if necessary. However, the software installation should properly select these options. If a pathway requires resetting, follow the instructions below.

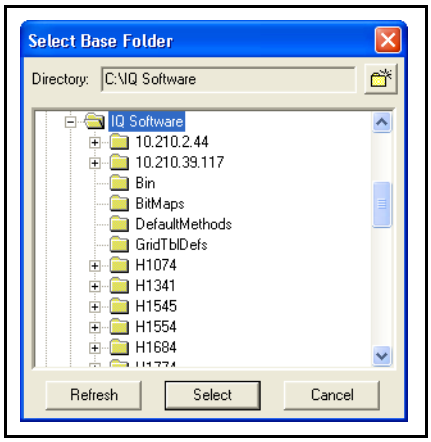
1 Click **Browse** for the **Default HAPSITE Folder**. (See Figure 7-14.)

Figure 7-14 Browse button



2 The **Select Base Folder** window will open. (See Figure 7-15.)

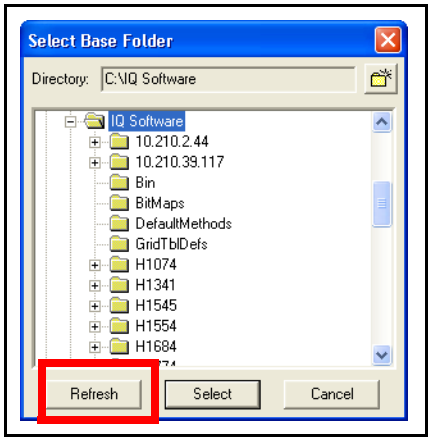
Figure 7-15 Select Base Folder window



3 Click to highlight the desired folder. (See Figure 7-16.)

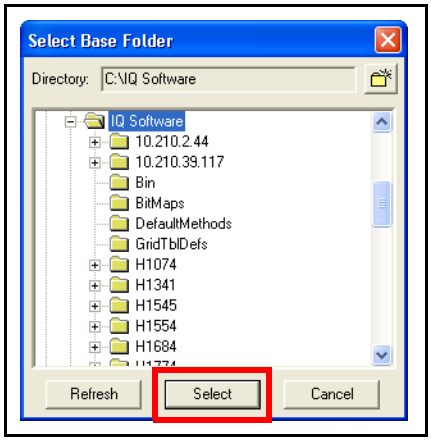
NOTE: Click **Refresh** to update the displayed folders if the desired folder is not displayed.

Figure 7-16 Clicking desired folder



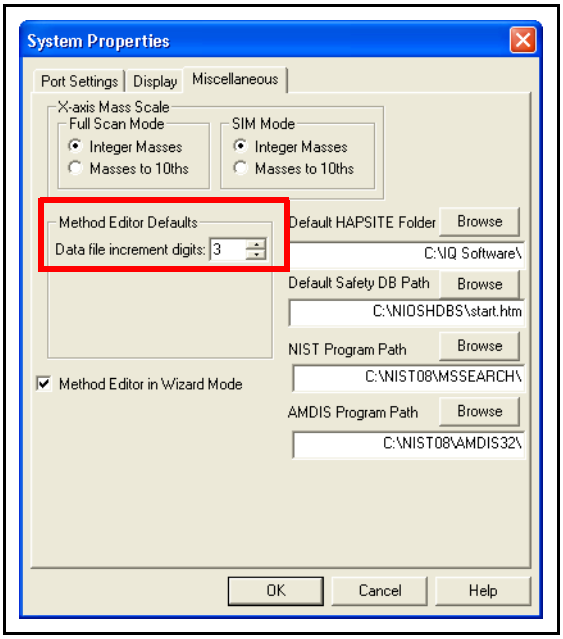
4 Once the desired file is highlighted, click **Select**. Once **Select** is clicked, the window will close. (See Figure 7-17.)

Figure 7-17 Selecting the pathway



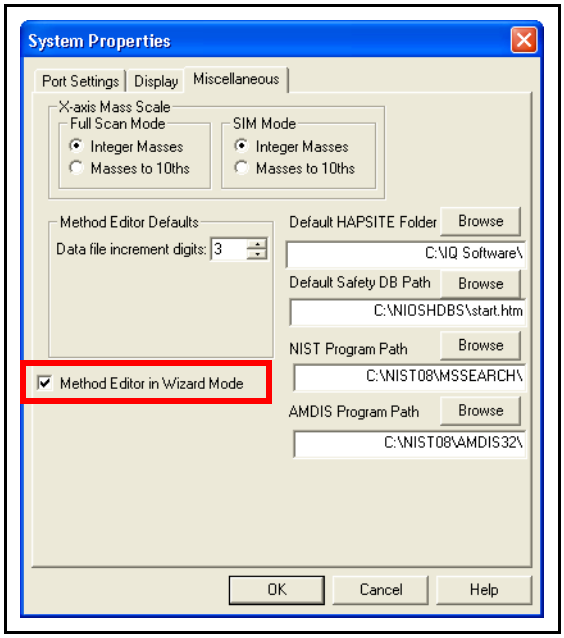
The **Data file increment digits** is used to select the number of digits that are to be appended to a data file. For example, if 2 is selected, the file name would read Method_yearmonthday_01. If 3 is selected, the file name would read Method_yearmonthday_001. (See Figure 7-18.) The data file increment digits can also be selected in Method Editor. See section 10.11.1, Data File Information, on page 10-60 for instructions.

Figure 7-18 Data file increment digits



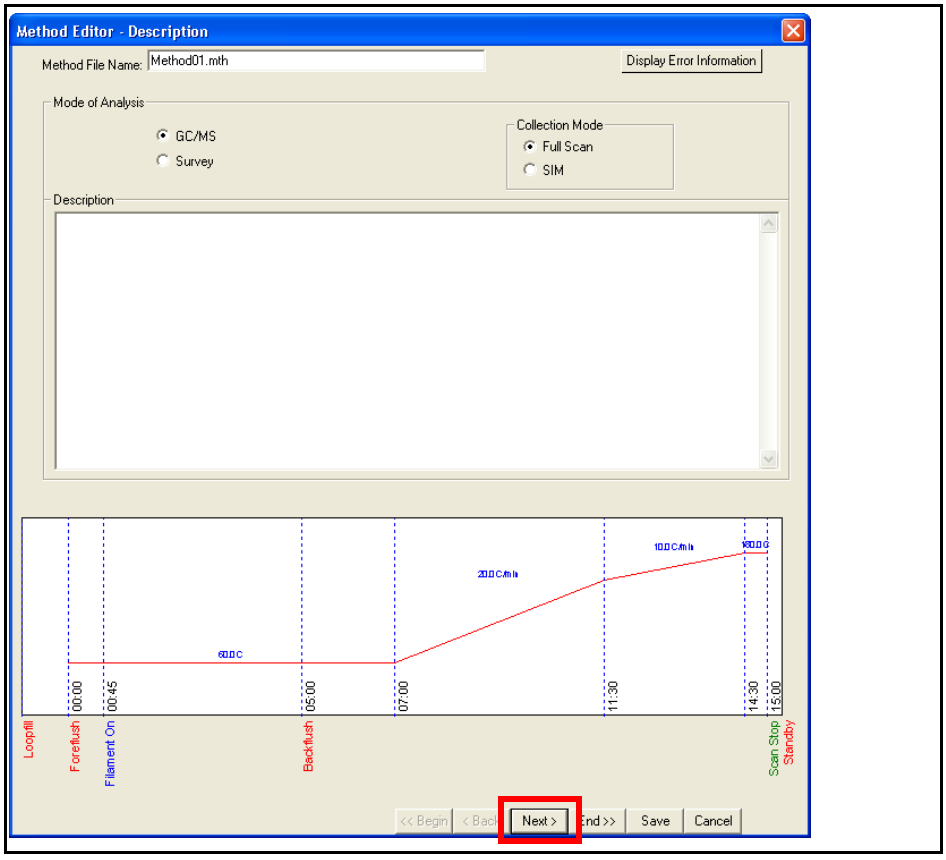
The **Method Editor in Wizard Mode** checkbox is the next option. (See Figure 7-19.)

Figure 7-19 Method Editor in Wizard Mode



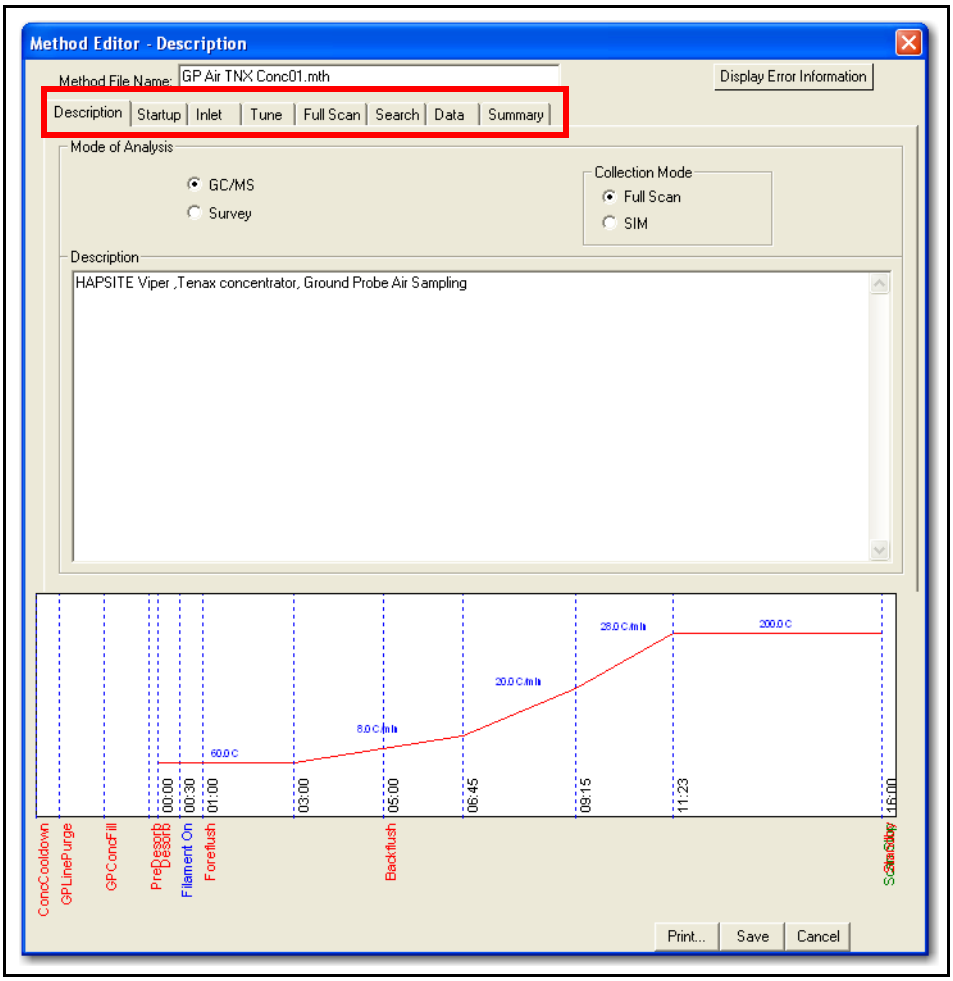
The Wizard Mode will guide the user through the Method Editor software by using **Next >** and **<Back** buttons at the bottom of the screen. (See Figure 7-20.)

Figure 7-20 Wizard mode



If the **Method Editor in Wizard Mode** box is not checked, tabs must be clicked at the top of the Method Editor screen to access method writing options. (See Figure 7-21.)

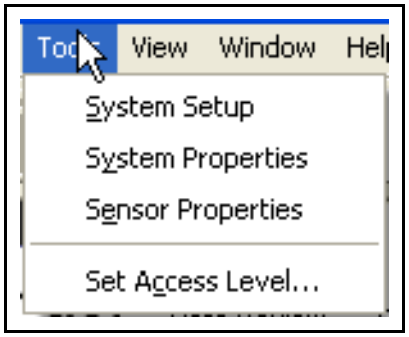
Figure 7-21 Non-Wizard Mode



7.3.4 Tools Menu

The **Tools** menu is shown below. (See Figure 7-22.)

Figure 7-22 Tools menu



System Setup closes the **System Setup** screen.

System Properties functions identically to the **System Properties** option in the System menu. Refer to section 7.3.3 on page 7-6.

Sensor Properties functions identically to the **Properties** option in the System Menu. Refer to section 7.3.3 on page 7-6 for further information.

7.3.4.1 Set Access Level

In the **Set Access Level** option there are two user levels which can be set in **ER IQ**, **Normal** and **Advanced**. Neither access level has a factory set password.

Normal level allows users to run samples, view results and perform basic operations with HAPSITE ER.

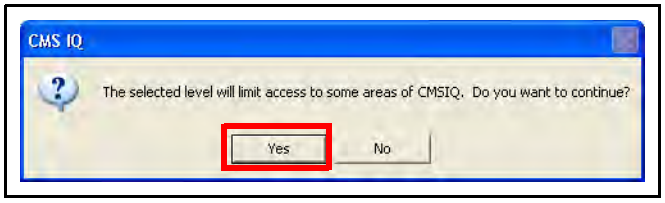
Advanced allows access to all user operations. This includes all normal user functions plus method creation and editing, file deletion, changing alarm parameters and changing network settings.

To restrict access to advanced functions, an advanced user password can be set. Once the password is set, it must be entered each time the **ER IQ** program is opened, or whenever the access level is changed from normal to advanced. See section 7.3.4.1.2 on page 7-15.

7.3.4.1.1 Changing Access Levels

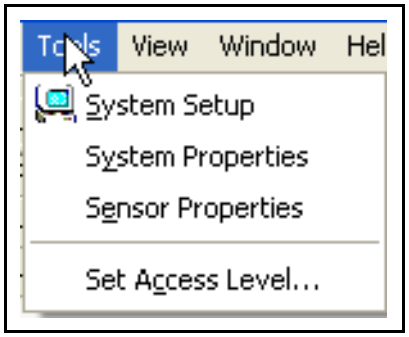
NOTE: When the **Normal** access level is selected, a prompt will be displayed stating that some areas of **ER IQ** will have restricted access. Click **Yes** if continuing is desired. (See Figure 7-23.)

Figure 7-23 Restricted access prompt



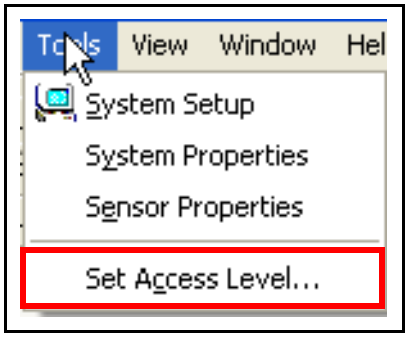
1 To change the access level, click on the **Tools** menu on the System Setup Screen. (See Figure 7-24.)

Figure 7-24 Tools menu



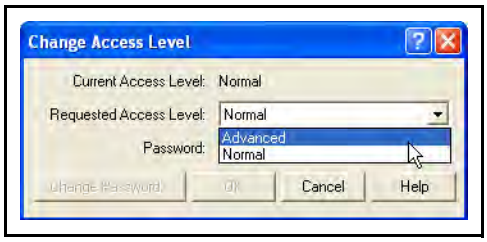
2 Select **Set Access Level...**. (See Figure 7-25.)

Figure 7-25 Set Access Level



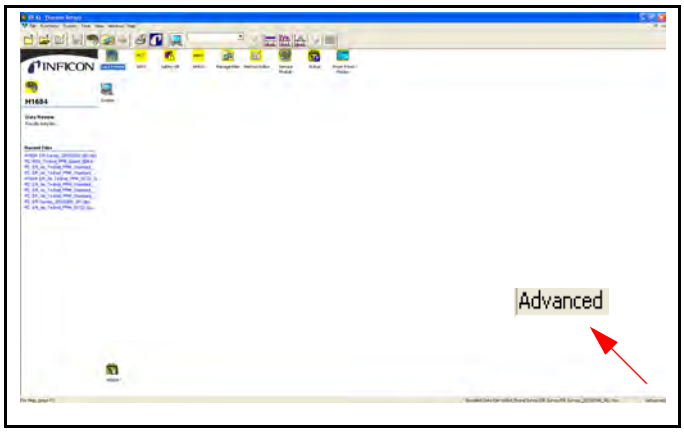
3 To select advanced access, click on **Requested Access Level** drop-down menu and select **Advanced**. If a password has been set, it will need to be entered in the password box before pressing **OK**. (See Figure 7-26.)

Figure 7-26 Change Access Level window



4 The current access level of the system is displayed at the bottom right corner of the **ER IQ** program, in the **Status Bar**. (See Figure 7-27.)

Figure 7-27 Current access level shown in system setup screen



7.3.4.1.2 Setting or Changing the Access Level Password

1 To change the Advanced password, first enter advanced mode.

2 Press the **Change Password** button. (See Figure 7-28.)

Figure 7-28 Change Password button

3 The window shown in Figure 7-29 will be displayed.

Figure 7-29 Change Password window

4 In order to change the password, the correct current password must be entered in the **Old Password** box. The Old Password box must be left blank if entering a password for the first time. The new password must be entered in both the **New Password** and **Verify New Password** boxes. Press **OK** to set the new password, or press cancel to exit without resetting the password.

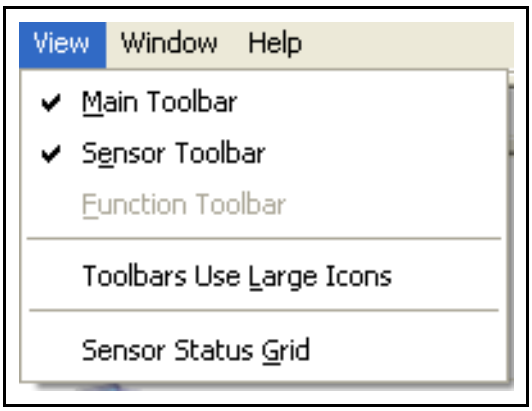
5 Click **OK** to close the **Change Access Level** window.

NOTE: ER IQ remembers the last access level when closed. Upon re-opening the program, the system will default to the last access level utilized. If a password has been set, the user will be required to enter the correct password for advanced access. If the password is not known, the user can select normal access and continue.

7.3.5 View Menu

The **View** menu is shown in Figure 7-30. It is used to select the desired toolbars.

Figure 7-30 View menu

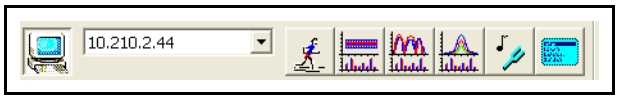


The **Main Toolbar** is shown in Figure 7-31. See Table 7-2 on page 7-40 for icon descriptions.

Figure 7-31 Main toolbar

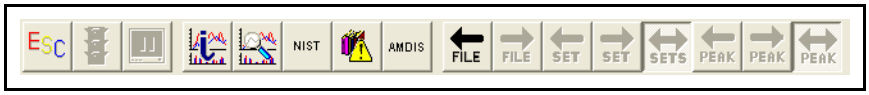
The **Sensor Toolbar** is shown in Figure 7-32. See Table 7-2 on page 7-40 for icon descriptions.

Figure 7-32 Sensor toolbar



The **Function Toolbar** is only available when the **Data Review** screen is open. (See Figure 7-33.) See section 8.1, Introduction, on page 8-1 for icon descriptions.

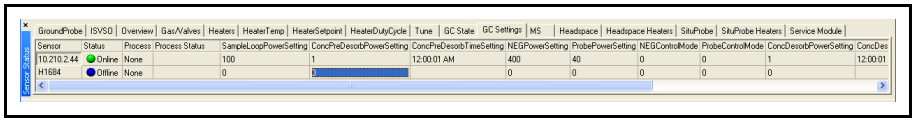
Figure 7-33 Function toolbar



Toolbars Use Large Icons increases the size of the toolbar icons.

Sensor Status Grid will open the **Sensor Status Grid** which shows the current condition of various components. (See Figure 7-34.)

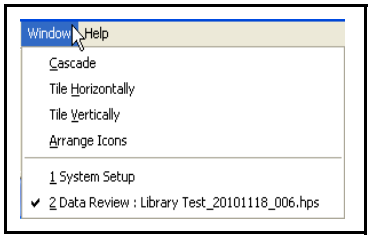
Figure 7-34 Sensor Status grid



7.3.6 Window Menu

The **Window** menu is shown below. (See Figure 7-35.)

Figure 7-35 Window menu



The first three options **Cascade**, **Tile Horizontally** and **Tile Vertically** determine the arrangement of open windows on the screen.

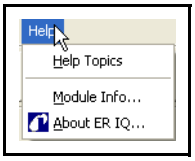
Arrange Icons aligns the icons along the top row.

The last options are **System Setup** and **Data Review**. The current view is the one that is checked. Select the unchecked option to switch views.

7.3.7 Help Menu

The **Help** menu is displayed below. (See Figure 7-36.)

Figure 7-36 Help menu



Help Topics is not available at this time.

Module Info shows the build version of various files and product number of the installed software.

About ER IQ shows the installed software version.

7.4 Safety DB

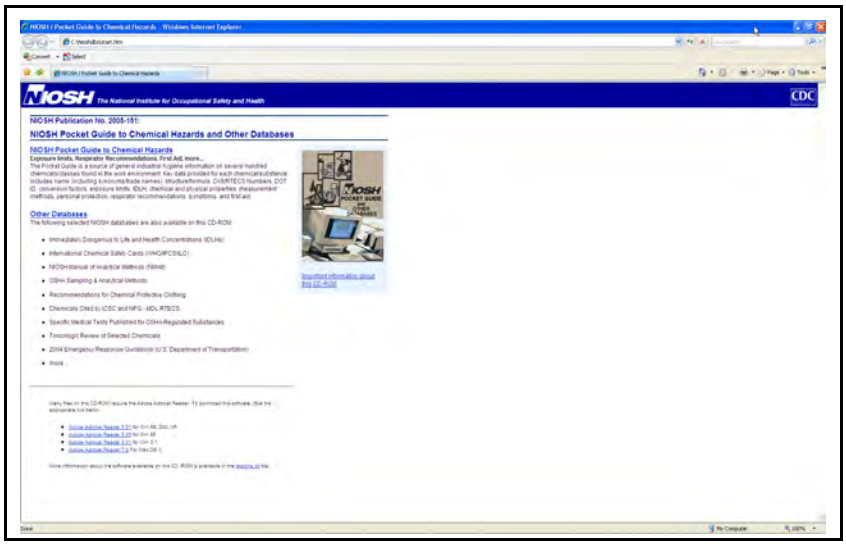
The **Safety DB** icon accesses the NIOSH Safety Database which is used to locate NIOSH REL, OSHA PEL, CAS Numbers, synonyms, IDLH's and safety recommendations. Follow the procedure below to access the Safety DB.

1 Double-click the **Safety DB** icon. (See Figure 7-37.)

Figure 7-37 Safety DB icon

2 The following screen will be displayed. (See Figure 7-38.)

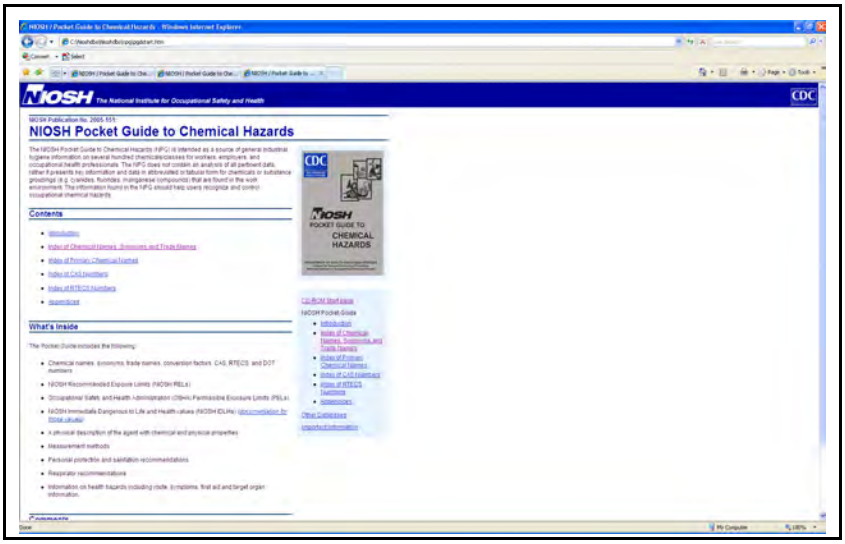
Figure 7-38 NIOSH screen



3 Double-click the **NIOSH Pocket Guide to Chemical Hazards** link or the link to the desired database.

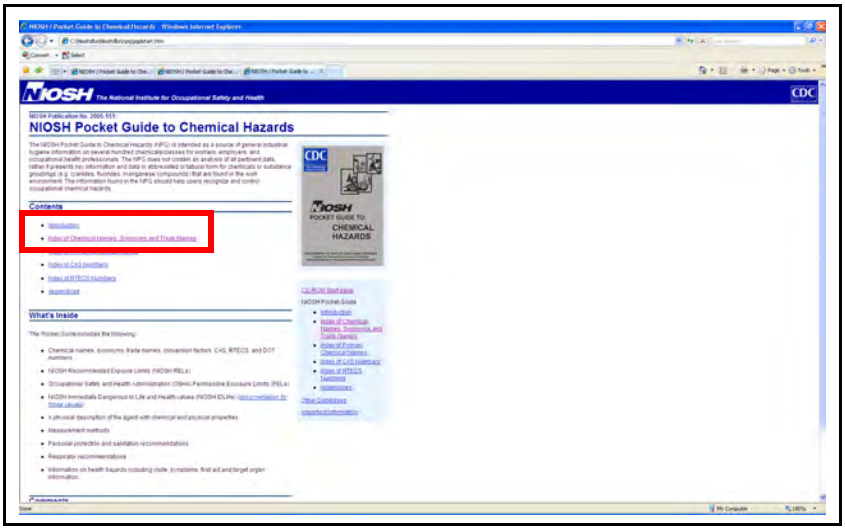
4 If clicking the **NIOSH Pocket Guide to Chemical Hazards** link, the following screen will be displayed. (See Figure 7-39.)

Figure 7-39 NIOSH Pocket Guide to Chemical Hazards Link



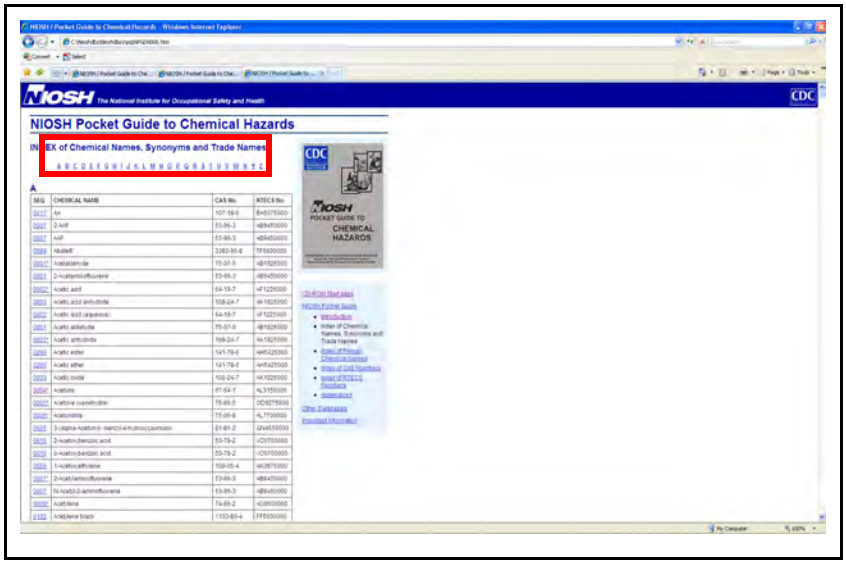
5 This screen will display the following options: **Introduction**, **Index of Chemical Names**, **Synonyms and Trade Names**, **Index of Primary Chemical Names**, **Index of CAS Numbers**, **Index of RTECS Numbers** and **Appendices**. In Figure 7-40 the **Index of Chemical Names, Synonyms and Trade Names** was selected.

Figure 7-40 Index of Chemical Names, Synonyms and Trade Names



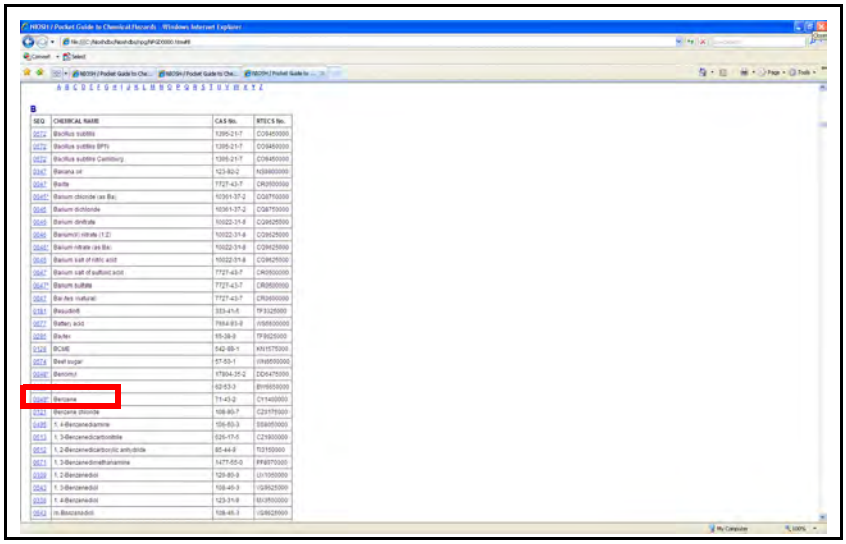
6 The following page, with the components of the database listed in alphabetical order, will be displayed. (See Figure 7-41.)

Figure 7-41 Index Of Chemical Names, Synonyms and Trade Names



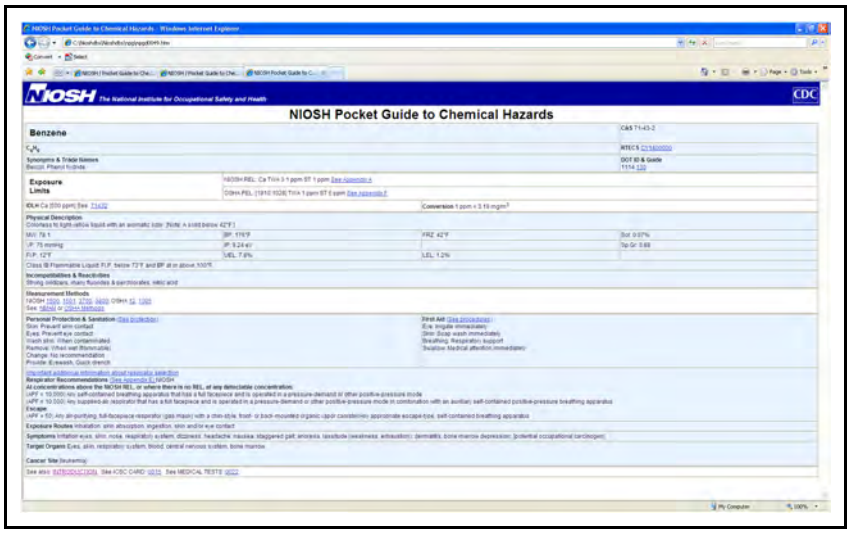
7 In Figure 7-42, Benzene was selected by clicking the **B** and then clicking the **SEQ** number, the database entry number, which is located to the left of the name.

Figure 7-42 Benzene Example



8 The screen shown in Figure 7-43 will be displayed.

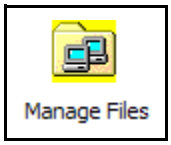
Figure 7-43 Benzene



7.5 Manage Files

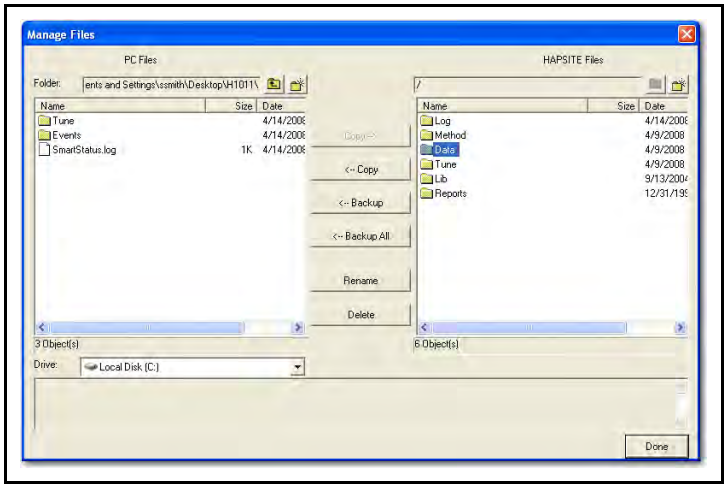
The **Manage Files** function transfers files between HAPSITE ER and the laptop. (See Figure 7-44.)

Figure 7-44 Manage Files icon



Double-clicking this icon will open the window shown below. (See Figure 7-45.)

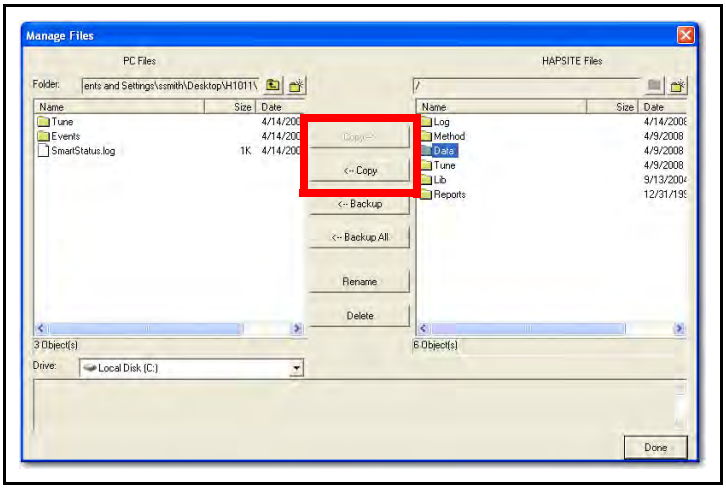
Figure 7-45 Manage Files



The **Copy-->** option allows methods only to be copied from the laptop to HAPSITE ER. The **<--Copy** option allows methods and data files to be copied from HAPSITE ER to the laptop. (See Figure 7-46.)

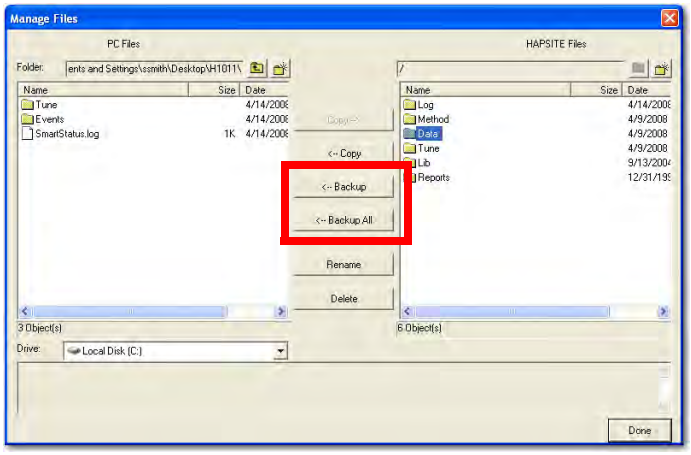
NOTE: Data files can only be transferred from the **ER IQ** to the laptop; they cannot be transferred from the laptop to HAPSITE ER. Method files can be transferred both from HAPSITE ER to the laptop and from the laptop to HAPSITE ER.

Figure 7-46 Copy function



The **<--Backup** option will backup the desired files from HAPSITE ER onto the laptop. The **<--Backup All** option will backup all of the files found on **HAPSITE ER** onto the laptop. The **Backup** options will copy the files with a .tgz extension, while the **Copy** option maintains the .hps or .mth file extensions. (See Figure 7-47.)

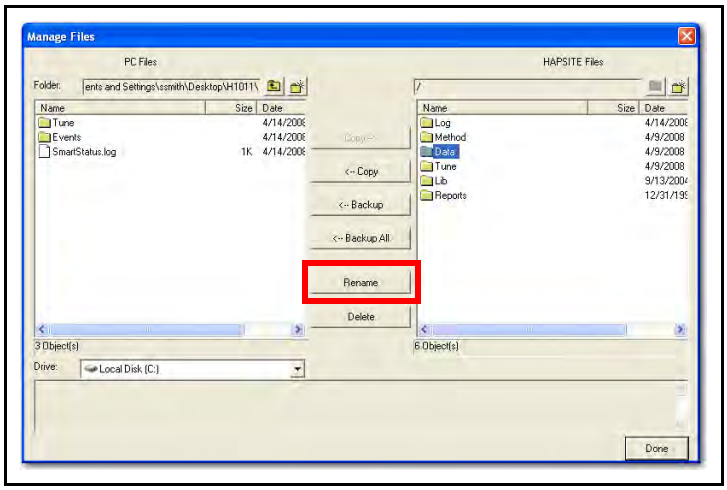
Figure 7-47 Backup function



NOTE: Renaming and/or deleting files are advanced user functions.

To rename a folder or file, click on the desired file and click **Rename**. (See Figure 7-48.)

Figure 7-48 Rename function



A new window will be displayed. The former name will be displayed on top and a box for typing in the new name will be displayed beneath it. Type in the new name and click **OK**. (See Figure 7-49 and Figure 7-50.)

Figure 7-49 Renaming folder

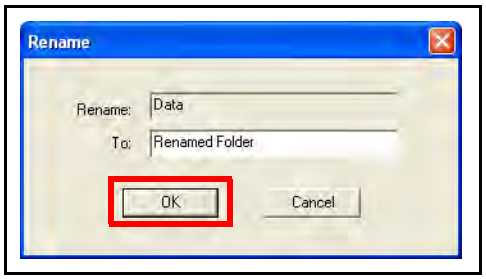
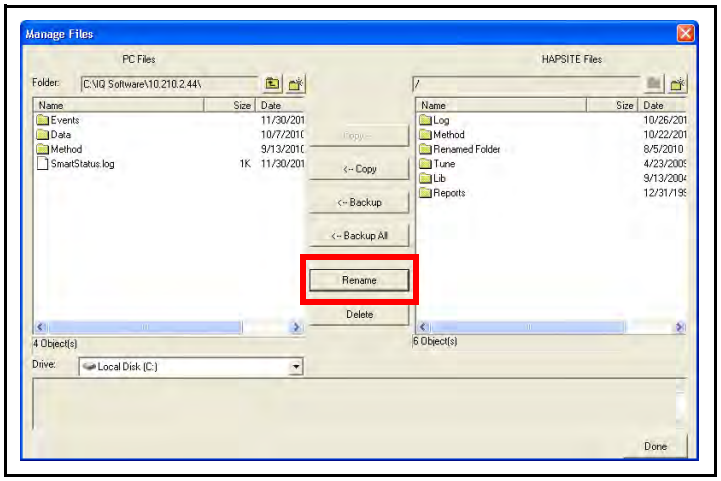
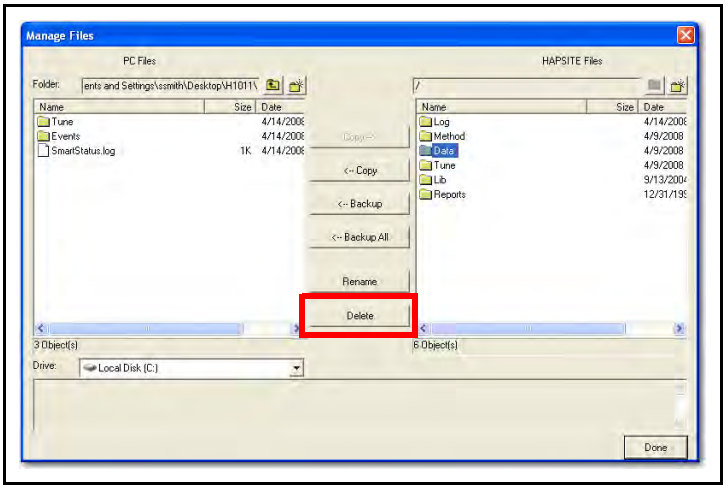


Figure 7-50 Renamed folder



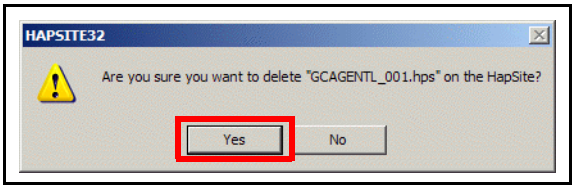
The **Delete** option will remove folders or files. To delete folders or files, highlight the desired folder or file and click **Delete**. (See Figure 7-51.)

Figure 7-51 Delete option



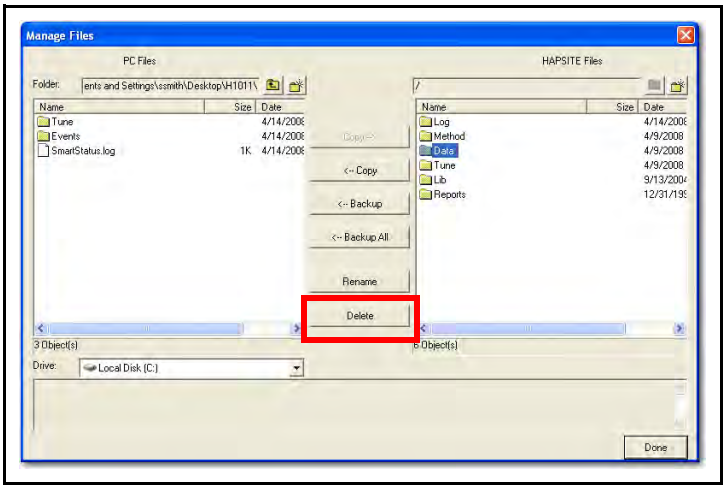
After **Delete** is clicked, a confirmation window will be displayed. Click **Yes** to delete the folder or file. (See Figure 7-52.)

Figure 7-52 Delete confirmation



To exit the screen, click **Done**. (See Figure 7-53.)

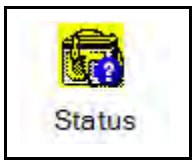
Figure 7-53 Folder or file deleted



7.6 Status Icon

The **Status** icon provides the status of various system parameters. Options, such as the time, data settings, NEG and ion pump status, and pressure flows can also be set by selecting the **Status** Icon. (See Figure 7-54.)

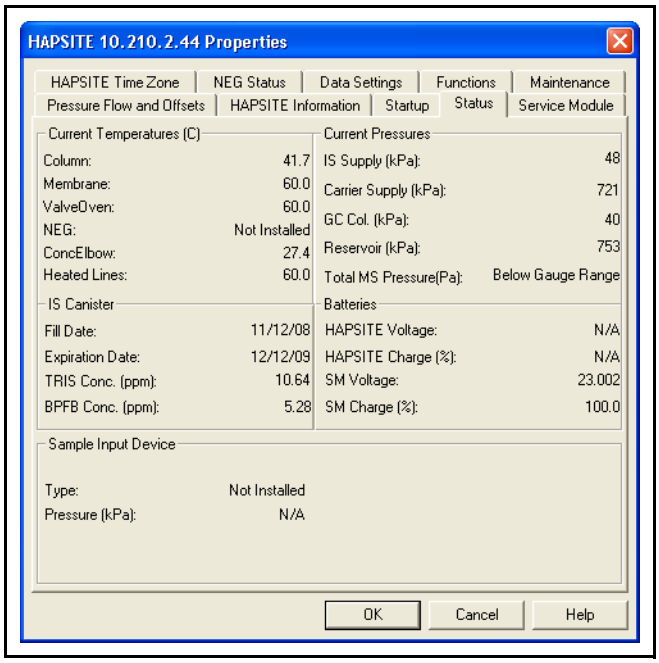
Figure 7-54 Status icon



7.6.1 Status Properties

After double-clicking the **Status** icon, the first window displayed is the **Status** window. This screen displays the current temperatures and pressures of the key components in HAPSITE ER. The battery status and internal standard canister status is also displayed. Additionally, the sample input device, i,e., probe, will be shown. (See Figure 7-55.)

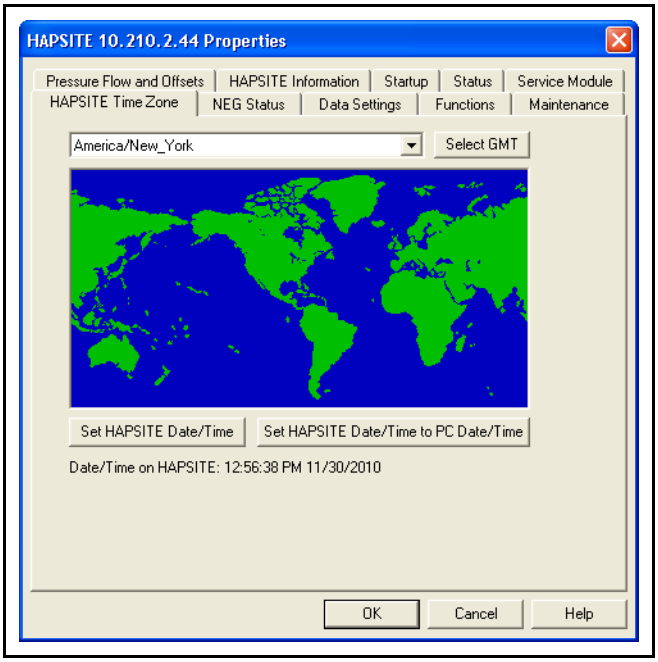
Figure 7-55 Status properties



7.6.2 HAPSITE ER Time Zone

The **HAPSITE ER Time Zone** tab allows the user to set the time on the HAPSITE ER. Setting this parameter will ensure that the data files are stamped with the proper date and time. (See Figure 7-56.)

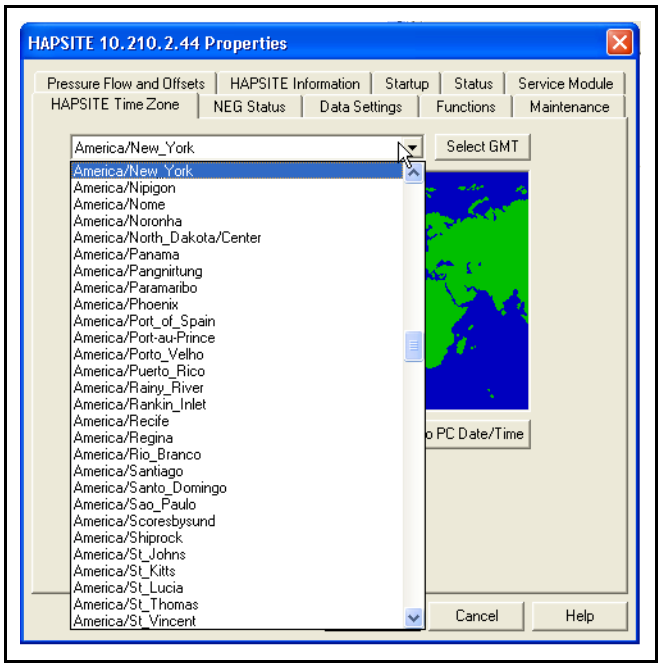
Figure 7-56 HAPSITE ER Time Zone



To set the time, select the desired time zone from the drop down menu. (See Figure 7-57.)

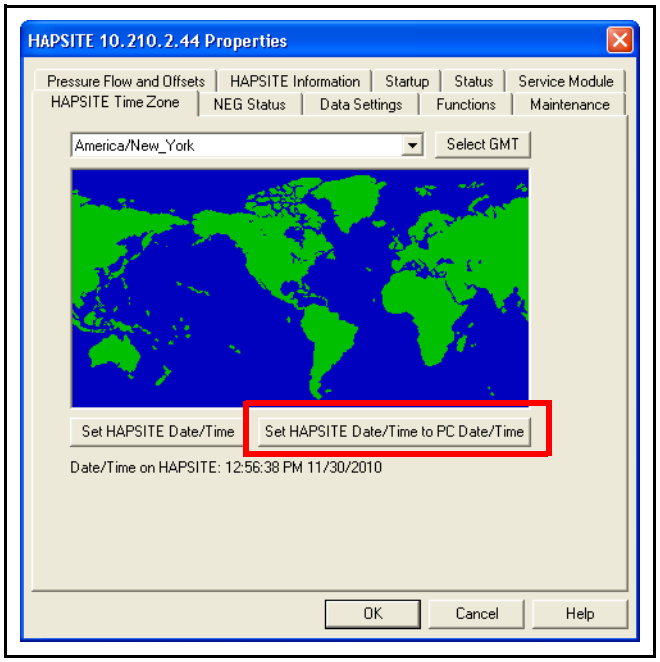
NOTE: Click **Select GMT** if Greenwich Mean Time is desired.

Figure 7-57 Selecting Time Zone



Clicking **Set HAPSITE Date/Time to PC Date/Time** will automatically synchronize HAPSITE to the laptop date and time. (See Figure 7-58.)

Figure 7-58 Set HAPSITE ER Date/Time to PC Date/Time



Clicking the **Set HAPSITE Date/Time** button will display a date/time window. (See Figure 7-59 and Figure 7-60.)

Figure 7-59 HAPSITE Date/Time button

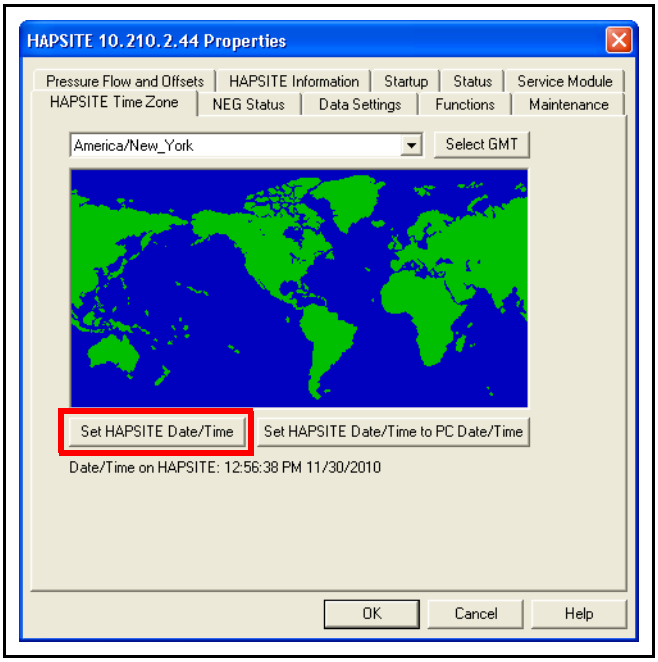
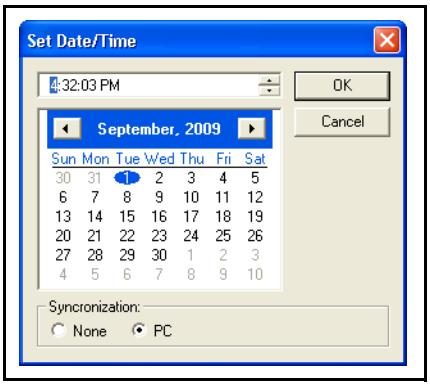
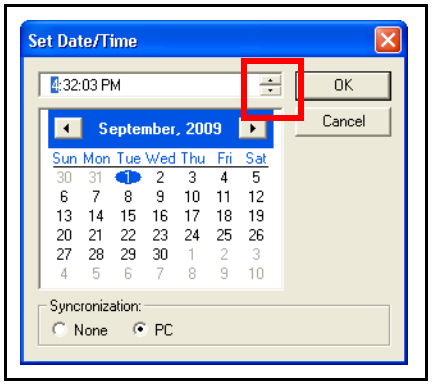


Figure 7-60 Set Date/Time



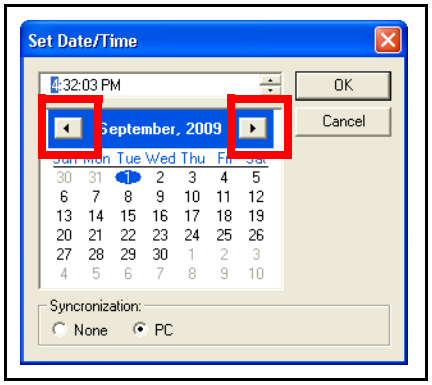
Use the top arrow keys to select the correct time. (See Figure 7-61.)

Figure 7-61 Time arrow keys



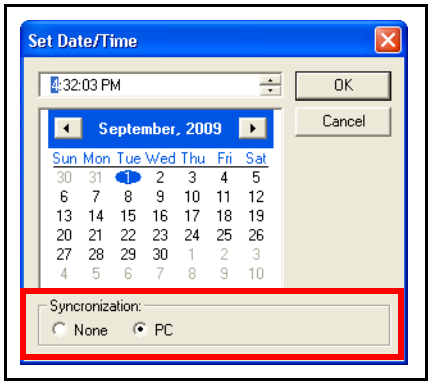
To select the proper date, use the arrow keys below the time to scroll to the current month. Click on the current date. (See Figure 7-62.)

Figure 7-62 Setting date



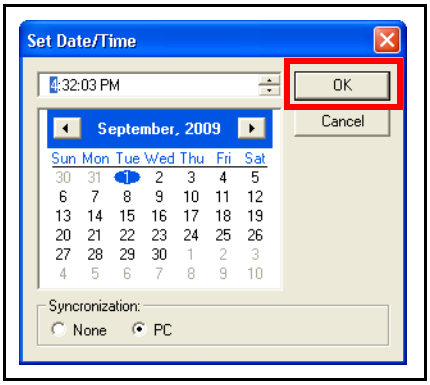
The **Synchronization** option synchronizes the time on the CMS5000 to the PC, GPS or both. If synchronization is not required, clicking **None** is also an option. (See Figure 7-63.)

Figure 7-63 Synchronization



When all the parameters have been set, click **OK**. (See Figure 7-64.)

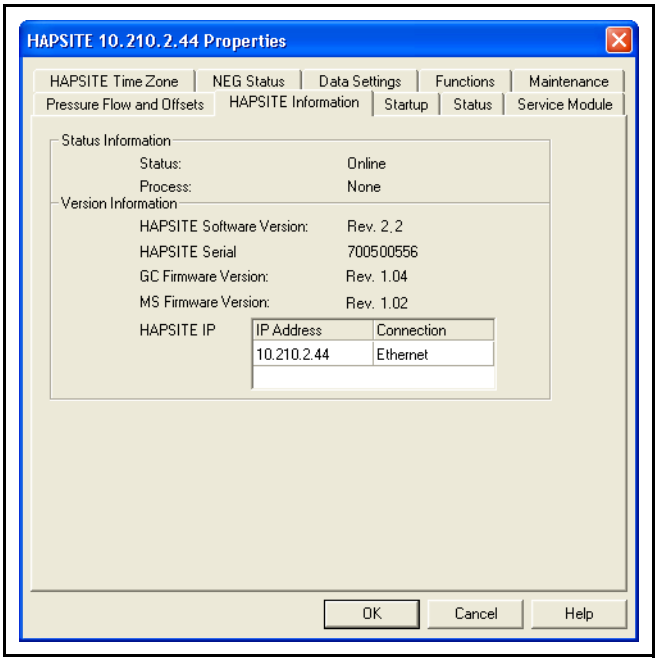
Figure 7-64 Setting Date and Time



7.6.3 HAPSITE ER Information

The **HAPSITE Information** tab provides general information regarding the HAPSITE ER system. The top portion, **Status Information**, provides verification that the system is online. It will also notify the user when a method is running. The **Version Information** box provides the **HAPSITE ER Software Version**, **HAPSITE Serial Number**, the **GC Firmware Version**, the **MS Firmware Version** the **HAPSITE IP Address** and the **Connection** type. (See Figure 7-65.)

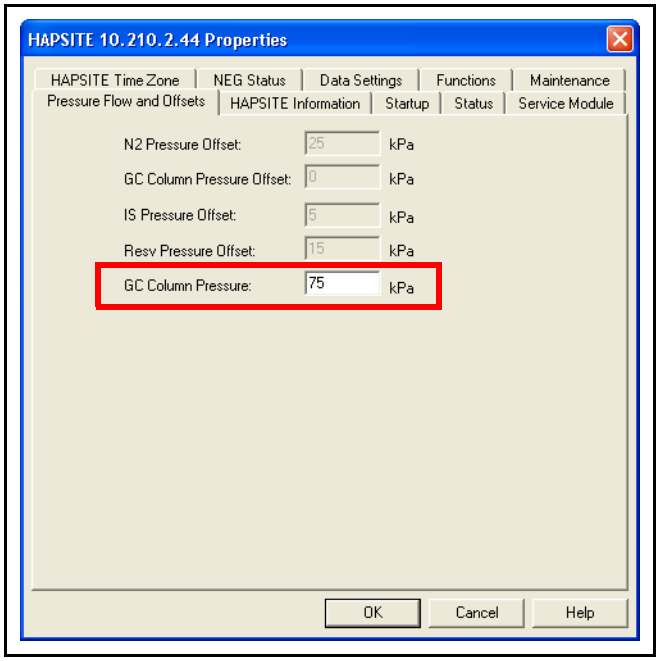
Figure 7-65 HAPSITE information



7.6.4 Pressure Flows and Temperatures

The **Pressure Flows and Temperatures** tab displays various pressures that have been set by the factory. The only pressure that can be changed by a user is the **GC Column Pressure**. When using HAPSITE ER, the BPFB internal standard should elute from the column between 3:40 and 3:50, with 3:45 being the optimal elution time. If the standard elutes outside of this range, the pressure can be adjusted. To increase the retention time by approximately three seconds, decrease the **GC Column Pressure** by 1 kPa. To decrease the retention by approximately three seconds, increase the **GC Column Pressure** by 1 kPa. After adjusting the retention time, it is recommended that the user run another blank to verify that the BPFB retention time is within range. (See Figure 7-66.)

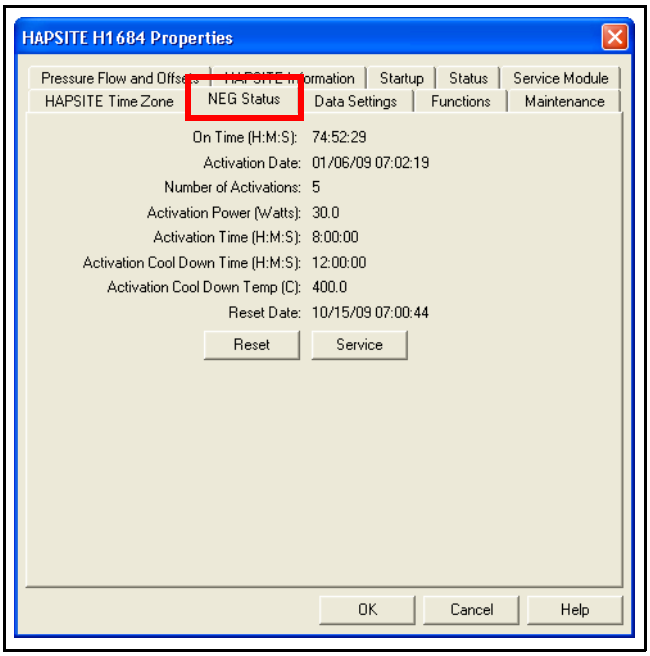
Figure 7-66 Pressure Flows and Offsets tab



7.6.5 NEG Status

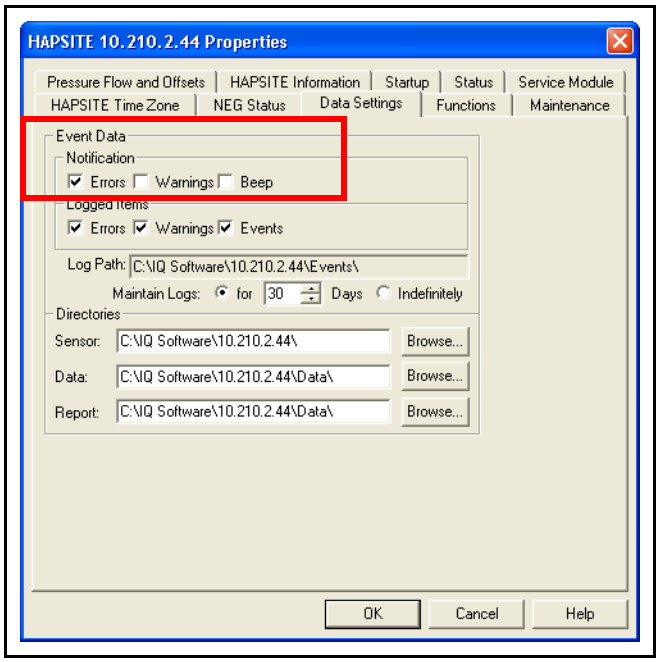
The NEG is a consumable item. NEG Status reports the number of hours that have been consumed. (See Figure 7-67.) See section 12.4 on page 12-5.

Figure 7-67 NEG Status



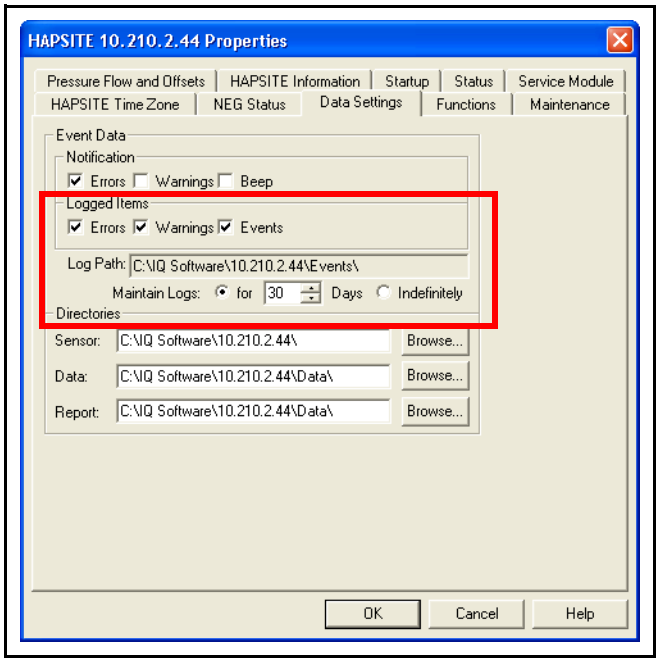
The **Data Settings** window displays the **Event Data** and the **Directories**. The **Event Data** allows for the user to set the type of **Notifications** that will be displayed on the HAPSITE ER front panel and laptop. An error will occur when a warning has been displayed, but the warning has been ignored. If **Error** is checked, an error message will be displayed. If **Warning** is checked, a warning message will be displayed, when a problem, such as high pressure, arises. If **Beep** is checked, HAPSITE will beep when an error or a warning occurs. (See Figure 7-68.)

Figure 7-68 Data settings



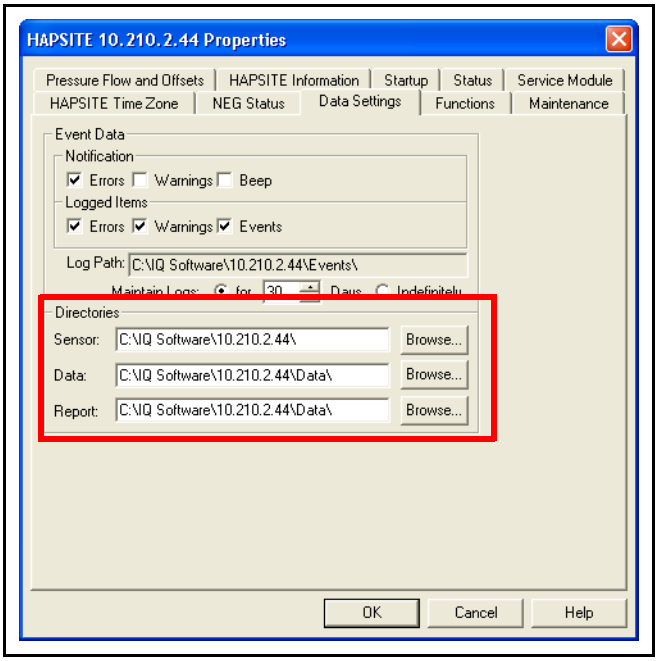
When an error, warning or event occurs, HAPSITE stores information about the occurrence and date it occurred. The pathway where this data is stored is displayed. The desired number of days for log storage can be set or the logs can be stored indefinitely. See for more information on accessing log files. (See Figure 7-69.)

Figure 7-69 Logged Items



The **Directories** folder allows for the file pathway for HAPSITE ER to be set. All data and information that has been created by HAPSITE ER will be stored in the folder that has been selected in the Sensor pathway. All data files that have been created by HAPSITE ER will be stored in the folder that was selected by the **Data** pathway. All report files which are text files of the quantitative, qualitative and summary report are stored in this folder. (See Figure 7-70.)

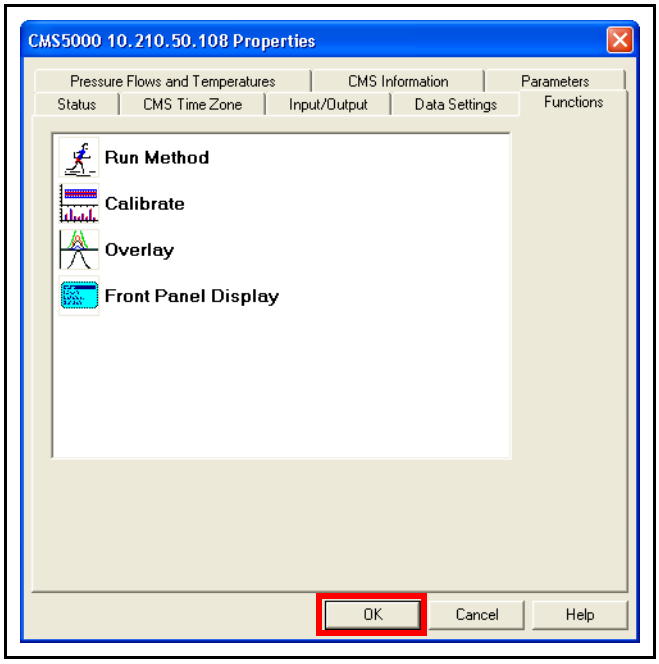
Figure 7-70 Directories



7.6.6 Functions

The icons shown on the **Functions** tab perform the same functions as the icons displayed in the **System Setup** screen. To activate a function, highlight the icon and press **OK**. (See Figure 7-71.)

Figure 7-71 Functions screen



For information on the **Run Method** function, refer to Chapter 6, Laptop Operation.

For information on the **Calibrate** function, see Chapter 11, Calibration.

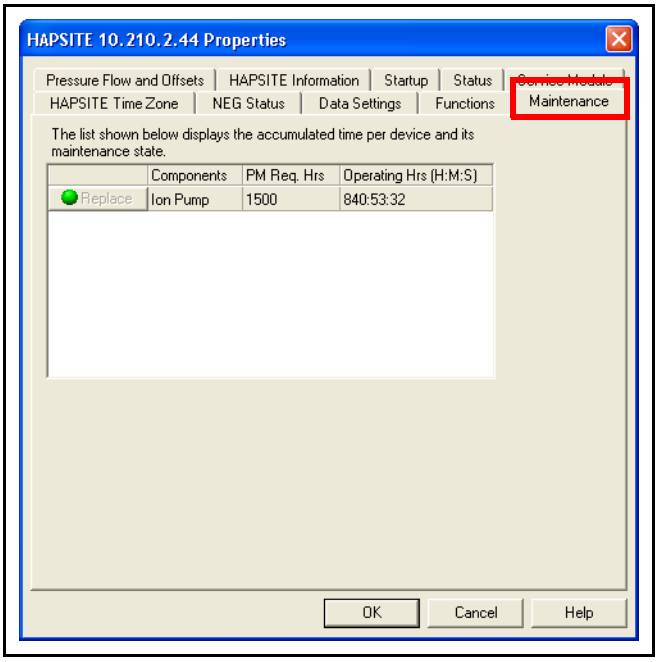
For information on the **Overlay** function, see section 8.8, Displaying Reconstructed Ion Chromatograms (RIC), on page 8-44.

For information on the **Front Panel Display** function, refer to section 7.7 on page 7-37.

7.6.7 Parameters

The **Maintenance** tab will display the number of hours that the ion pump has been running. It will also display the recommended preventative maintenance guideline of 1500 hours. If it needs replaced, the **Replace** button will activate. (See Figure 7-72.) See for information on contacting customer support for service.

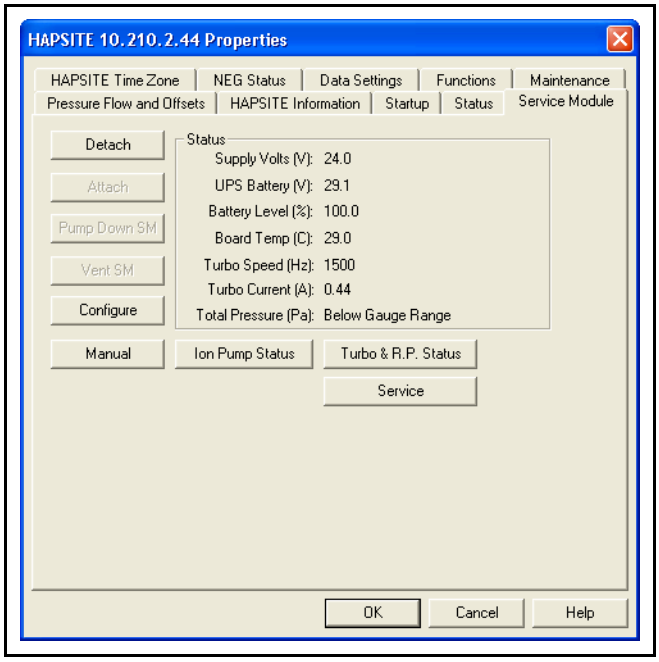
Figure 7-72 Maintenance



7.6.8 Service Module

The Service Module can be used as an alternate vacuum source or as a troubleshooting accessory. (See Figure 7-73.) For more information on using the Service Module, see Chapter 12, Maintenance or refer to the *Service Module Operating Manual.*

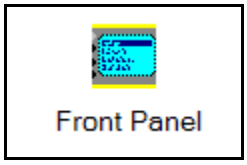
Figure 7-73 Service module



7.7 Front Panel Display Icon

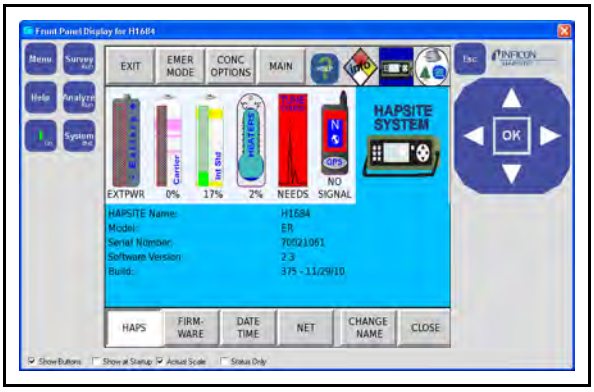
Double-clicking on the **Front Panel Display** icon will reveal an emulation on the laptop of the HAPSITE ER front panel screen, which can be used to control the front panel. (See Figure 7-74.)

Figure 7-74 Front Panel display icon



Double-click the **Front Panel Display** icon to open the emulation. (See Figure 7-75.)

Figure 7-75 Front panel display

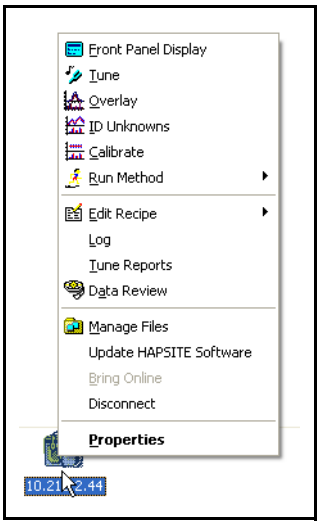


All of the buttons on the emulation operate identically to their front panel counterparts. To utilize the emulation, click on the desired button.

7.8 HAPSITE Sensor Icon

Right-clicking on the **HAPSITE ER Sensor Status** icon will display the following menu. (See Figure 7-76.)

Figure 7-76 Sensor status menu



The first five options perform the same functions as their counterpart located in the System Setup screen. The **Edit Recipe** option performs the same functions as Method Editor. Refer to Table 7-2 on page 7-40 for more information.

The **Log** and **Tune Report** options can also be accessed through the **File** menu. Refer to section 7.3.1.1 on page 7-3 for more details.

The **Data Review** and **Manage Files** options perform the same functions as their icon counterpart located on the System Setup Screen. Refer to Table 7-2 on page 7-40 for more information.

7.8.1 Update HAPSITE Software

Periodically, a software update for HAPSITE ER may be available. Clicking the **Update HAPSITE Software** option, allows the user to select the software update file. Once selected, the update will be loaded onto the analytical module and the analytical module will restart. For complete installation instructions, refer to the Software Installation Instructions that are located on the update CD, as instructions for each update may vary.

NOTE: All update files will have the .upd extension.

Latest versions of the HAPSITE software, along with instructions for loading these onto the unit, can be downloaded from the INFICON website, Software Downloads page: http://www.inficon.com/tabid/244/en-US/default.aspx.

7.8.2 Bring Online

If HAPSITE ER is not communicating when connecting through the Ethernet cable, clicking on the **Bring Online** option will attempt to re-establish communication. If the connection has been manually disabled, clicking **Bring Online** will re-enable the connection. When the connection is active, the **HAPSITE Sensor** icon will not be overlaid with an “X”.

7.8.2.1 Communication Messages

If the laptop is not communicating with HAPSITE ER, there are three types of “X’s” that may be displayed.

The red “X” signifies that communication was suddenly lost. For example, an Ethernet cable was disconnected.

The blue “X” signifies that communication has yet to be established.

The gray “X” signifies that communication has been disabled through ER IQ by using the **Disconnect** option.

7.8.3 Disconnect

The **Disconnect** option will manually disconnect the laptop from HAPSITE ER and will remain disconnected until **Bring Online** is selected.

CAUTION

The Laptop and HAPSITE ER should always have the most current version of the software installed. Verify that the unit software and ER IQ software have the save version number. Do not try to run incompatible versions of software together. (For example ER IQ 1.05 and HAPSITE ER Analytical Module software 1.16)

7.9 HAPSITE Icons

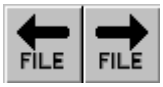
Table 7-2 HAPSITE Icons

Icon	Description
	Starts **ER IQ** Software from desktop.
 System	System properties (Communications, Display, Miscellaneous)
 haps4	HAPSITE sensor. Right-click to access menu.
 Data Review	Accesses all saved data files.
 Run Method	Accesses methods to initiate a run.
 NIST	Accesses the NIST software and library.

Table 7-2 HAPSITE Icons (continued)

Icon	Description
	Accesses the NIOSH database.
 AMDIS	Accesses the AMDIS software and library.
 Manage Files	Allows transfer of files between HAPSITE and laptop.
 Method Editor	Allows editing and creating methods.
 Service Module	Accesses the Service Module when attached.
 Status	Accesses HAPSITE properties.
 Tune	Accesses the HAPSITE tune program.
 Front Panel	Opens the HAPSITE front panel display on the laptop screen.
	Accesses Data File information.
	Returns the current screen to the System Setup screen.

Table 7-2 HAPSITE Icons (continued)

Icon	Description
	Displays the software version of **ER IQ** software that is installed on the laptop.
	Accesses the Calibrate function.
	Accesses the ID Unknowns function.
	Accesses **Chromatogram Overlay** function.
	Navigates through files in **Data Review**.
	Navigates through peaks in “search for peaks”.
	Returns to the complete full chromatogram (TIC) display in “search for peaks”.

Chapter 8
Data Review

8.1 Introduction

This chapter provides information regarding the analysis of data samples. Topics include opening data files, compound identification using the AMDIS and NIST Libraries, overviews of all data review menus, **Background Subtract** and **Chromatogram Overlay**.

8.2 Data Review Toolbar

The **Data Review** toolbar is shown in Figure 8-1.

Figure 8-1 Data Review toolbar

. . . . . Aborts a running method.


. . . . . Start/stops a method.


. . . . . Pauses the data updates to the laptop during a run. This does not pause the analysis of the data by the HAPSITE ER.


. . . . . Accesses the **Data File Information** window.


. . . . . Views **Search Reports** for this data file.

. . . . . Opens the **NIST** program.


. . . . . Opens the **NIOSH** database.

. . . . . Opens the **AMDIS** program.

. . . . . Opens the previous file in the current directory.

. . . . . Opens the next file in the current directory.

. . . . . Opens the previous **SIM** Set.

. . . . . Opens the next **SIM** Set.

. . . . . Opens all **SIM** Sets.

. . . . . Selects the previous peak when using the **Search for Peaks** function.

. . . . . Selects the next peak when using the **Search for Peaks** function.

. . . . . Returns to the full chromatogram display.

8.3 Accessing the Data Review Feature

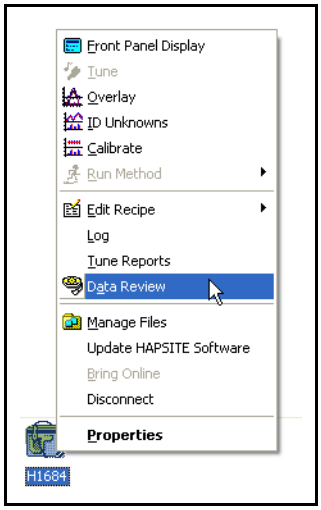
The **Data Review** feature can be accessed as follows:

1 Double-click the **Data Review** icon. (See Figure 8-2.)

Figure 8-2 Data Review icon

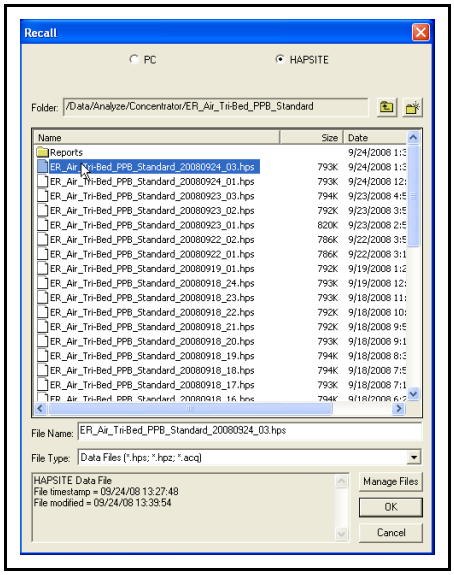
2 Alternately, right-click the **HAPSITE Sensor** icon. The menu shown in Figure 8-3 will be displayed. Click **Data Review**.

Figure 8-3 Data Review Menu



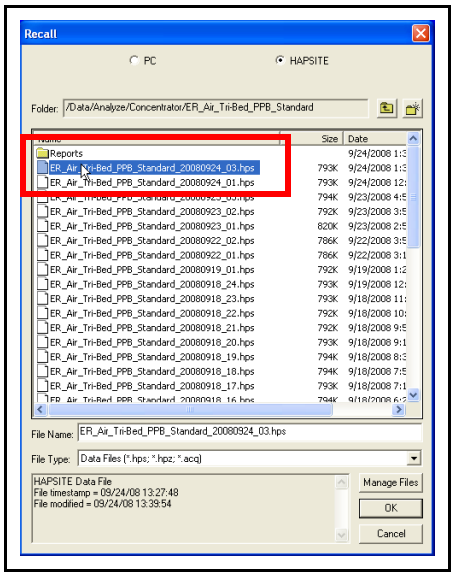
3 The **Recall** window will be displayed. Select **PC** if the file was run using the laptop. Select **HAPSITE** if the file was run using the HAPSITE ER front panel and the laptop was not connected at the time of sample collection. (See Figure 8-4.)

Figure 8-4 Data Recall window



4 Double-click on the desired data file. (See Figure 8-5.)

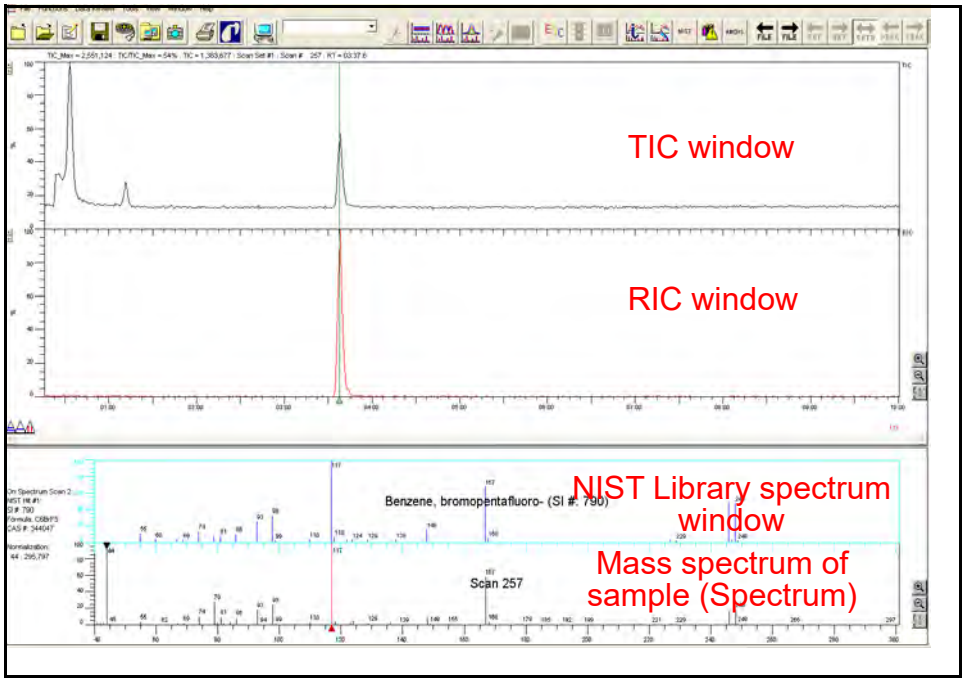
Figure 8-5 Selecting the data file



NOTE: HAPSITE data file extensions end in **.hps**.

5 The **Data Review** screen with the selected data file will be displayed. The **Data Review** screen is divided into four sections, as shown in Figure 8-6.

Figure 8-6 Sections of the Data Review Screen



TIC window . . . . . The total ion chromatogram, which is the total intensity of the mass fragments, is plotted in this screen. Basic data analysis, such as background subtraction and peak identification, is also conducted here.

RIC window . . . . . The intensity of a specific mass fragment is plotted in this screen.

NIST Library spectrum . . . . . This window will display NIST matches if **Search NIST/User** is checked in the **Control Panel**.

Mass spectrum of sample (Spectrum) . . . . . The mass spectrum generated from the sample is displayed in this window.

8.4 Reports

1 To access data reports, double-click the **View Search Results** icon on the **Data Review** screen. (See Figure 8-7 and Figure 8-8.)

Figure 8-7 View Search Results icon

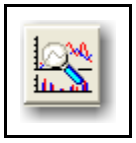
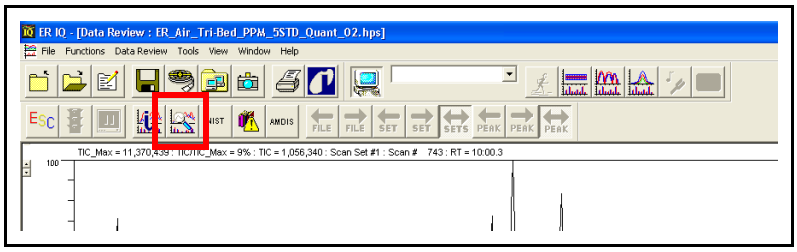
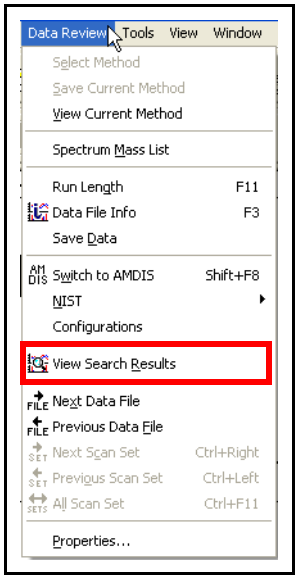


Figure 8-8 Location of View Search Results icon



2 Alternately, **View Search Results** may be accessed from **Data Review** drop-down menu. (See Figure 8-9.)

Figure 8-9 Data Review Drop-down menu

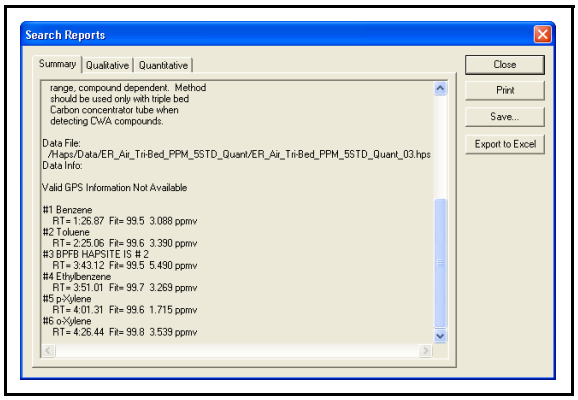


3 There are a maximum of three reports available, depending on how the method was configured.

3a The **Summary** report provides an overview of the **Qualitative** and/or **Quantitative** reports. (See Figure 8-10.) The **Summary** report includes:

- date
- time
- method name
- method description
- GPS info
- analyte identification
- retention time
- fit (see section 8.5 on page 8-16)
- concentration

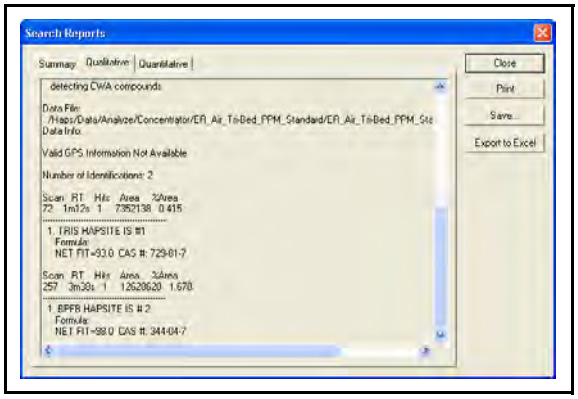
Figure 8-10 Summary Reports screen



3b The **Qualitative** report (see Figure 8-11) includes:

- date
- time
- method name
- method description
- GPS info
- scan number
- retention time
- number of hits (possible identifications)
- area
- percent area
- analyte identification
- formula
- fit (see section 8.5 on page 8-16)
- CAS number

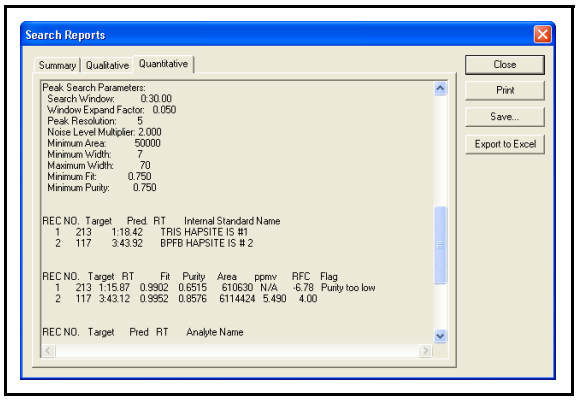
Figure 8-11 Qualititative Reports screen



3c The **Quantitative** report (see Figure 8-12) includes:

- date
- time
- method name
- method description
- GPS info
- target library
- date of the last library calibration
- peak search parameters
- target ion
- predicted retention time
- actual retention time
- internal standard
- scan number
- retention time
- number of hits (possible identifications)
- area
- percent area
- analyte identification
- formula
- fit (see section 8.5 on page 8-16)
- purity
- CAS number
- concentration with units
- RFC
- The flag, which provides the reason that the compound was not identified

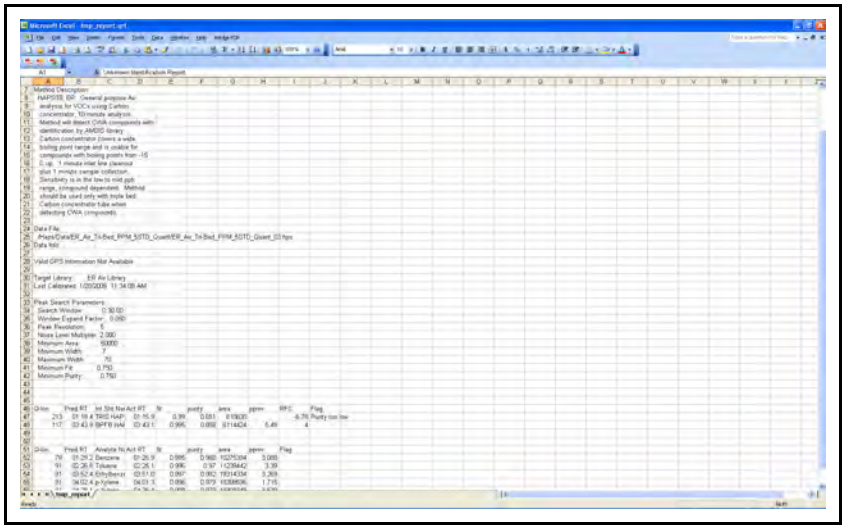
Figure 8-12 Quantitative Report



NOTE: If the method does not contain a calibrated library, the **Quantitative** tab will display **No Report**.

4 The **Quantitative** report can be exported to Excel for further analysis by clicking on the **Export to Excel** button. (See Figure 8-13.)

Figure 8-13 Export to Excel



8.4.1 Using the Zoom Function in the TIC/RIC Window

In order to magnify the peaks, **ER IQ** has a zoom capability.

1 Click the **Zoom** icon. (See Figure 8-14 and Figure 8-15.)

Figure 8-14 Zoom

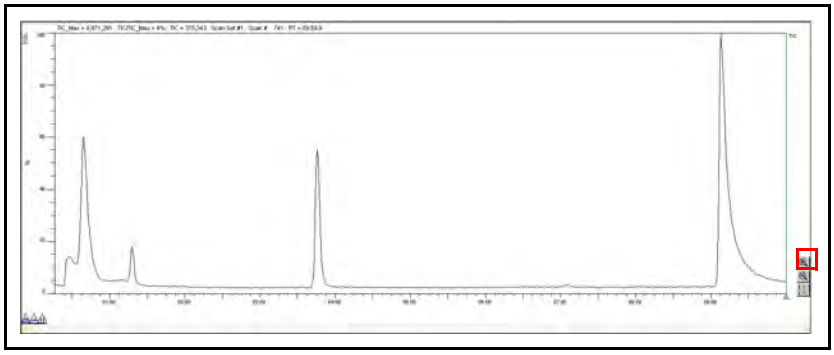
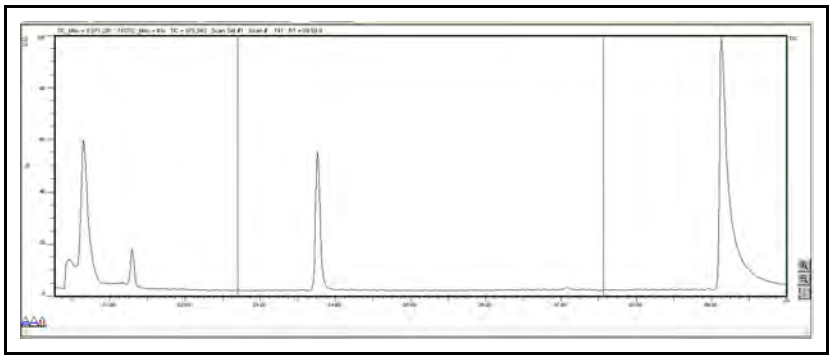


Figure 8-15 Zoom icon

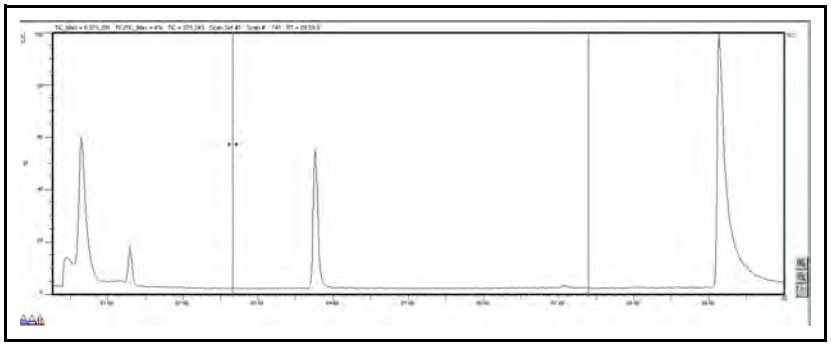
2 Two vertical lines will be displayed. (See Figure 8-16.)

Figure 8-16 Displaying vertical lines



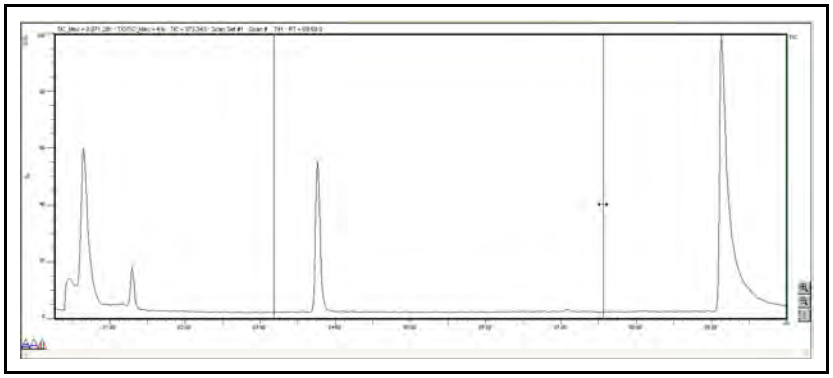
3 Mouse over one of the lines. The cursor will become a double-sided arrow. Move the line to the desired point. (See Figure 8-17.)

Figure 8-17 Moving the first line



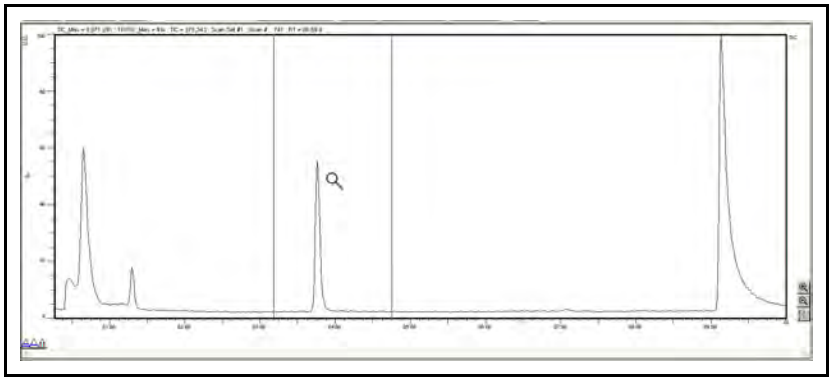
4 Mouse over the other line. The cursor will again become a double-sided arrow. Move the line to the desired point. (See Figure 8-18.)

Figure 8-18 Moving the second line



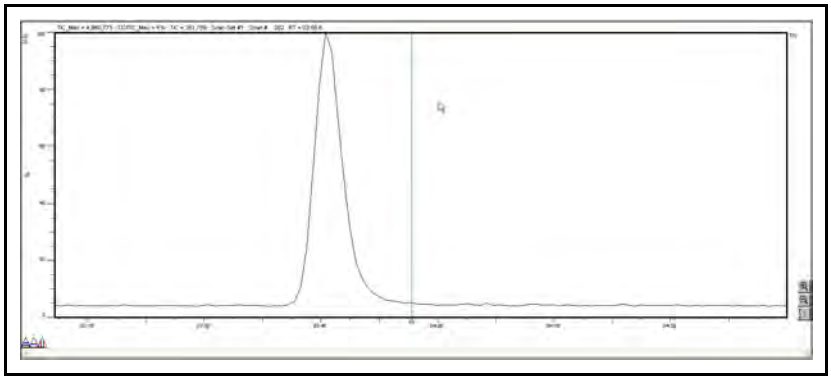
5 Move the cursor between the two vertical lines. The cursor will become a magnifying glass. (See Figure 8-19.)

Figure 8-19 Moving the cursor



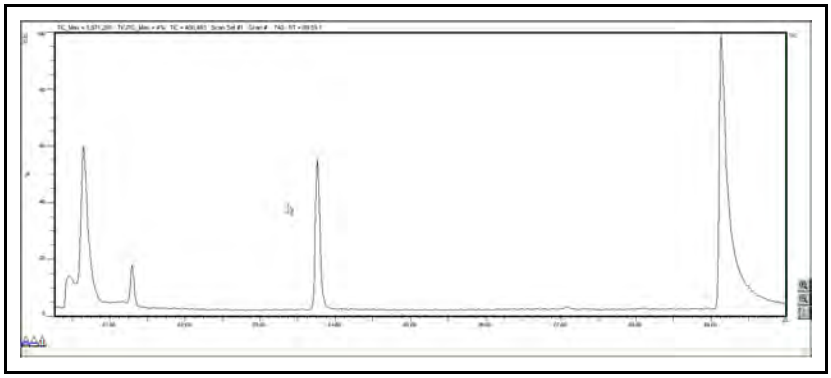
6 Click between the lines to zoom. (See Figure 8-20.)

Figure 8-20 Zooming



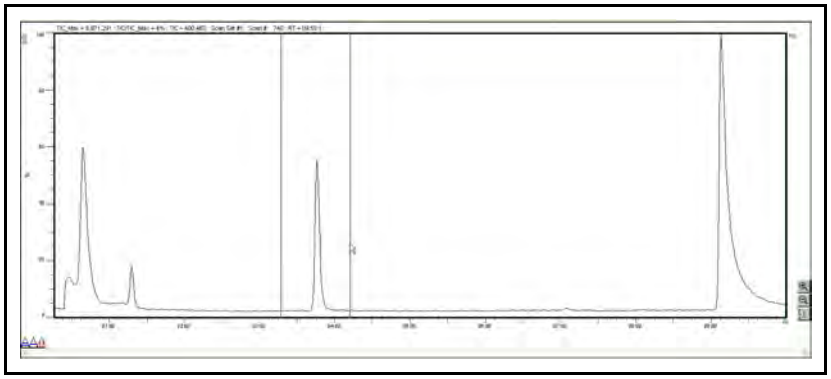
7 Alternately, a zoom can be completed by clicking and holding the left mouse button at the desired zoom starting point. (See Figure 8-21.)

Figure 8-21 Zooming using the left mouse button



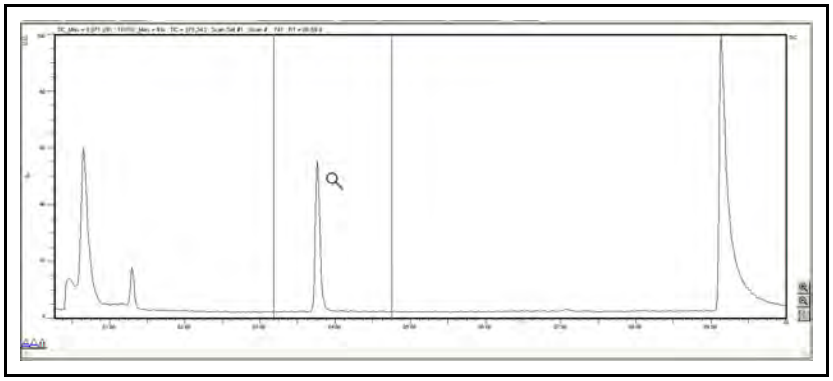
8 Continue to hold the left mouse button and drag the mouse to the desired zoom ending point. Two vertical lines will be displayed. (See Figure 8-22.)

Figure 8-22 Zoom end point



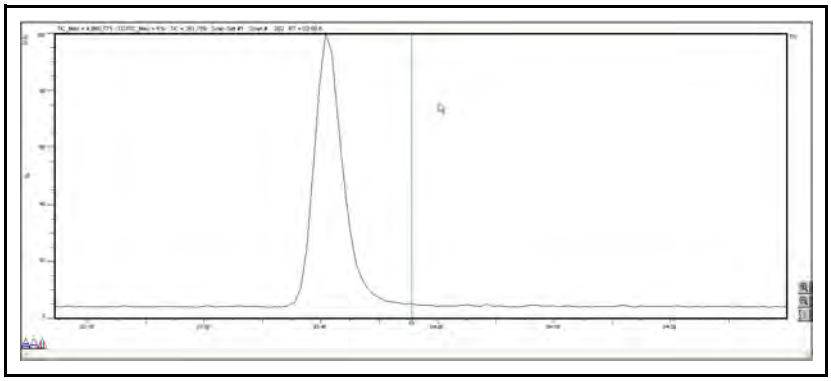
9 Release the left mouse button. Move the cursor in between the two vertical lines. The cursor will become a magnifying glass. (See Figure 8-23.)

Figure 8-23 Magnifying glass



10 Click between the lines to zoom. (See Figure 8-24.)

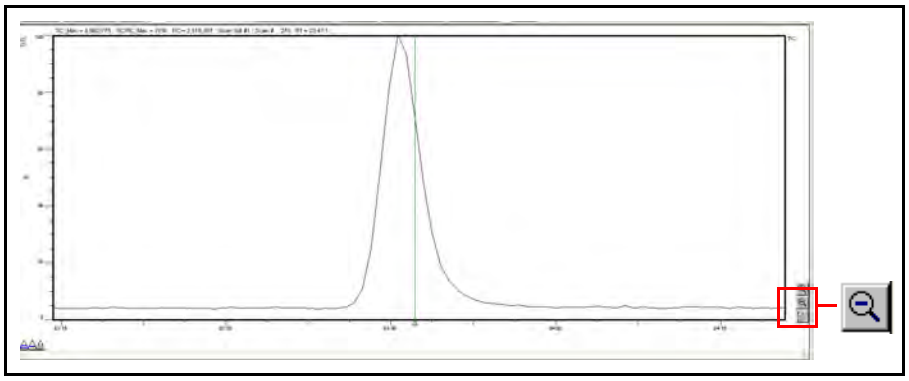
Figure 8-24 Click between the lines



8.4.2 Zooming Out

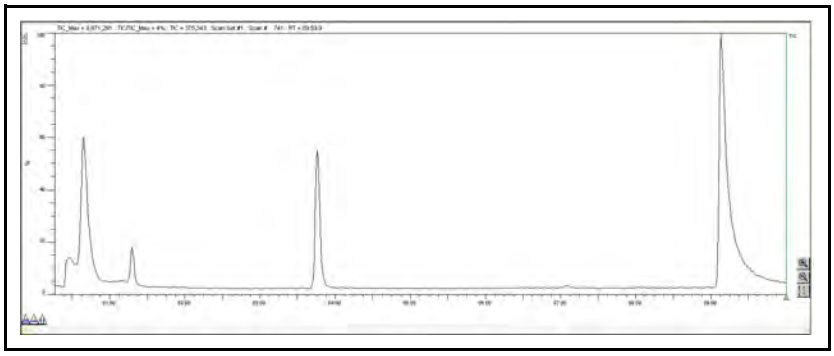
1 Click on the **Zoom Out** icon. (See Figure 8-25.)

Figure 8-25 Zoom out



2 The screen will return to the expanded view. (See Figure 8-26.)

Figure 8-26 Expanded view



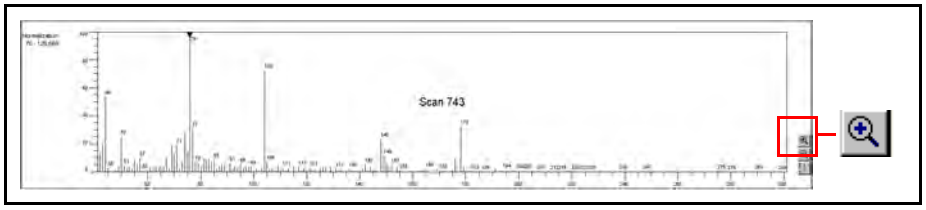
3 Alternately, click **F11** to return the expanded view.

8.4.3 Using the Zoom Spectrum Function

The **Spectrum** window has a zoom function to magnify the spectra.

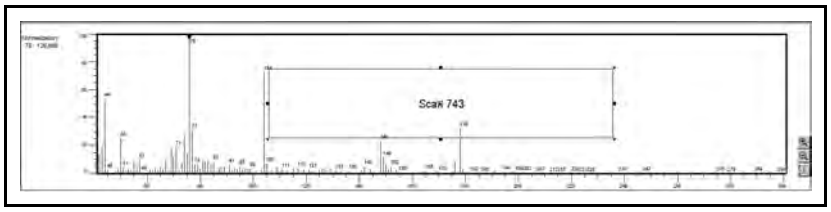
1 Click the **Zoom** icon. (See Figure 8-27.)

Figure 8-27 Zoom icon



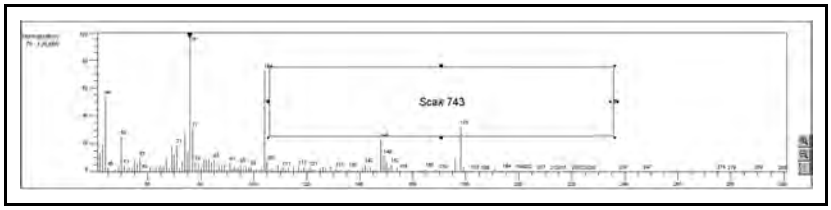
2 A rectangle will be displayed in the **Spectrum** window. (See Figure 8-28.)

Figure 8-28 Rectangle in spectrum window



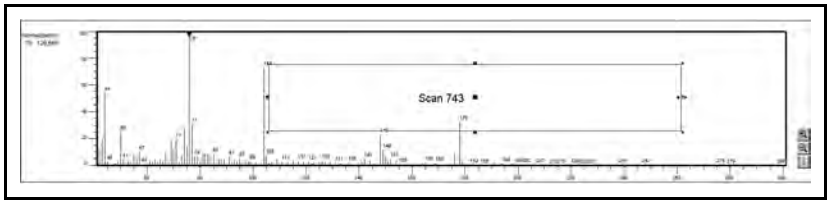
3 Mouse over a side of the rectangle. The cursor will become a double-sided arrow. (See Figure 8-29.)

Figure 8-29 Mouse over a side



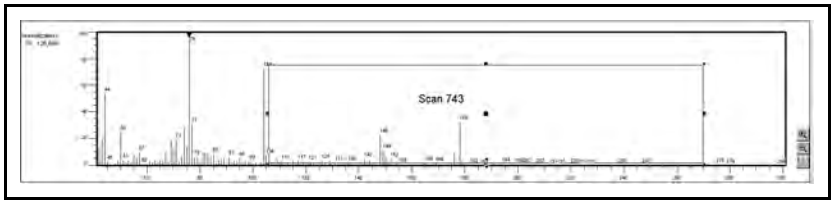
4 Drag the side to the desired end zoom point. (See Figure 8-30.)

Figure 8-30 Zoom end point



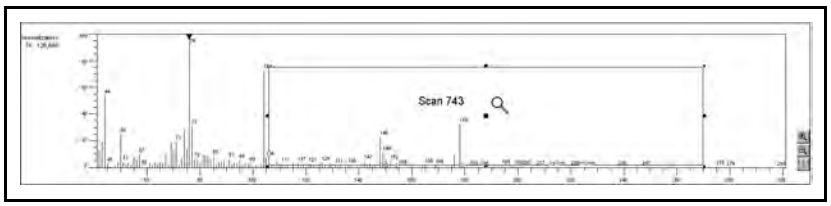
5 If necessary, repeat with other sides of the rectangle in order to adjust the desired zoom area. (See Figure 8-31.)

Figure 8-31 Adjusting zoom area



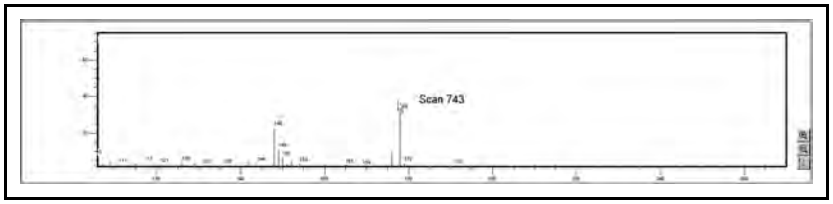
6 Move the cursor into the center of the rectangle. The cursor will become a magnifying glass. (See Figure 8-32.)

Figure 8-32 Magnifying glass



7 Click inside the rectangle to zoom. (See Figure 8-33.)

Figure 8-33 Clicking to zoom

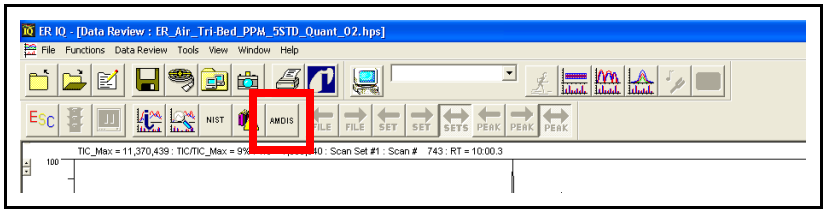


8.5 Analyzing Data Using AMDIS

AMDIS is an acronym for Automated Mass Spectrum Deconvolution and Identification System, a tool which was developed by the National Institute of Science and Technology. HAPSITE utilizes an on-board library, **HAPSITE.msl**, and the AMDIS deconvolution algorithm to make identifications. This library contains approximately 750 chemicals including chemical warfare agents and is able to identify complex mixtures, including co-eluting chemicals. The on-board library can be updated to include several thousand compounds. The laptop AMDIS software can be accessed through ER IQ, enhancing the quality of data analysis by including access to the NIST mass spectral library.

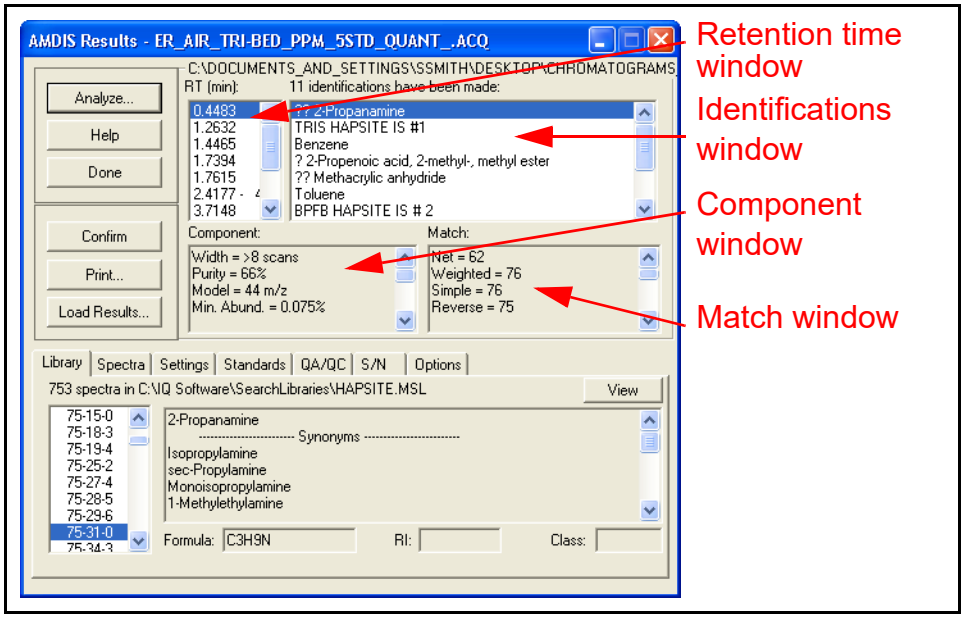
1 Double-click on the **AMDIS** icon. (See Figure 8-34.)

Figure 8-34 AMDIS icon



2 The following window will be displayed. (See Figure 8-35.)

Figure 8-35 AMDIS window



The results screen includes:

Retention time window . . . . . AMDIS uses a decimal time format. Multiply the numbers after the decimal point to convert to a seconds format.

Identifications window. . . . . Lists the identifications in order of retention time. If a question mark is displayed before the identification, the match is between 70-79. If two question marks are displayed, the fit is between 60-69, and if three question marks are displayed, the fit is less than 60.

Component window. . . . . Displays the width of the peak in terms of scans, the purity of the peak and the min. abund (minimum abundance). This is the abundance of the smallest observable mass spectral peak and model, which is the m/z value or TIC used to determine the peak shape. It is generally the ion that rises and falls the fastest.

Match window. . . . . Displays the quality of the spectral match. If the Net is greater than 70, the identification is considered to be a good match. If the Net is greater than 80, the identification is considered to be a very good match. If the Net is greater than 90, the identification is considered to be an excellent match.

Library Tab . . . . . Displays the search library, CAS number, synonyms and formula for the compound that is highlighted in the identifications box.

Analyze Button. . . . . Sets the library pathway, which may be necessary when reloading the **ER IQ** program. See section 8.5.1, Setting the AMDIS Pathway, on page 8-18.

Help . . . . . Detailed **Help** instructions about AMDIS.

Done . . . . . Closes the AMDIS screen.

Confirm . . . . . Labels the peaks in the chromatogram that were not identified by AMDIS and allows the peaks to be exported to NIST for further identification. See section 8.5.3, Confirm Screen in AMDIS, on page 8-22 for further information.

Print. . . . . Prints the AMDIS data in a report format.

Load Results . . . . . Allows for the analyst to select a different data file and perform an AMDIS search on the newly selected file.

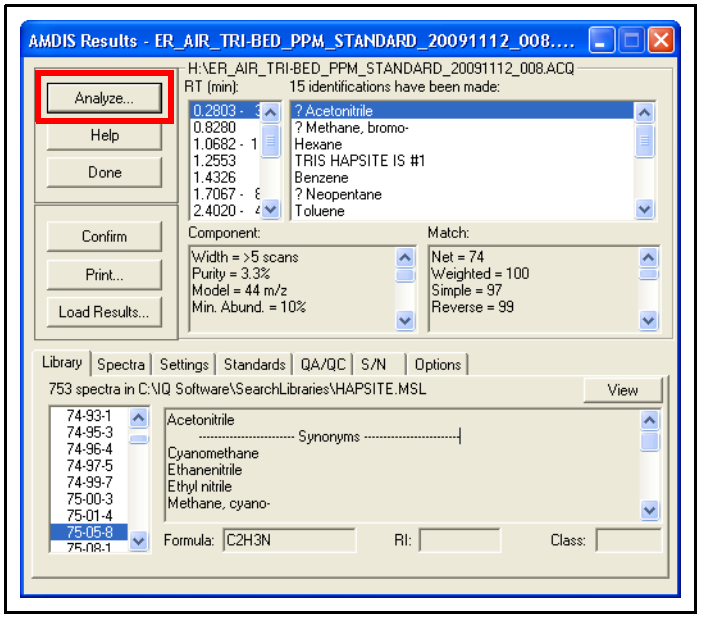
View . . . . . Allows the analyst to view the library components. See section 8.5.2, View Function in AMDIS, on page 8-21.

8.5.1 Setting the AMDIS Pathway

If AMDIS is reloaded onto the laptop, the library pathway may need to be reset. To reset the pathway:

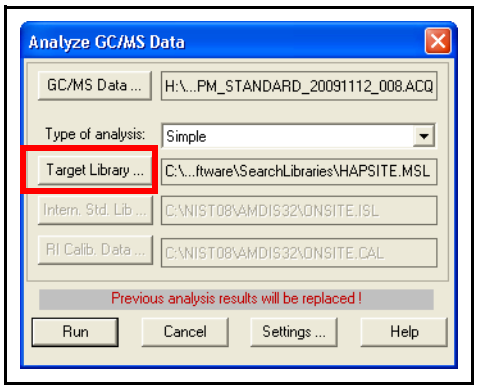
1 Double-click on **Analyze...**. (See Figure 8-36.)

Figure 8-36 Analyze button



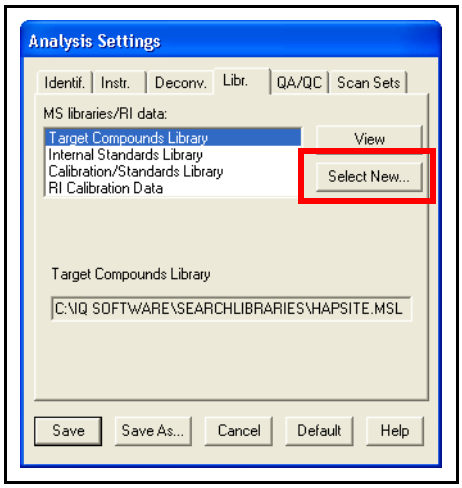
2 Double-click on **Target Library**. (See Figure 8-37.)

Figure 8-37 Target Library



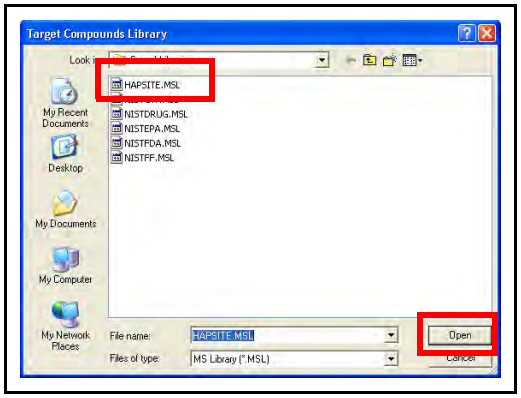
3 Click **Select New** to change the library pathway. (See Figure 8-38.)

Figure 8-38 Select New



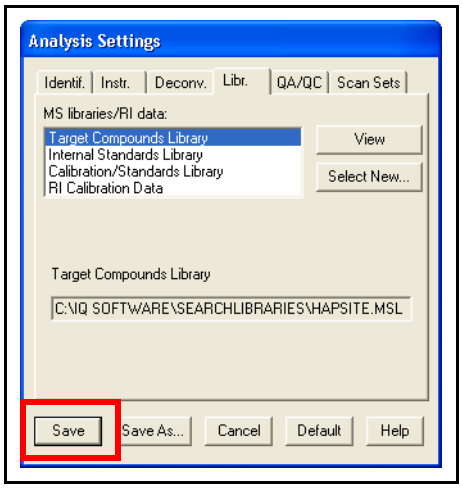
4 The **HAPSITE.msl** is located at the following pathway: C:\IQ Software\SearchLibraries. If custom libraries are used, they must be located in this directory. Highlight the library and click **Open**. (See Figure 8-39.)

Figure 8-39 HAPSITE.msl



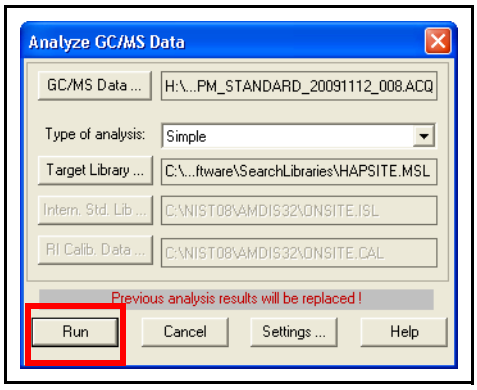
5 Click **Save**. (See Figure 8-40.)

Figure 8-40 Save



6 Click **Run**. (See Figure 8-41.)

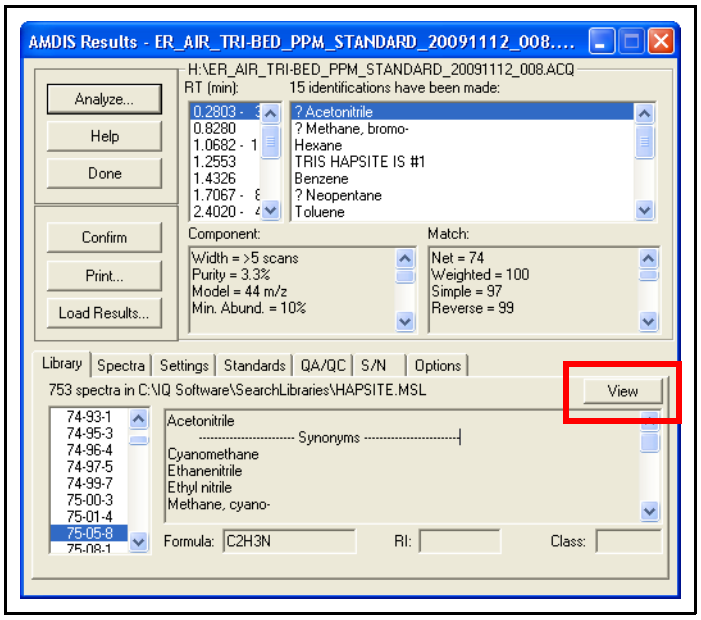
Figure 8-41 Run



8.5.2 View Function in AMDIS

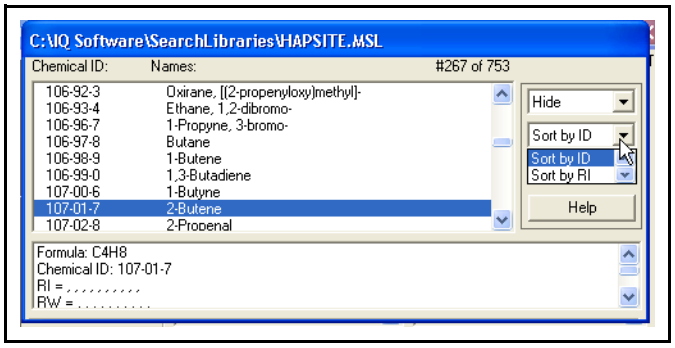
The **View** function can be accessed by selecting the **View** button displayed below or by following through step 3 of the previous section and selecting **View**. (See Figure 8-42.)

Figure 8-42 AMDIS



This function displays the components of the **HAPSITE.msl** library. This list can be sorted by retention index, name or CAS number. (See Figure 8-43.)

Figure 8-43 View screen

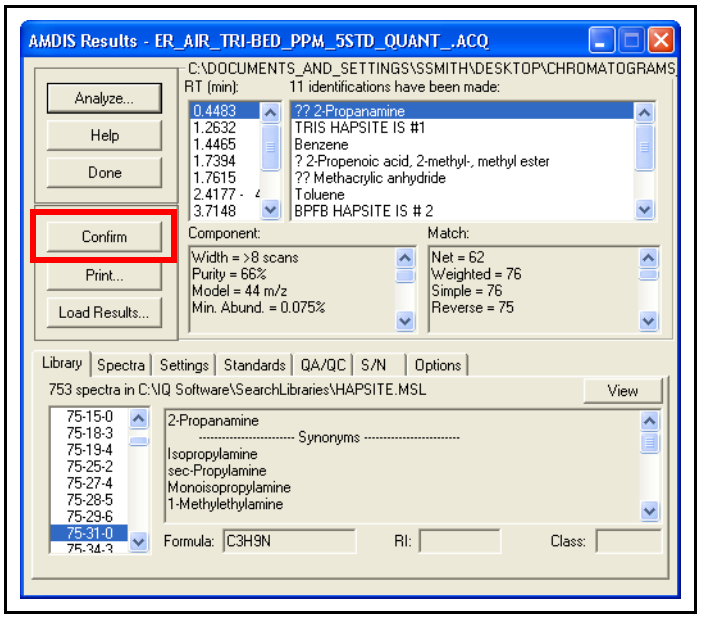


8.5.3 Confirm Screen in AMDIS

The **Confirm** function in AMDIS allows for unidentified peaks to be located by AMDIS and export them to NIST for identification. See below for instructions on using **Confirm**.

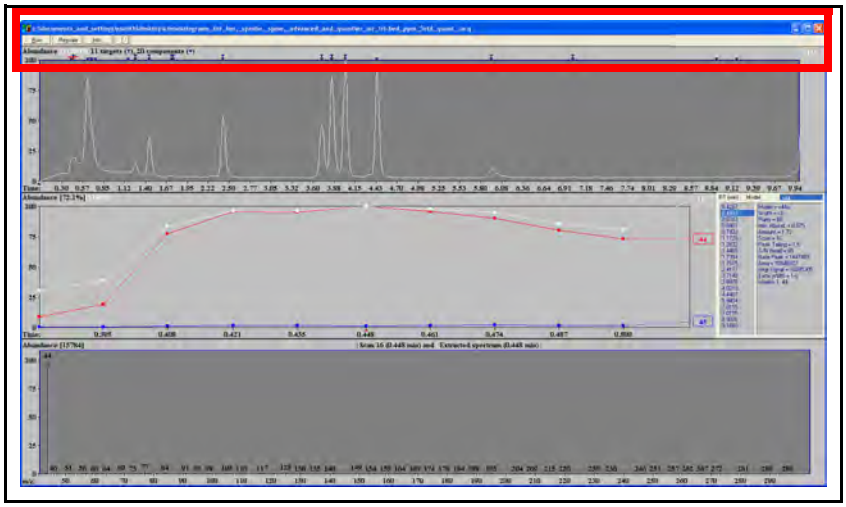
1 Click the **Confirm** button. (See Figure 8-44.)

Figure 8-44 Confirm button



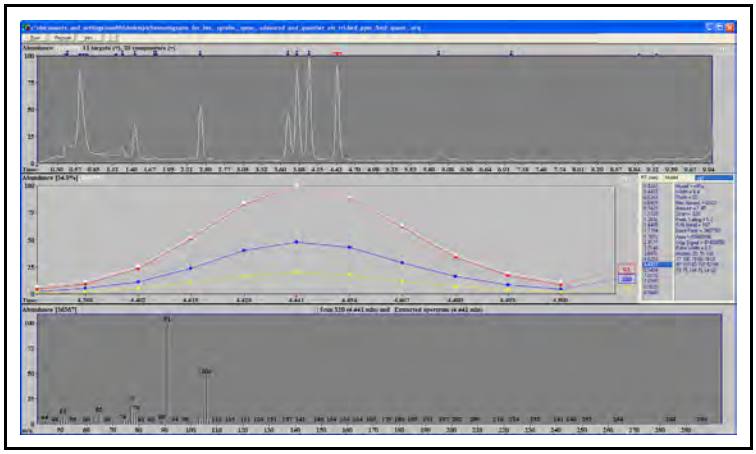
2 The **Confirm** page will be displayed. An arrow located above the peak indicates that a compound has been found. A **T** over the arrow indicates that the compound has been identified by AMDIS. (See Figure 8-45.)

Figure 8-45 Confirm page



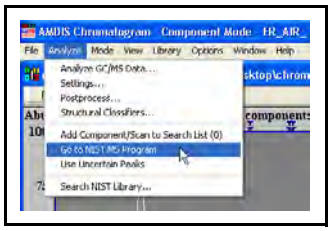
3 If a peak has not been identified, click on the arrow above it. The arrow will turn red. (See Figure 8-46.)

Figure 8-46 Arrow



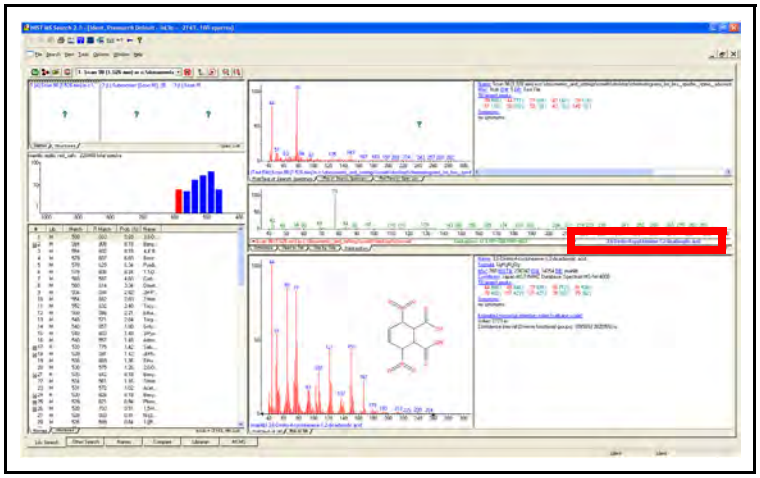
4 Click **Analyze** and click **Go to NIST MS Program**. (See Figure 8-47.)

Figure 8-47 Go To NIST MS Program



5 The spectra will be exported to NIST. NIST will identify the unknown compound. (See Figure 8-48.)

Figure 8-48 Exporting Spectra to NIST



6 Alternately, if a NIST Search is not desired, select **File** followed by **Go to Results** to return to the Results page.

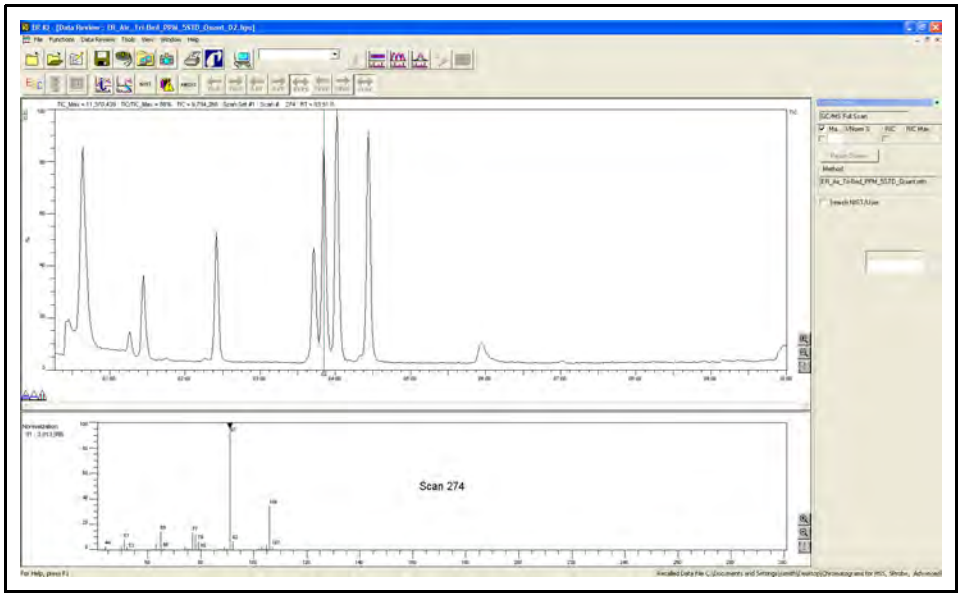
8.6 NIST Library Searches

The laptop will come pre-loaded with identification software from the National Institute of Standards and Technology's (NIST) Mass Spectral Search Program, which contains approximately 192,000 spectra. This library compares the sample spectra to the library spectra in order to determine the SI number based upon purity and fit, the ratio of the intensities of the unknown spectra to the library spectra.

1. Refer to section 8.3, Accessing the Data Review Feature, on page 8-2 to open a data file.

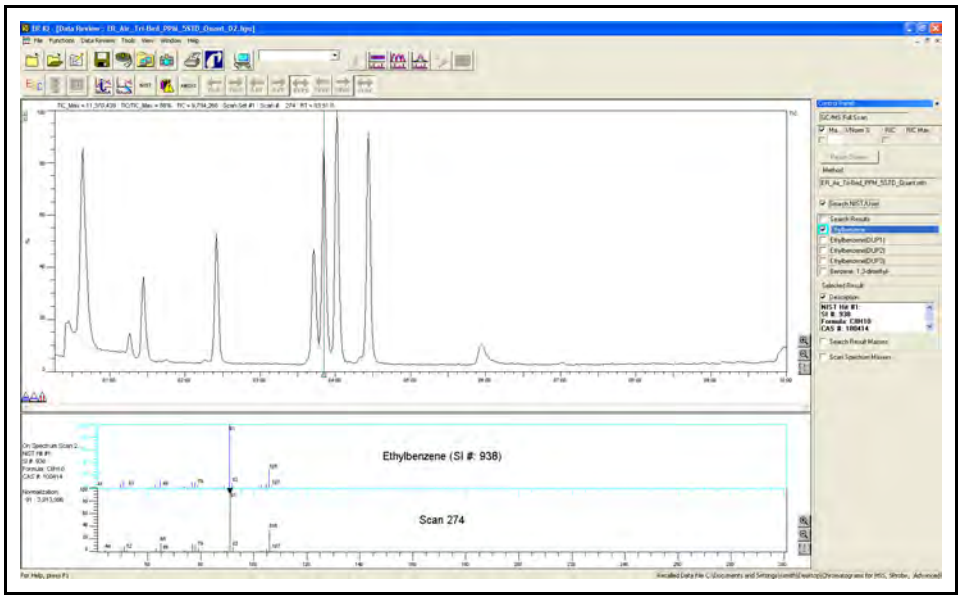
2. Double-click on the peak of interest. The green scan cursor will relocate to the peak. Use the arrow keys on the laptop to adjust the scan cursor. The optimal location of the scan cursor is at the apex of the peak. (See Figure 8-49.)

Figure 8-49 Green scan cursor



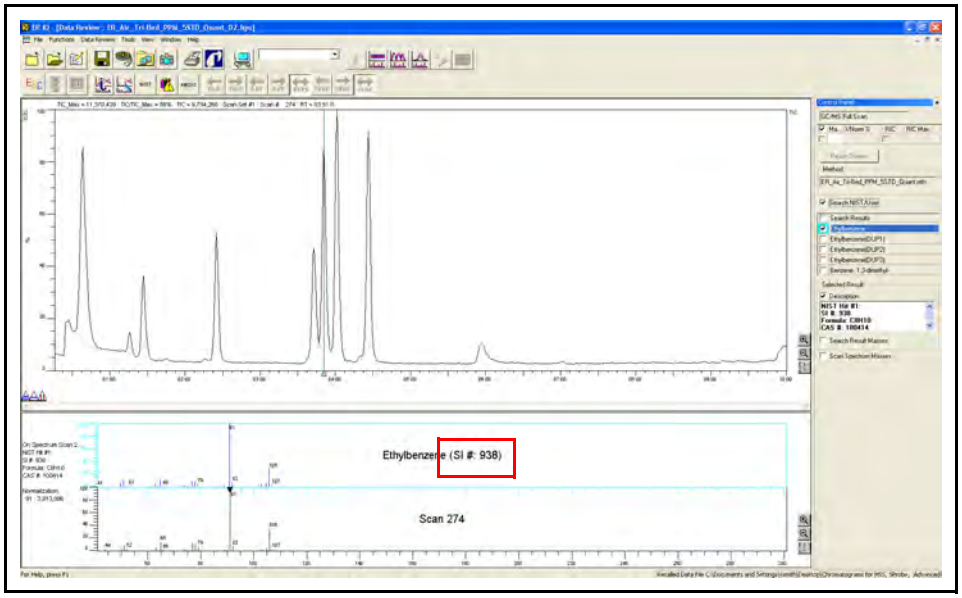
3 Check the **Search NIST/User** box in the **Control Panel**. The library identification and the library spectra will be displayed above the spectra of the sample. (See Figure 8-50.)

Figure 8-50 Search NIST/User



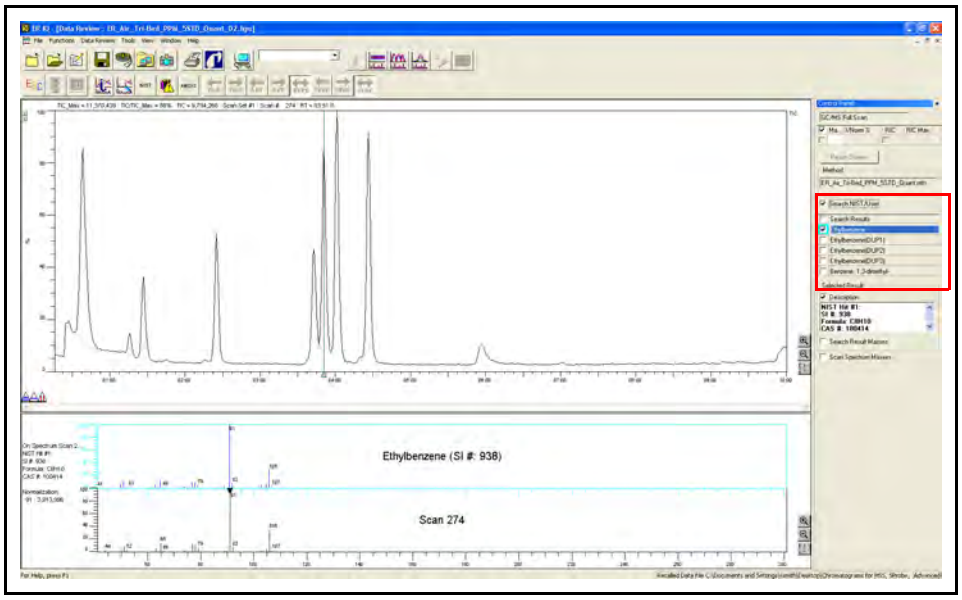
4 The **Similarity Index Number (SI #)** will be located next to the library identification. A number of 700 and above indicates a good match. A number of 800 and above indicates a very good match. A number of 900 and above is an excellent match. A match of 1000 is a perfect match. (See Figure 8-51.)

Figure 8-51 SI Number



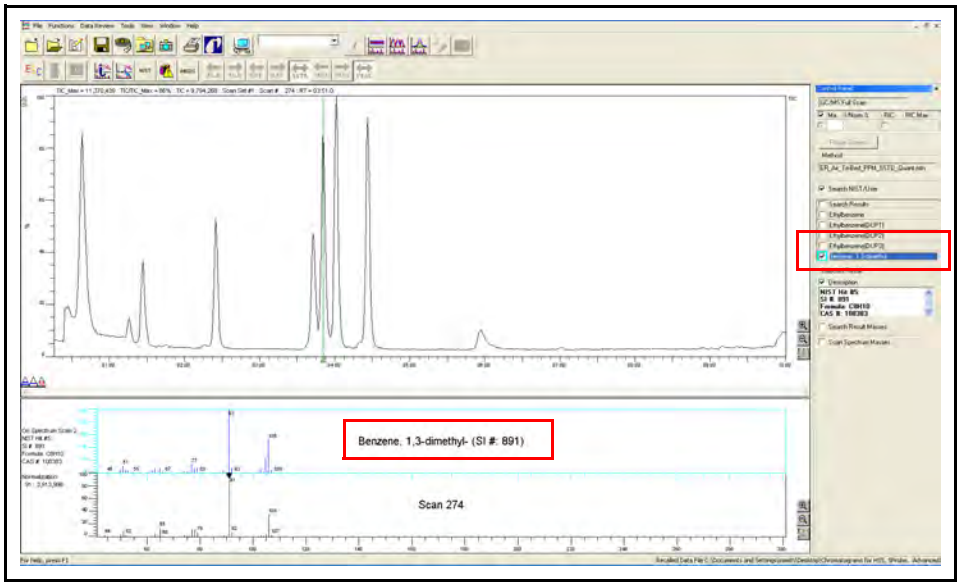
5 The **Search Results** box will show five identifications from the spectral search. The result with the highest SI number will be displayed first. If the program identifies the same compound more than once, it will display **DUP**, for duplicate, next to the name of the compound. Duplication increases the confidence in the identification. Therefore, if a compound has four duplicates and a high SI number, the confidence in the identification would be high. (See Figure 8-52.)

Figure 8-52 Duplication in NIST



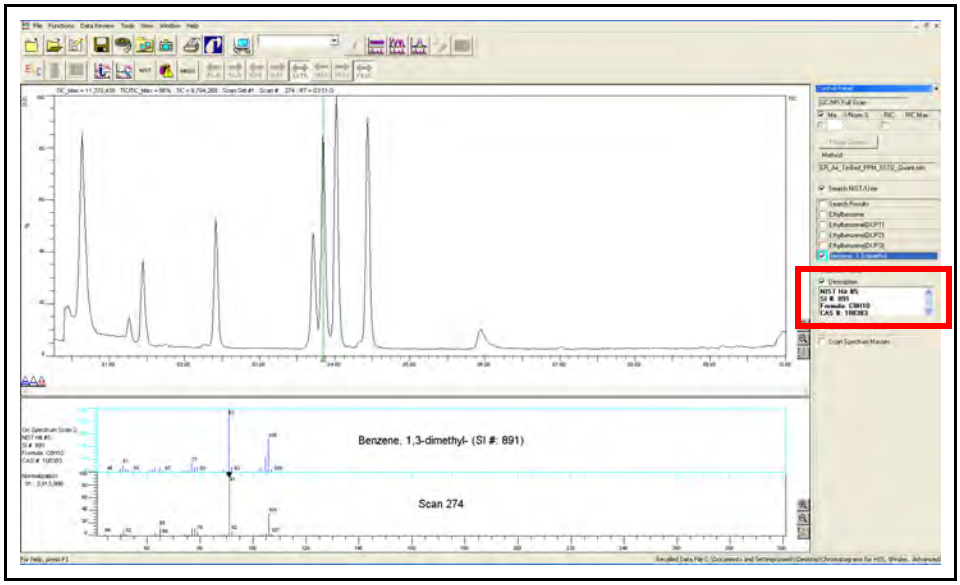
6 To view the spectra for a different library identification, highlight the name of the desired compound. (See Figure 8-53.)

Figure 8-53 Viewing different spectra



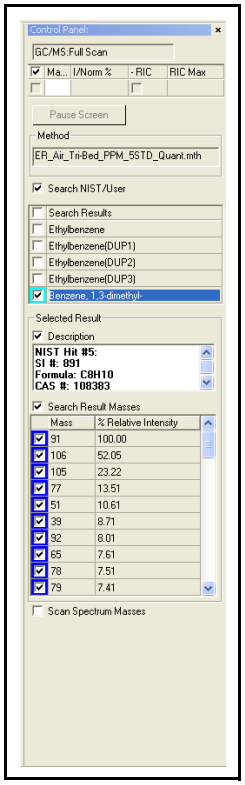
7 If the **Description** box is checked, the highlighted hit, the SI, the formula, and CAS number will be displayed. (See Figure 8-54.)

Figure 8-54 Description box



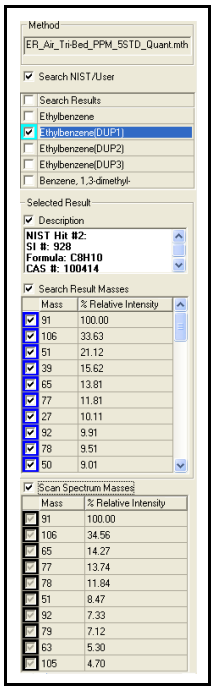
8 If the **Search Result Masses** box is checked, the masses and relative intensities for the current scan will be displayed as a table for the NIST library spectrum. (See Figure 8-55.)

Figure 8-55 Search Result Masses



9 If the **Scan Spectrum Masses** box is checked, the masses and relative intensities are displayed as a table for the unknown spectrum. (See Figure 8-56.)

Figure 8-56 Scan Spectrum Masses

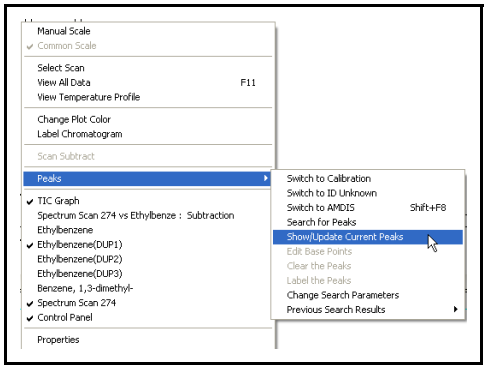


8.7 Show/Update Current Peaks

The **Show/Update Current Peaks** function will search the entire chromatogram to qualitatively identify each peak. The **Show/Update Current Peaks** function searches in the same manner as the **Search NIST/User** function. After performing the search, the software will list all of the compounds that were identified in the chromatogram.

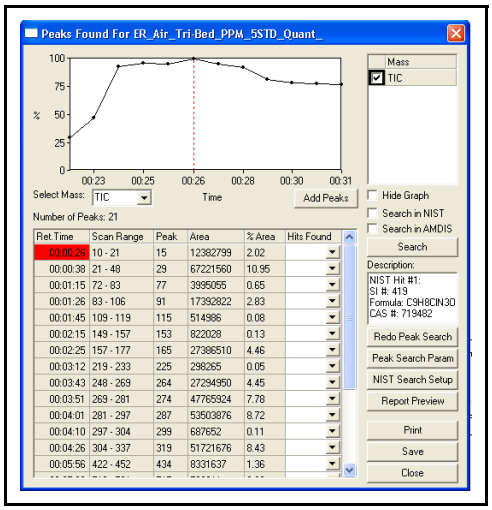
1 The **Show/Update Current Peaks** function is accessed by right-clicking on the chromatogram. Mouse over **Peaks** and click on **Show/Update Current Peaks**. (See Figure 8-57.)

Figure 8-57 Show/Update Current Peaks



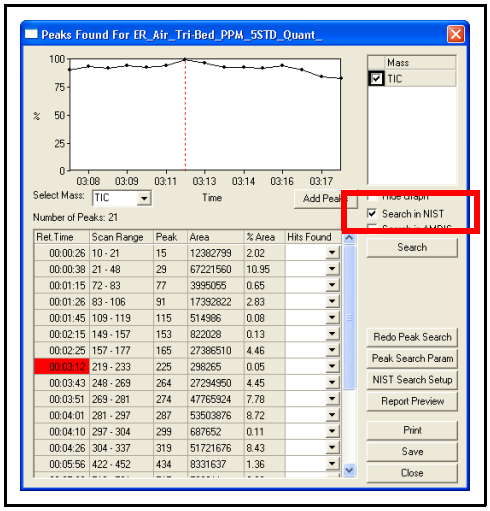
2 The **Show/Update Current Peaks** window will display. (See Figure 8-58.)

Figure 8-58 Show/Update Current Peaks



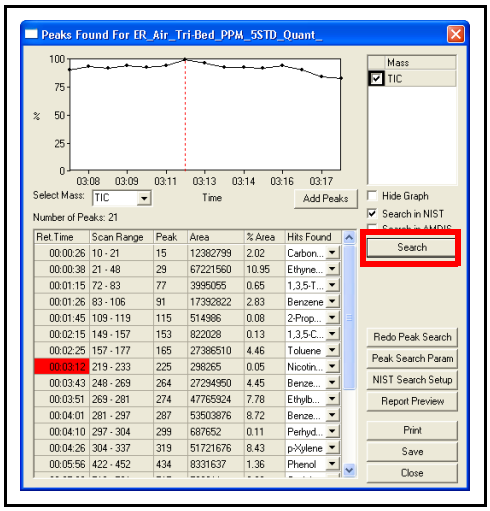
3 Check the **Search in NIST** box. (See Figure 8-59.)

Figure 8-59 Search In NIST



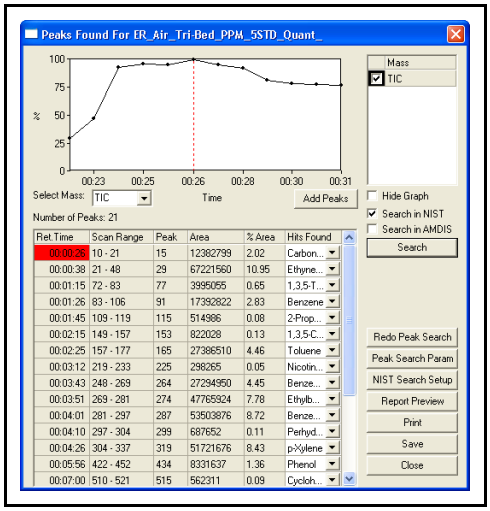
4 Click **Search**. (See Figure 8-60.)

Figure 8-60 Search



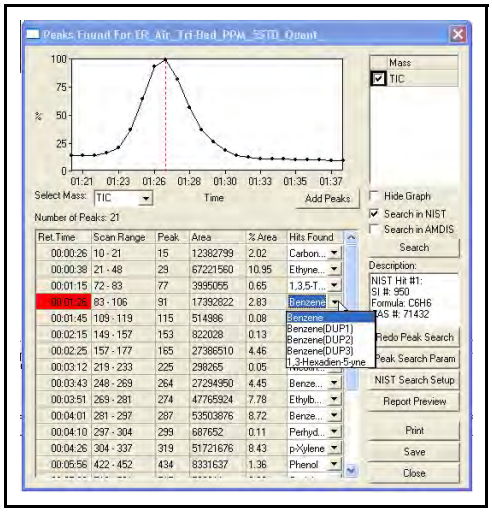
5 A NIST search will be performed on the peaks that NIST has located. The **Hits Found** column will be populated. (See Figure 8-61.)

Figure 8-61 Hits Found



6 Each identification has a drop-down menu. Five hits will be displayed in each menu. (See Figure 8-62.)

Figure 8-62 Drop-Down Menu



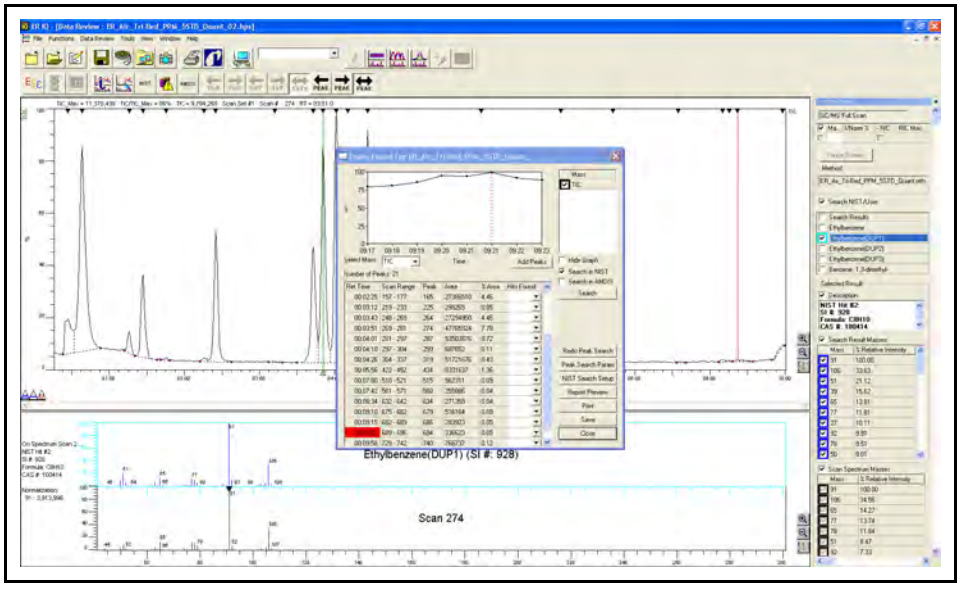
7 Check the **Search in AMDIS** box. The software will search the peaks using the AMDIS library. The AMDIS identification will be located in the drop-down menu below the NIST hits.

NOTE: This is not a true AMDIS search. AMDIS will not search the entire chromatogram. It will only search the peaks that NIST has located.

8.7.0.1 Show/Update Current Peaks Window Description

In the chromatogram beneath the **Show/Update Current Peaks** window, each detected peak will be labeled with a black triangle. Pink dots will appear at the base of each peak. These dots are used to determine the peak area. (See Figure 8-63.)

Figure 8-63 View Beneath the Window



On the **Show/Update Current Peaks** window, the highlighted peak will be displayed with the dots along the peak representing each individual scan. The following will also be displayed:

Number of Peaks . . . . . The number of peaks that have been identified by the **Show/Update Current Peaks** program.

Retention Time . . . . . The time the compound elutes from the column.

Scan Range . . . . . The range of scans that encompass the peak.

Area . . . . . The area of the peak.

Percent Area . . . . . The ratio of the TIC of the peak to the total TIC multiplied by 100.

Add Peaks . . . . . The peaks that were not automatically located by the software can be added to the **Show/Update Current Peaks** window using the **Range Tool**. See section 8.7.2, Range Tool, on page 8-42.

Hide Graph . . . . . Checking the **Hide Graph** box will remove the graph from the **Show/Update Current Peaks** window.

Redo Peak Search . . . . . The software will clear the identifications from the **Hits Found** column.

Peak Search Parameters . . . . . See section 10.10.2, Setting Up a Quantitative Search, on page 10-43 for more information.

NIST Search Setup . . . . . Allows the pathway for the NIST libraries to be set. The library pathways are set at the factory, but may need reset if the software is reloaded. See section 8.7.0.3, NIST Search Setup, on page 8-33 for instructions.

Report Preview . . . . . The information in the **Show/Update Current Peaks** is displayed in a text format. See section 8.7, Show/Update Current Peaks, on page 8-28 for instructions.

8.7.0.2 Peak Search Parameters

Some of the parameters for peak searching can be selected. These include the **Min RIC Area**, **Min TIC Area**, the **Min** and **Max Width**, the **mass range**, the **Net fit**, the NIST library used for identification and the number of identifications that are displayed by the NIST library.

Library Name . . . . . The selected library will be used to make AMDIS identifications.

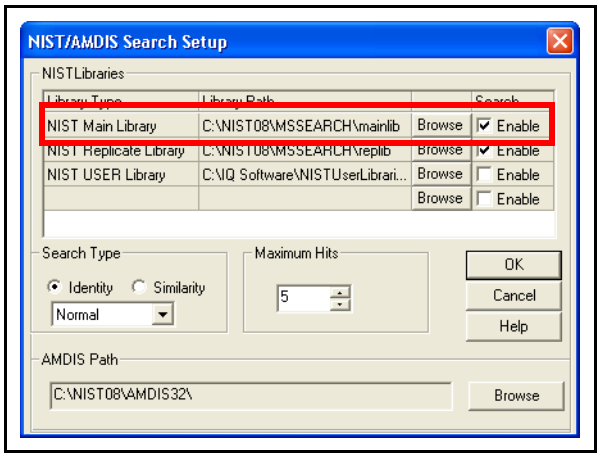
Maximum NIST Hits . . . . . NIST will display the setpoint number of identifications.

8.7.0.3 NIST Search Setup

If NIST is reloaded onto the laptop, the library pathway may need to be reset.

If the libraries have properly loaded, the pathways will be set to folders displayed in Figure 8-64.

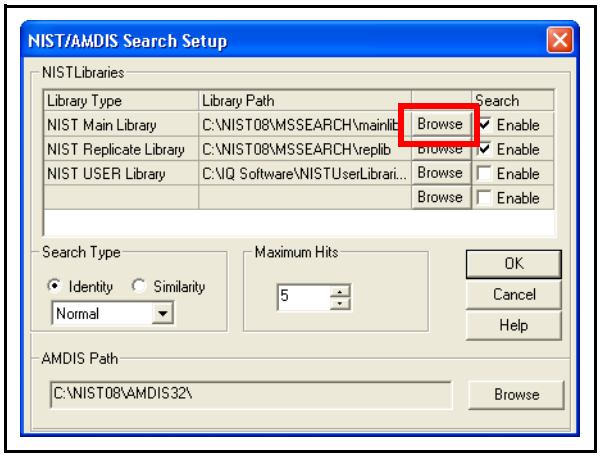
Figure 8-64 NIST Main Library



To reset the **NIST Main Library**:

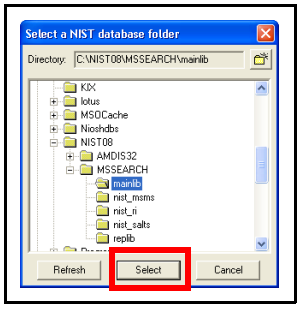
1 Click **Browse...**. (See Figure 8-65.)

Figure 8-65 Browse...



2 Select the **NIST Main Library** from the folder displayed. Click **Select** to set the library. (See Figure 8-66.)

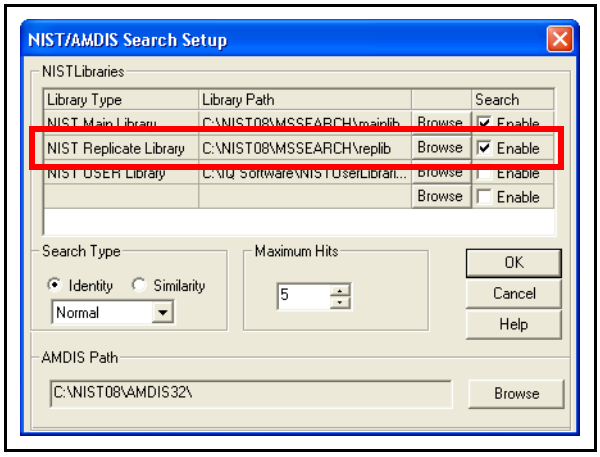
Figure 8-66 NIST Main Library



To reset the **NIST Replicate Library**:

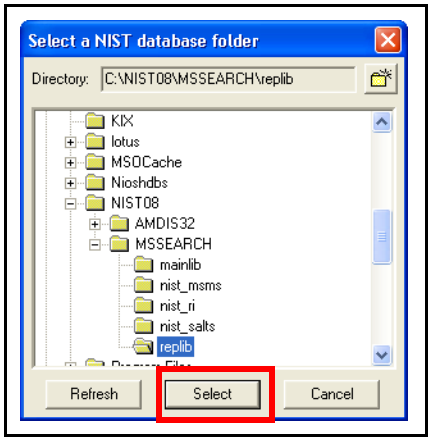
1 Click **Browse...**. (See Figure 8-67.)

Figure 8-67 Browse...



2 Select the **NIST Replicate Library** from the folder displayed. Click **Select** to set the library. (See Figure 8-68.)

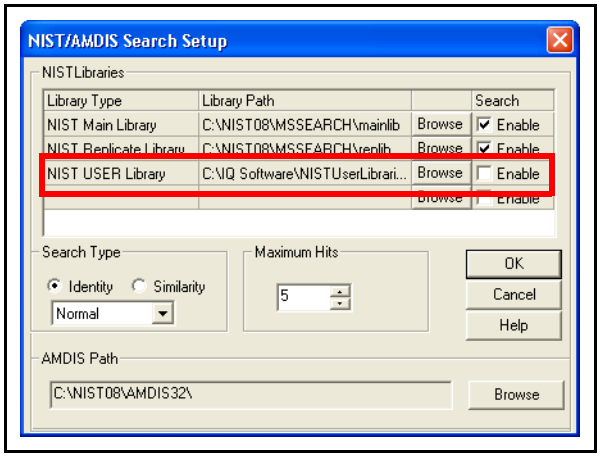
Figure 8-68 NIST Replicate Library



To reset the **NIST USER Library**:

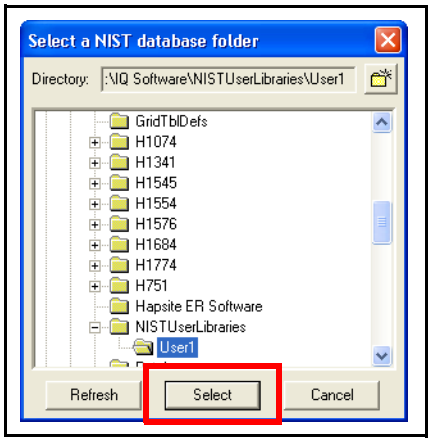
1 Click **Browse...**. (See Figure 8-69.)

Figure 8-69 NIST USER Library



2 Select the **NIST USER Library** from the folder displayed. Click **Select** to set the library. (See Figure 8-70.)

Figure 8-70 NIST USER Library

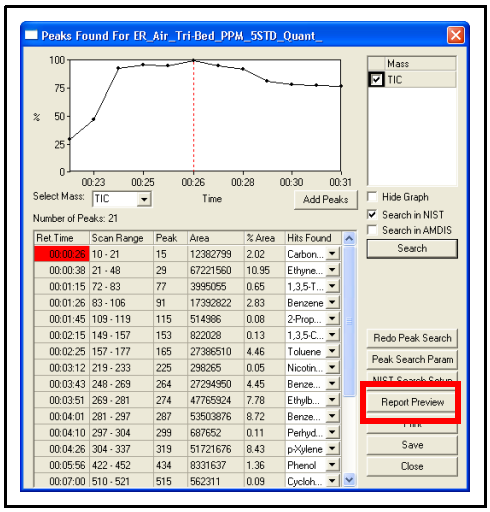


8.7.0.4 Report Preview

Report Preview will reformat the **Show/Update Current Peaks** window into a text file.

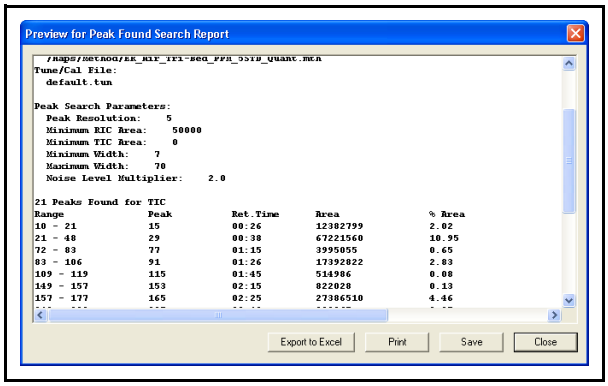
1 To view the report, click the **Report Preview** button. (See Figure 8-71.)

Figure 8-71 Report Preview



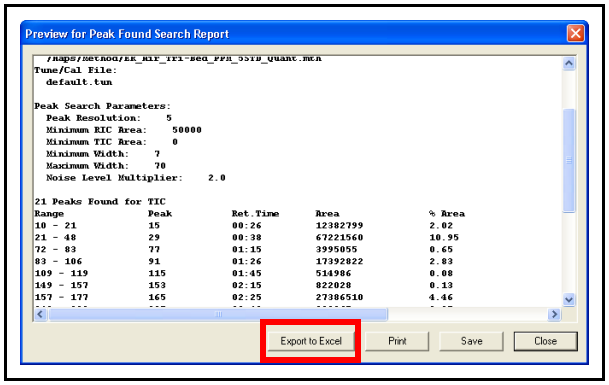
2 The report will be displayed. (See Figure 8-72.)

Figure 8-72 Displaying Report



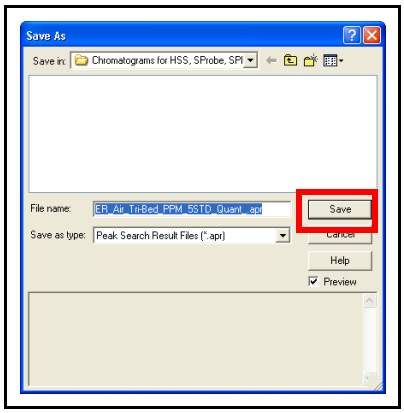
3 The report can exported to Excel for further data analysis. Click **Export to Excel**. (See Figure 8-73.)

Figure 8-73 Export to Excel



4 The report will need to be saved before Excel will open. Click **Save**. (See Figure 8-74.)

Figure 8-74 Saving Report



5 The report will open in Excel. (See Figure 8-75 and Figure 8-76.)

Figure 8-75 Opening Report

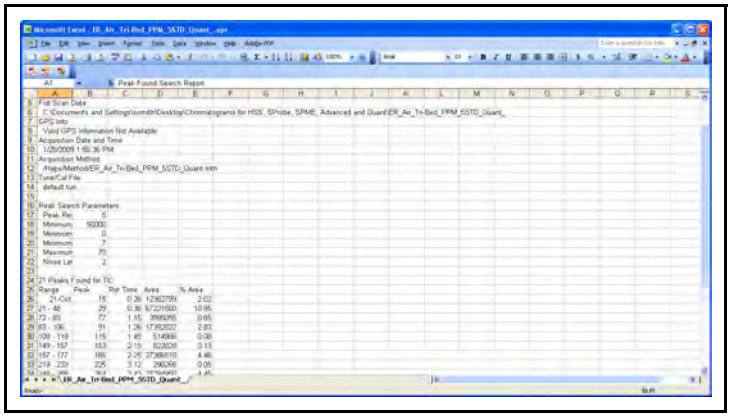
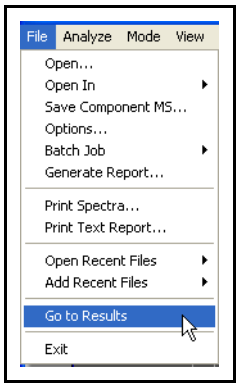


Figure 8-76 File Menu

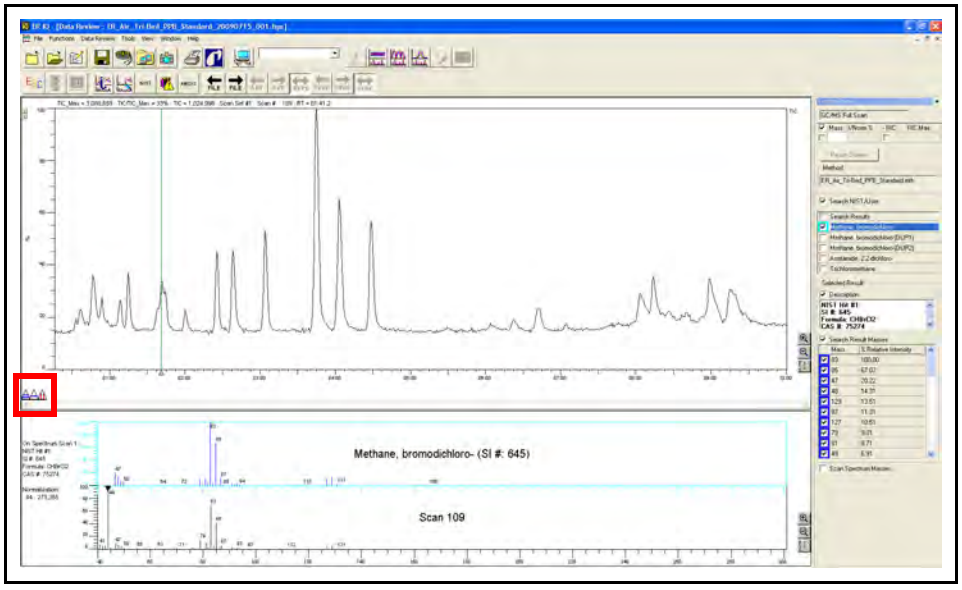


8.7.1 Background Subtract

Background Subtract will remove masses in the spectrum that are caused by background interference. Using **Background Subtract** will increase the SI number of the identification when the low SI number is a result of high background. Follow the instructions below to perform a **Background Subtract**.

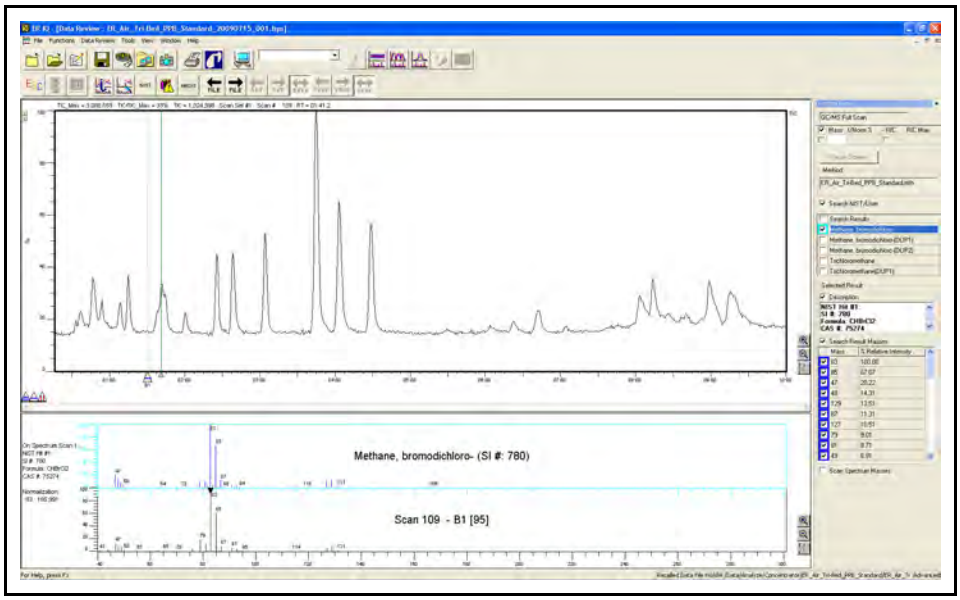
1. Perform a **NIST Library Search** by checking the **Search NIST/User** box in the **Control Panel**.
2. If the SI number is low and the background is high, select the blue **Background Subtract** triangle from the lower left side of the chromatogram. (See Figure 8-77.)

Figure 8-77 Background Subtract Triangle



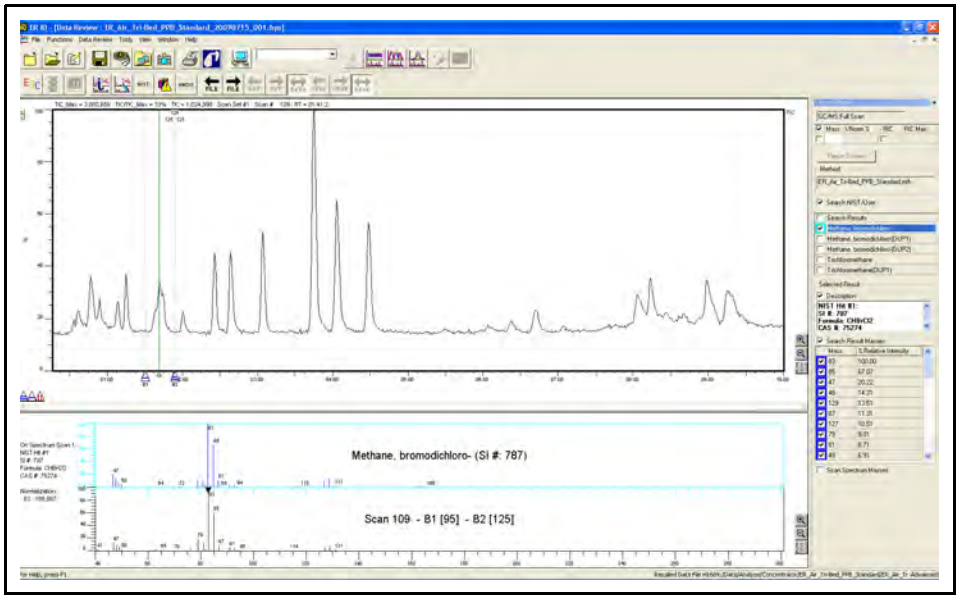
3 Drag to an area that is representative of the background on either side of the selected peak. The background masses at this location are automatically subtracted from the peak. (See Figure 8-78.)

Figure 8-78 Placing the Subtract Triangle



4 If the background on the opposite side of the peak differs from the subtracted background, a second background subtract can be used. (See Figure 8-79.)

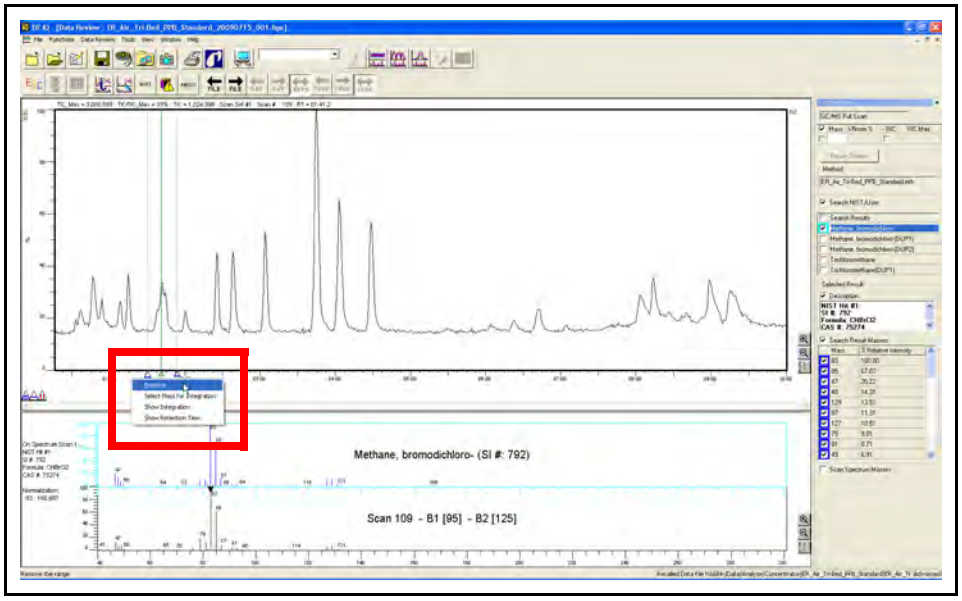
Figure 8-79 Second Background Subtract



NOTE: All background subtractions are indicated in the **Spectrum** window by the designation **Scan Number - B1(range) - B2(range)**.

5 To remove **Background Subtract** from the chromatogram, place the cursor over the **Background Subtract** triangle, right-click and select **Remove**. (See Figure 8-80.)

Figure 8-80 Removing Background Subtract

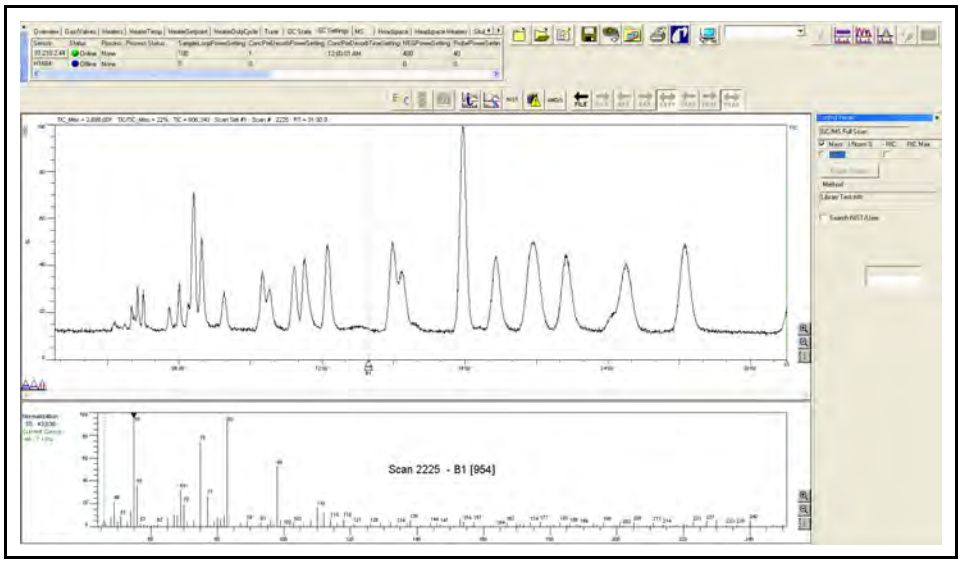


8.7.1.1 Background Subtraction Using a Range of Points

Background from a range of points can be subtracted if desired.

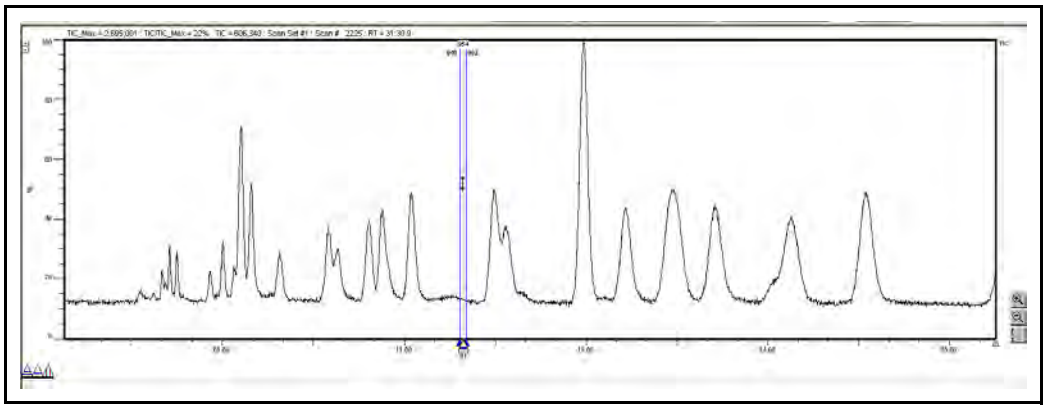
1 Place the **Background Subtract** triangle at the apex of the small peak. (See Figure 8-81.)

Figure 8-81 Placing the Background Subtract Triangle



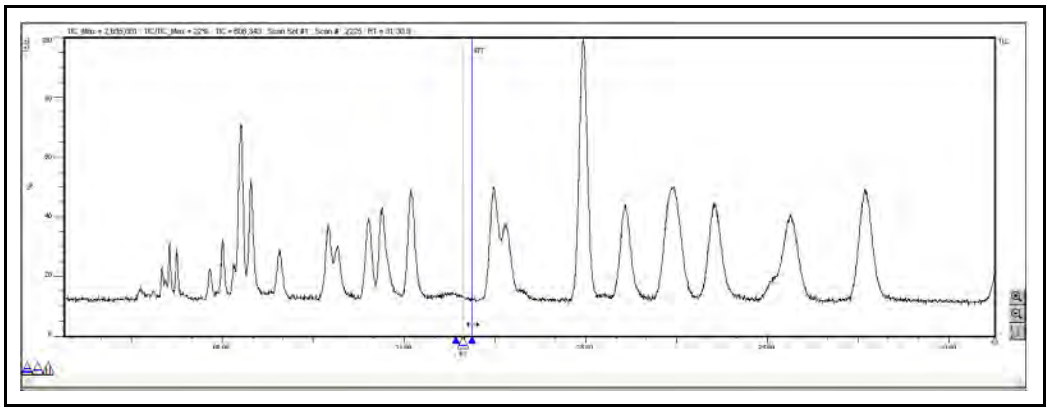
2 Mouse over the gray line located above the **Background Subtract** triangle. The cursor will change to a vertical double headed arrow. Left-clicking and holding, while moving the double headed arrow upwards, widens the background range. Moving the arrow downwards, narrows the range of the background. The width of the range is represented by two small, blue triangles. (See Figure 8-82.)

Figure 8-82 Adjusting the Range



3 The left and right side boundaries can be manually adjusted by clicking on the smaller blue triangle and dragging it to the desired location. (See Figure 8-83.)

Figure 8-83 Adjusting the Smaller, Blue Triangles

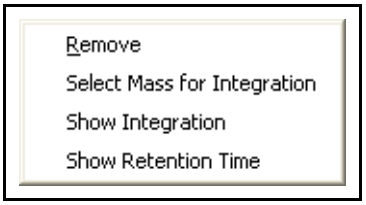


NOTE: This procedure can be repeated by using the second **Background Subtract** triangle.

8.7.1.2 Additional Features of the Background Tool

By placing the mouse over a **Background Subtract** triangle and right-clicking, see Figure 8-84, the following menu will be displayed:

Figure 8-84 Background Subtract Menu



Remove . . . . . Removes the **Background Subtract** triangle.

Select Mass for Integration . . . . . Selects either the TIC or a mass fragment for integration.

Show Integration . . . . . Displays the integration on the x-axis.

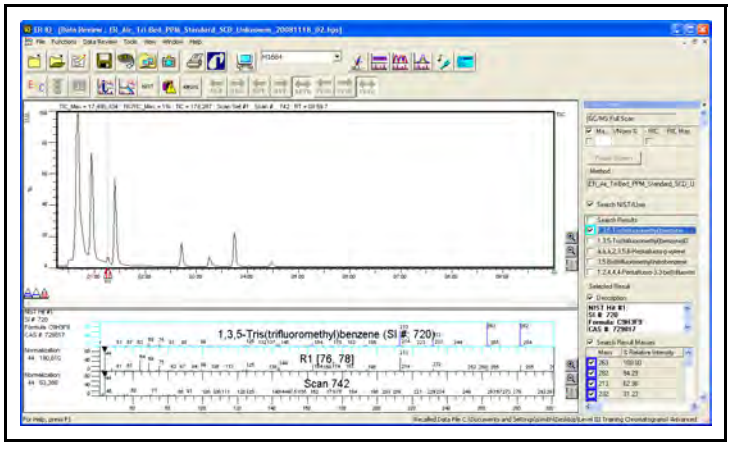
Show Retention Time . . . . . Displays the retention time on the x-axis.

8.7.2 Range Tool

The Range Tool is a red-striped triangle located at the bottom left side of the chromatogram. It is used to average spectra over a “range” of scans across a given peak, especially when the analytes are low in concentration. It can also be used to select a section of a peak or reintegrate peaks. The SI numbers for the selected compound will increase when using the **Range Tool**. Follow the instructions below to use the **Range Tool**.

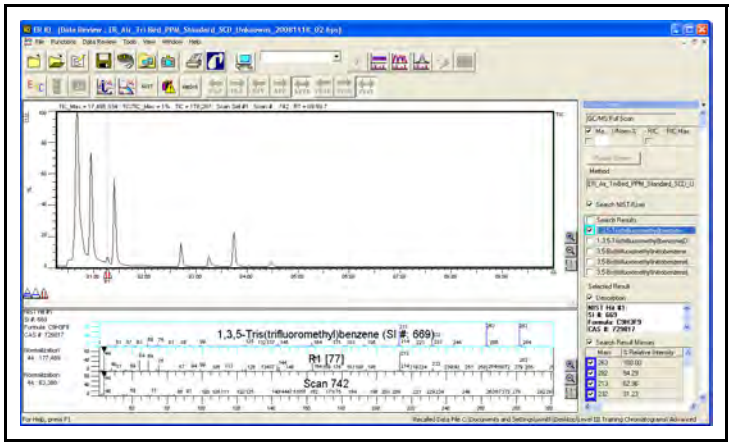
1 Place cursor on the red-striped triangle, which is the **Range Tool**. Left-click, hold and drag the triangle to the location where the scans should be averaged. (See Figure 8-85.)

Figure 8-85 Range Tool



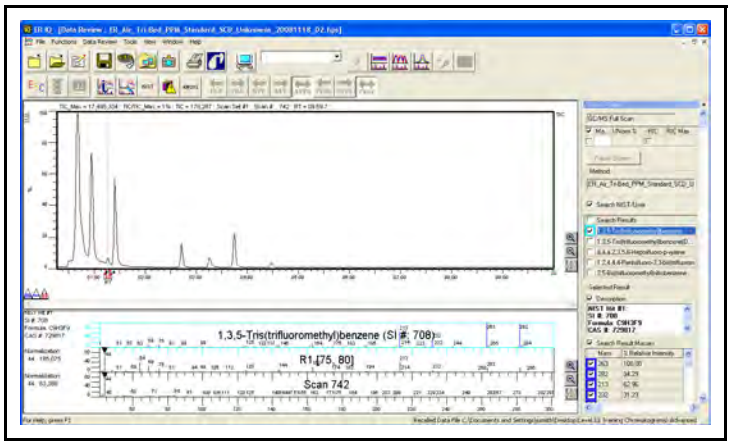
2 Move the cursor to the tip of the **Range Tool** triangle. The cursor will change to a vertical double-headed arrow. Left-click, hold and move the double-headed arrow upwards to widen a range. Moving the arrow downwards narrows the range. The red range lines should intersect the peak sides at 50% of their height. (See Figure 8-86.)

Figure 8-86 Adjusting the Range



3 The left and right side boundaries can be manually adjusted by clicking on the smaller red triangle and dragging it to the desired location. (See Figure 8-87.)

Figure 8-87 Adjusting the Smaller, Red Triangles

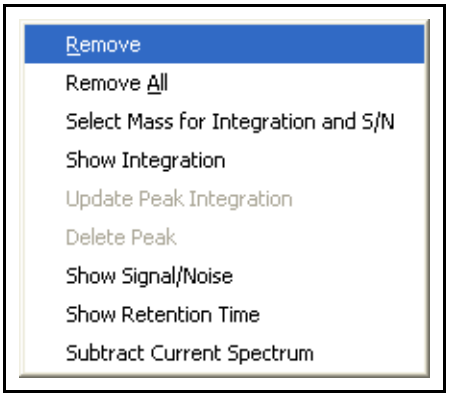


NOTE: All ranges are indicated in the spectrum window by the designation: R1 [Range Start Scan, Range End Scan].

8.7.2.1 Additional Features of the Range Tool

By placing the mouse over the **Range Tool** triangle and right-clicking, the following menu will be displayed. (See Figure 8-88.)

Figure 8-88 Range Tool Menu



Remove . . . . . Removes the range cursor.

Select Mass for Integration . . . . . Selects the TIC or a specific mass fragment for reintegration.

Show Integration . . . . . Displays the integration on the x-axis.

Show Retention Time . . . . . Displays the retention time on the x-axis.

Show Signal/Noise . . . . . Shows **Signal to Noise** ratio. A background must be selected using **Background Subtract** first. Refer to section 8.7.1, Background Subtract, on page 8-38.

Subtract Current Spectrum . . . . . Subtracts the spectrum at the point where the green scan cursor is located from the range.

8.8 Displaying Reconstructed Ion Chromatograms (RIC)

RIC plots are used to locate specific compounds in a chromatogram. A RIC plot of the top three or more mass fragments can help locate the peak of interest. Follow the instructions below to create a RIC plot.

NOTE: The NIST program uses the term peak instead of mass fragment. However, the terms are synonymous.

Alternately, double-clicking on a mass in the **Scan** window will automatically insert the selected mass in the **Control Panel** table and display the RIC for the selected mass.

When the box in the **Control Panel** labeled **-RIC** is checked, the TIC/RIC window will display the TIC minus the RIC selected.

1 Either from the **System Setup** screen or the **Data Review** screen, double-click on the **NIST** icon. (See Figure 8-89.)

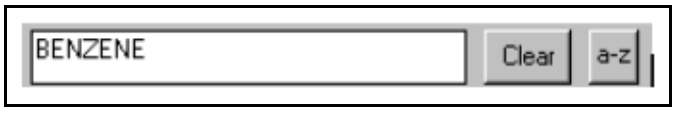
Figure 8-89 NIST icon

2 Click on the **Names** tab at the bottom of the NIST screen. (See Figure 8-90.)

Figure 8-90 NIST Names tab

3 Enter the name of the compound in the box on the top left of the screen. (i.e., benzene). (See Figure 8-91.)

Figure 8-91 NIST Name Entry



4 In the bottom right box, the **10 Largest Peaks** will be listed. Make a note of the three largest mass peaks that are between 45-300 amu.

NOTE: Peaks are listed in order from the largest to the smallest. For example, benzene's three largest peaks are masses 78, 77 and 51. (See Figure 8-92 and Figure 8-93.)

Figure 8-92 Location of Box

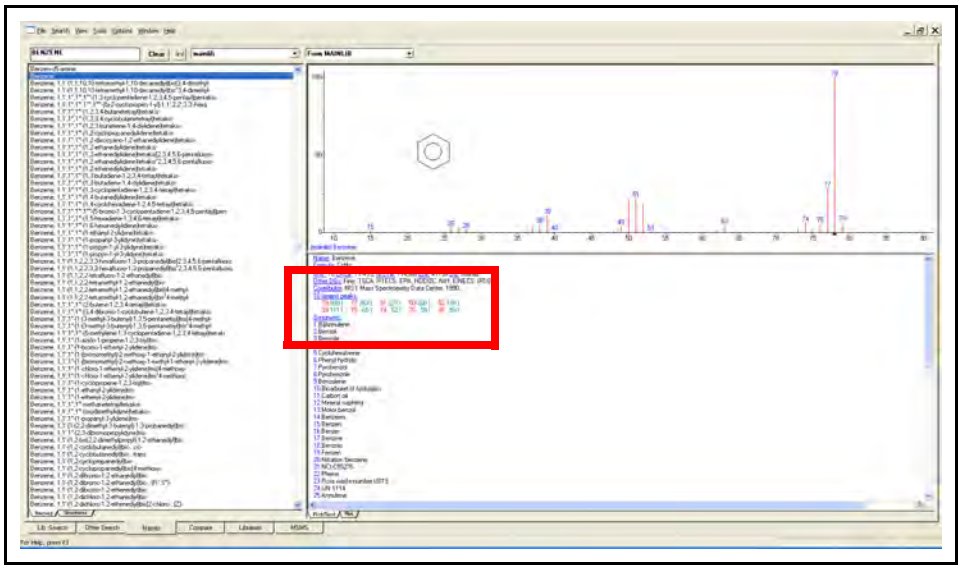
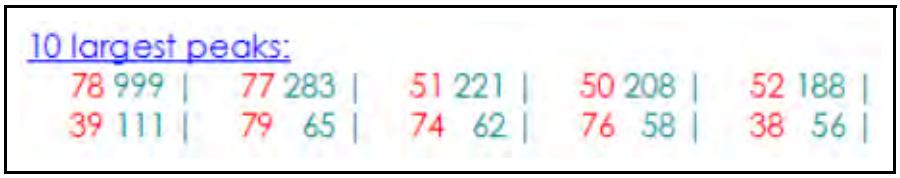


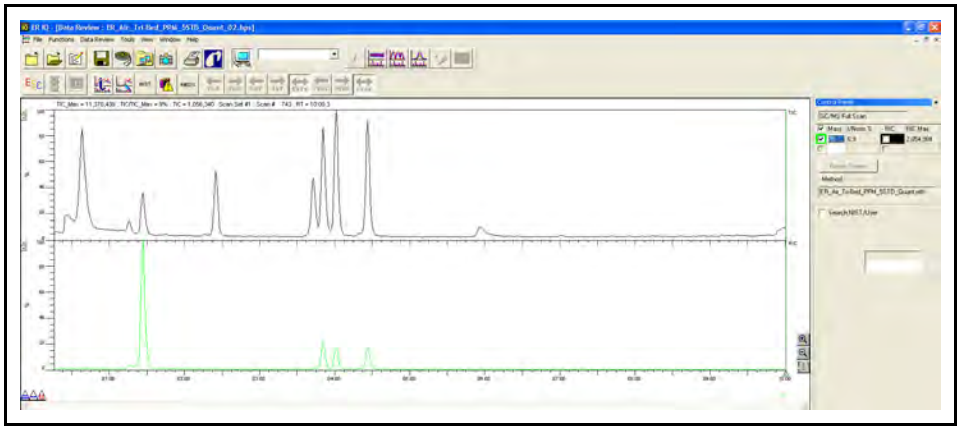
Figure 8-93 Top 10 Masses



5 Minimize the NIST window and return to the **Data Review** screen displaying the chromatogram.

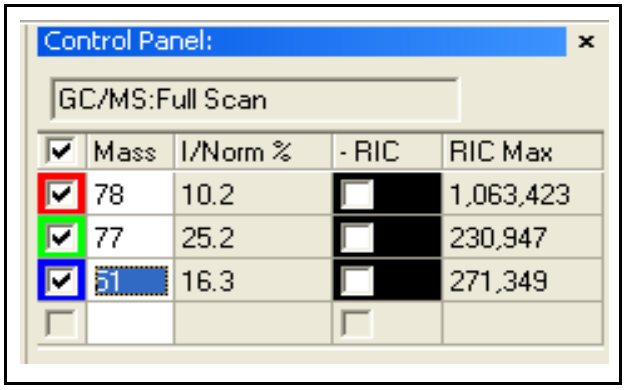
6 Enter the largest peak, 78 for benzene, into the **Control Panel** underneath the **Mass** column. Press **Enter**. The RIC plot will be displayed underneath the TIC window. A new row will be created in the **Control Panel** for entering additional peaks. (See Figure 8-94.)

Figure 8-94 Creating a RIC Plot



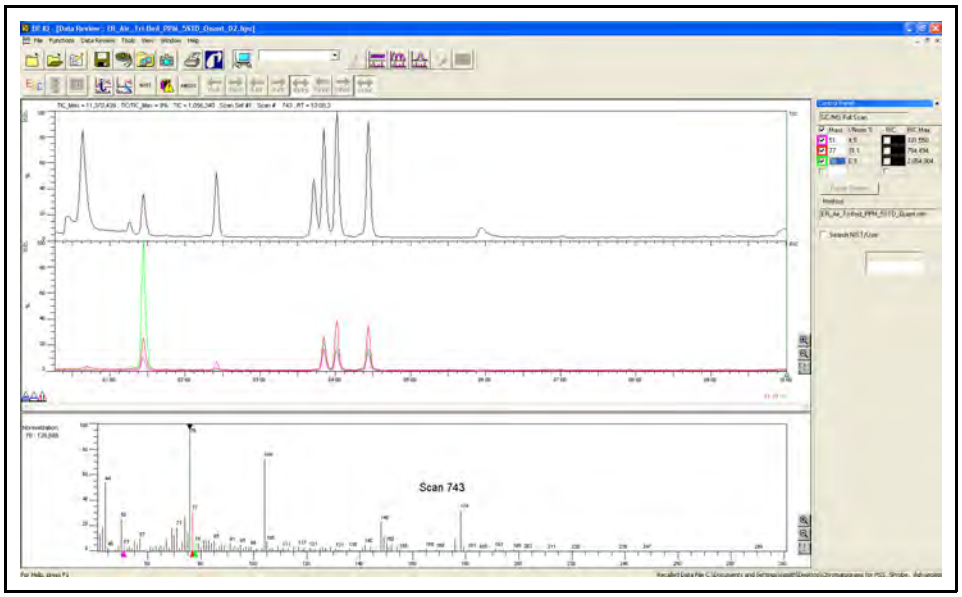
7 Enter the two or more remaining peaks into the **Control Panel**. (See Figure 8-95.)

Figure 8-95 Entering Masses in the Control Panel



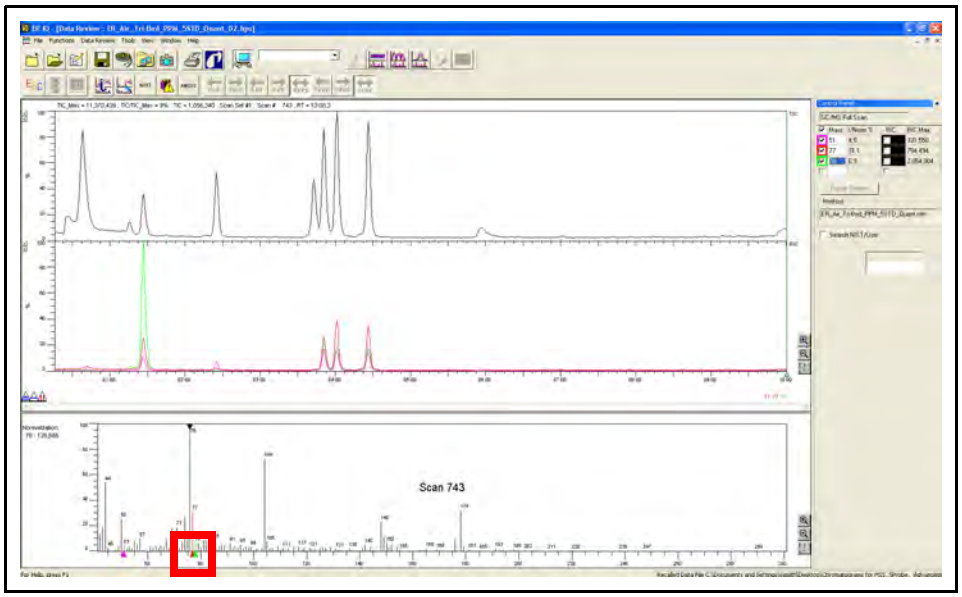
NOTE: This RIC window can be closed by unchecking the masses selected in the **Control Panel**. (See Figure 8-96.)

Figure 8-96 RIC Plot for Benzene



8 Alternately, click on the desired mass fragments in the **Spectrum** window to create a RIC plot. (See Figure 8-97.)

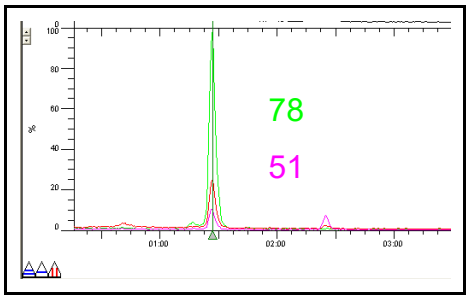
Figure 8-97 Clicking on Mass Fragment



9 The compound may be present in the unknown sample if all three peaks (mass fragments) align in the RIC plot. Use the **Search NIST/User** program to confirm identification of the suspected compound. (See Figure 8-98.)

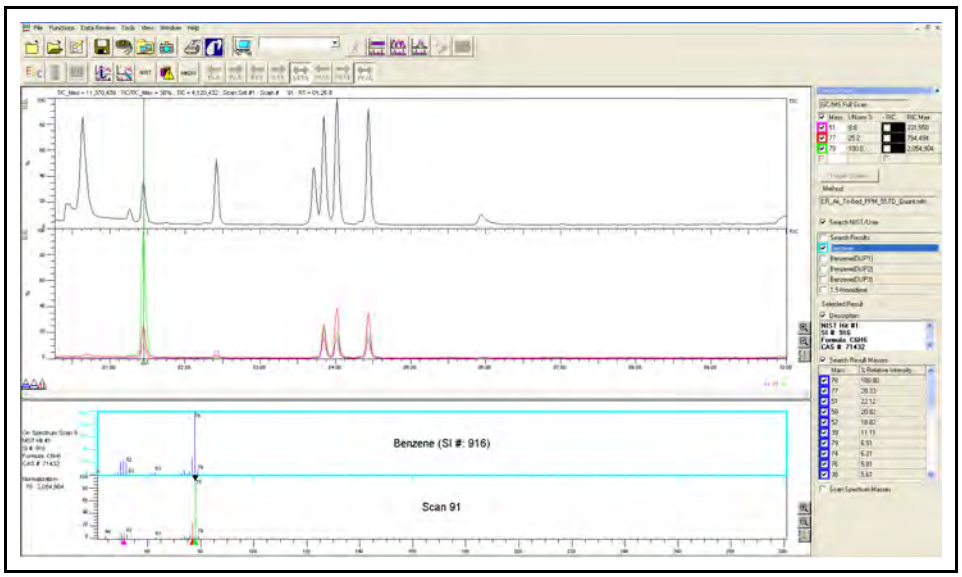
NOTE: In this example, the largest peak (mass fragment) is 78, which is displayed in green. This will be the highest RIC plot peak. The smallest peak was 51, which is displayed in pink. This will be the lowest RIC plot peak.

Figure 8-98 RIC Plot Heights



NOTE: There may or may not be a peak present in the TIC window. (See Figure 8-99.)

Figure 8-99 RIC Plot to Locate Benzene



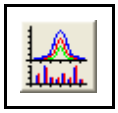
10 The compound was not detected in the sample if all three peaks (mass fragments) are not present or do not align in the RIC plot.

8.9 Chromatogram Overlay

In order to compare multiple chromatograms, **Chromatogram Overlay** allows chromatograms to be superimposed in the same window. Follow the instructions below to overlay chromatograms.

1 Click on the **Chromatogram Overlay** icon. (See Figure 8-100.)

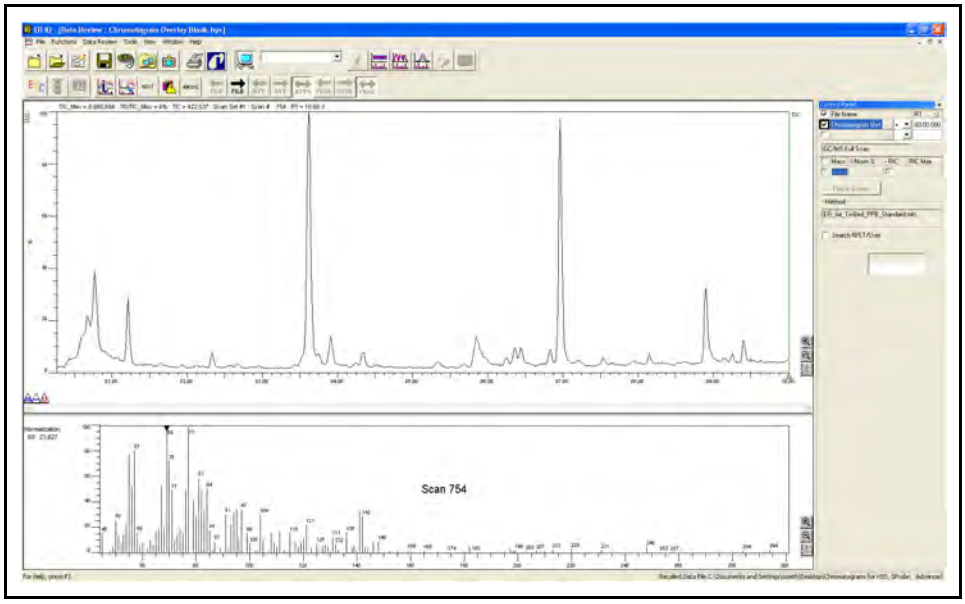
Figure 8-100 Chromatogram Overlay Icon



2 Follow the **Data Review** icon instructions in order to locate the desired file. Refer to section 8.1 on page 8-1.

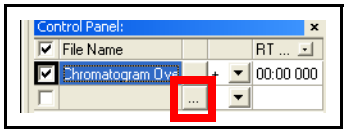
3 The data file will be displayed in the **Control Panel**. (See Figure 8-101.)

Figure 8-101 Displaying the File in the Control Panel



4 Click the icon displayed below in the row below the data file. (See Figure 8-102.)

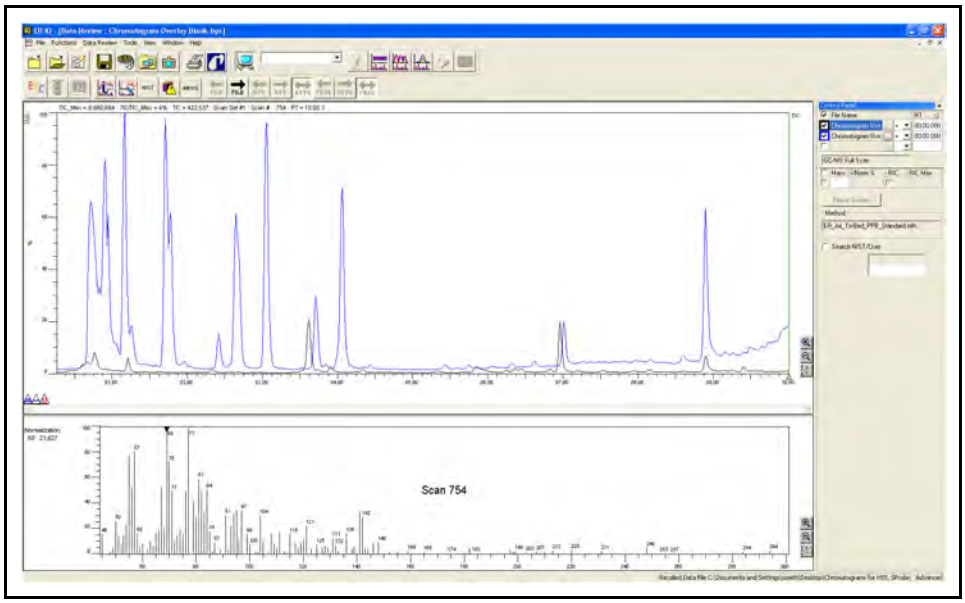
Figure 8-102 Adding the Second File



5 Follow the file selection procedure that was used in Step 2.

6 Both chromatograms will be displayed in the chromatogram window. The color displayed in the check box correlates with the color of the chromatogram. (See Figure 8-103.)

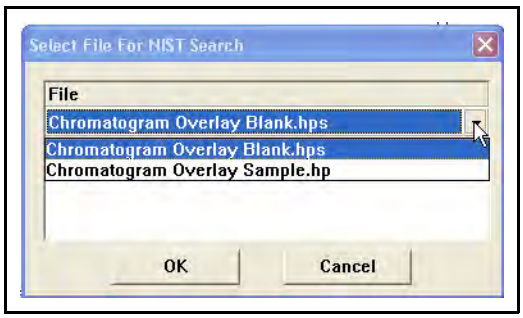
Figure 8-103 Displaying Chromatograms



NOTE: The mass spectrum will be displayed for the highlighted file.

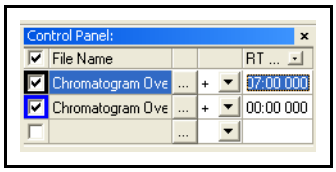
NOTE: A NIST search can be performed on either chromatogram. Select **Search NIST/User** (refer to section 8.6, NIST Library Searches, on page 8-24 for instructions) and select the desired file from the drop-down menu. (See Figure 8-104.) The NIST identification will be displayed for the highlighted file.

Figure 8-104 NIST Search



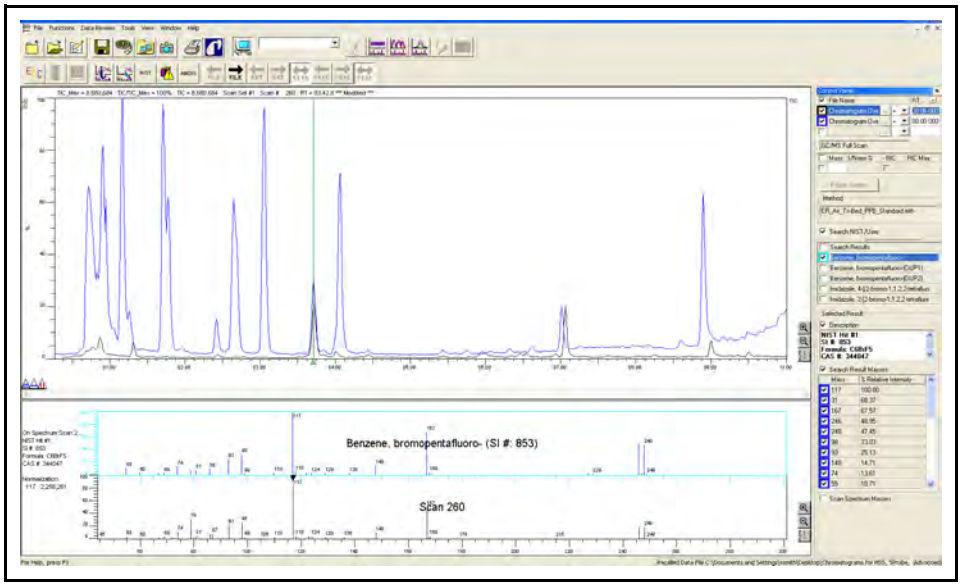
7 Peaks can be aligned by retention time for further comparison. Determine the time difference between the peaks being compared. The chromatogram will be shifted the desired amount of time by selecting **+** or **-** and typing in the time difference. (See Figure 8-105.)

Figure 8-105 Aligning the Chromatogram



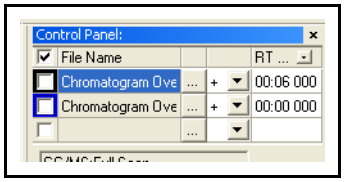
8 Press **Enter**. The chromatogram will shift by the time selected. (See Figure 8-106.)

Figure 8-106 Shifting the Chromatogram



9 To close the **Chromatogram Overlay** feature, uncheck the box located to the left of the data file's name. (See Figure 8-107.)

Figure 8-107 Closing Chromatogram Overlay

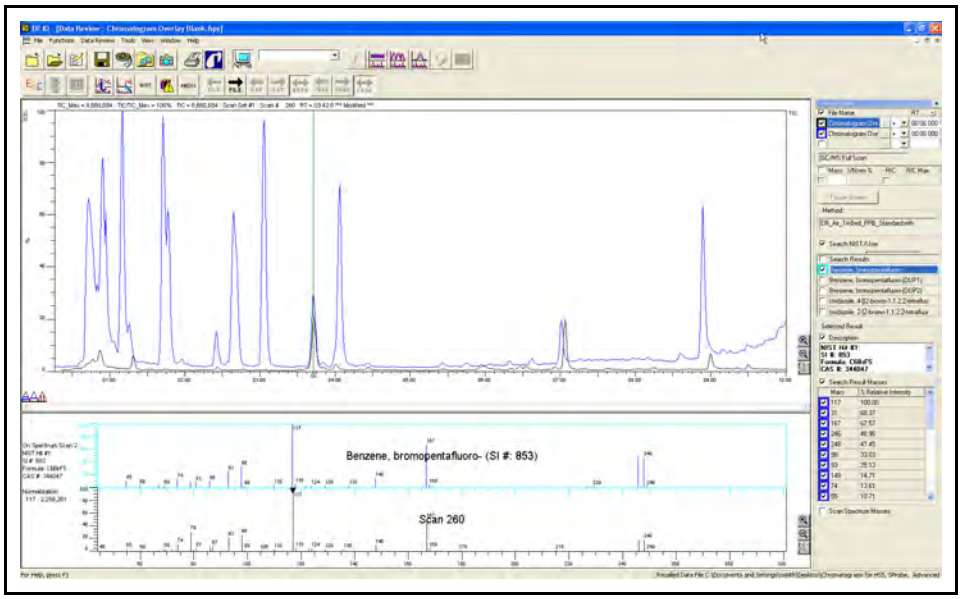


8.10 Chromatogram Subtract

This feature will subtract the TIC from one chromatogram from the TIC of another chromatogram. This is generally used to subtract the blank from the sample and verify the presence of a compound of concern.

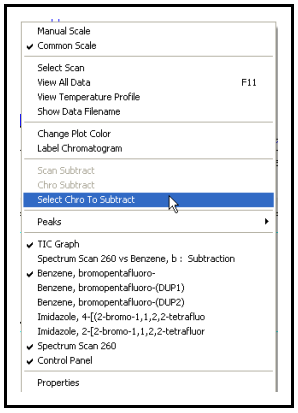
1. Overlay the desired chromatograms by using **Chromatogram Overlay**. Refer to section 8.9, Chromatogram Overlay, on page 8-49.
2. Select the peak for the desired compound. Record the TIC. (See Figure 8-108.)

Figure 8-108 Selecting the Peak



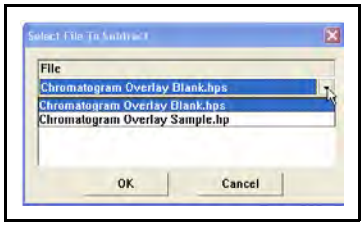
3. Right-click on the chromatogram. Click **Select Chro to Subtract**. (See Figure 8-109.)

Figure 8-109 Select Chro to Subtract



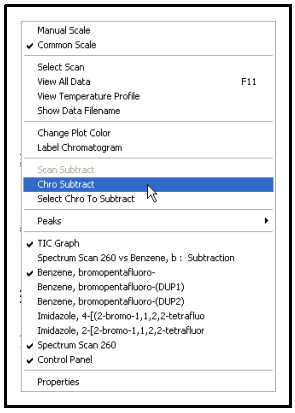
4 Select the desired file for subtraction from the drop-down menu. This will generally be the file for the blank. (See Figure 8-110.)

Figure 8-110 Selecting the Desired File



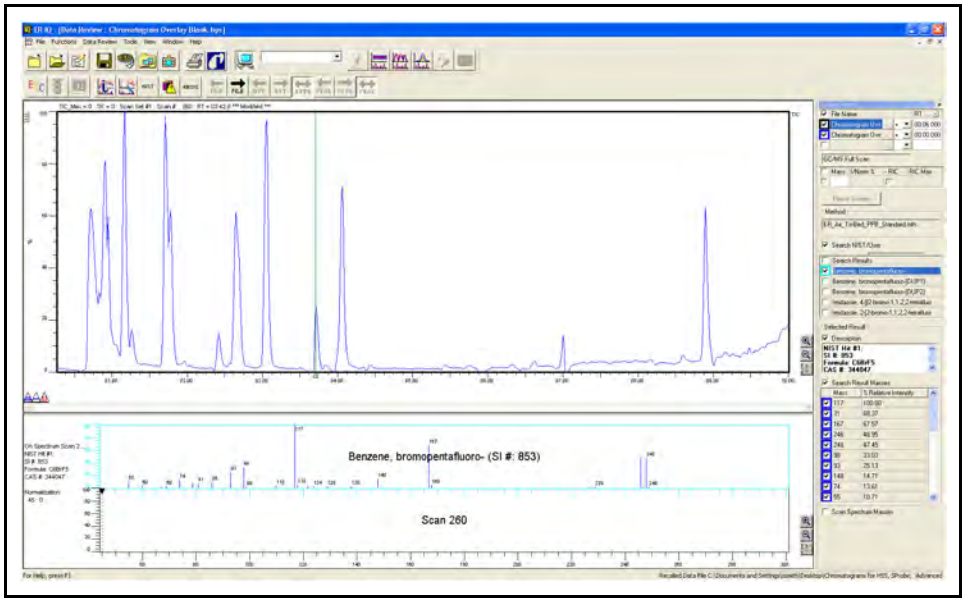
5 Right-click on the chromatogram. Right-click on the chromatogram. Click **Select Chro to Subtract**. (See Figure 8-111.)

Figure 8-111 Select Chro to Subtract



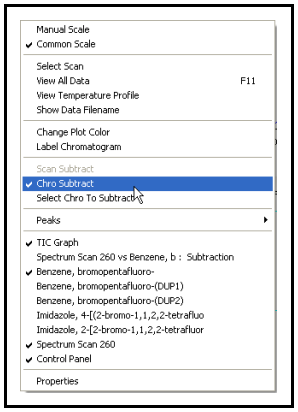
6 The desired chromatogram will be subtracted. Note the new TIC of the selected peak. (See Figure 8-112.)

Figure 8-112 New TIC



7 To return to the previous view, right click on the chromatogram and click **Chro Subtract** from the menu to deselect. (See Figure 8-113.)

Figure 8-113 Deselecting Chromatogram Subtract

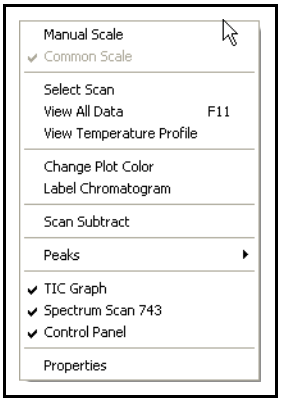


8.11 Right-Click Menus Within Data Review

8.11.1 Right-Clicking in the TIC Window

Figure 8-114 shows the functions available when right-clicking on the TIC window.

Figure 8-114 Right Clicking in the TIC Window



Common Scale . . . . . When checked, all RIC plots will be plotted to the same scale; when not checked all RIC plots will be individually scaled to 100%.

Select Scan . . . . . Allows the scan cursor to select a specific scan in order to view the desired mass spectrum.

View All Data . . . . . Rescales the plot to display the entire run. Also accessed by **F-11**.

View Temperature Profile. . . . . Plots the GC temperature profile of the method.

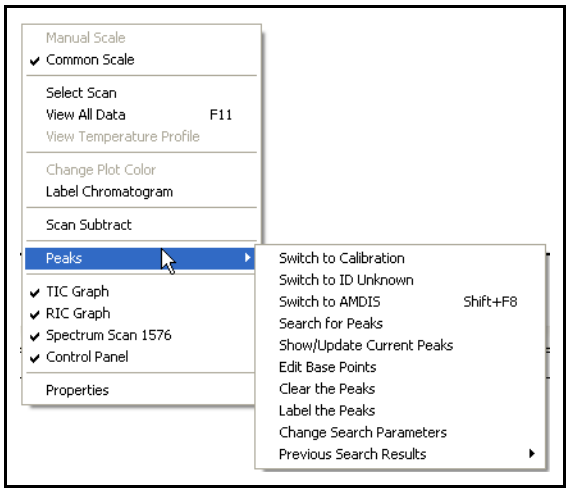
Change Plot Color . . . . . Changes the color of the TIC plot.

Label Chromatogram . . . . . Displays a text box to label the chromatogram. The location of the label can be adjusted with the cursor and saved with the data file.

Scan Subtract . . . . . Subtracts the current scan from the displayed RIC plots.

Peaks submenu (See Figure 8-115.)

Figure 8-115 Peaks



Switch to Calibration . . . . . Opens the **Calibrate** function. See Chapter 11, Calibration.

Switch to ID Unknowns . . . . . Opens the **ID Unknowns** function. See ID Unknowns, see section 11.5 on page 11-24.

Switch to AMDIS . . . . . Opens the AMDIS program. See section 8.5, Analyzing Data Using AMDIS, on page 8-16.

Search for Peaks . . . . . Searches the chromatogram for peaks. Performs the same function as **Show/Update Current Peaks**. Refer to section 8.7, Show/Update Current Peaks, on page 8-28.

Show/Update Current Peaks . . Searches the chromatogram for peaks. Refer to section 8.7, Show/Update Current Peaks, on page 8-28.

Edit Base Points . . . . . To move the base point, double-click on the desired new location for the base point. This function is used to manually reintegrate the peak.

Clear the Peaks . . . . . Clears the identification of peaks from the TIC graph after using **Search for Peaks**.

Label the Peaks . . . . . Labels identified peaks with retention time and area.

Change Search Parameters . . . Modifies current peak search parameters. Refer to section 10.10.2, Setting Up a Quantitative Search, on page 10-43.

Previous Search Results . . . . . View results from a previous search. (Drop-down menu of previously opened data files.)

TIC Graph . . . . . When checked, displays TIC window.

RIC Graph . . . . . When checked, displays the RIC window.

Spectrum Scan ### . . . . . When checked, displays **Spectrum** window for the current scan.

Control Panel . . . . . When checked, displays the **Control Panel**.

Properties . . . . . Allows access to the **Properties** of the display. See section 8.11.1.1, Properties Menu, on page 8-56.

8.11.1.1 Properties Menu

The **Properties** option displays the following options: (See Figure 8-116.)

Current Width . . . . . The width of the graph can be set to the desired time point.

Show Spectrum . . . . . The **Spectrum** will be automatically displayed upon opening a data file when this box is checked.

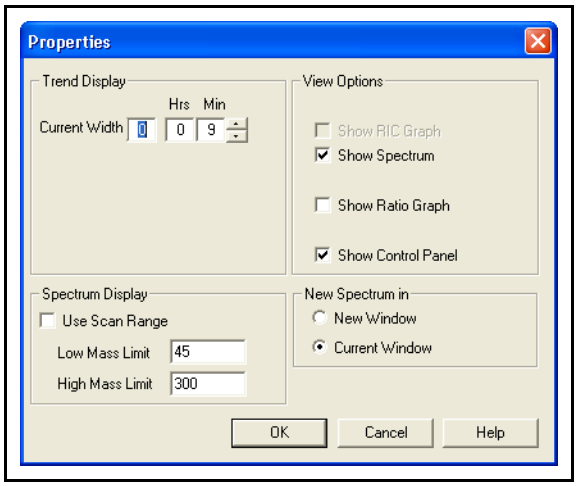
Show Control Panel . . . . . The **Control Panel** will be automatically displayed upon opening a data file when this box is checked.

Use Scan Range . . . . . The masses for the scan range of the method will be displayed.

Low Mass Limit . . . . . HAPSITE will display masses in the spectrum above this limit.

High Mass Limit . . . . . HAPSITE will display masses in the spectrum below this limit.

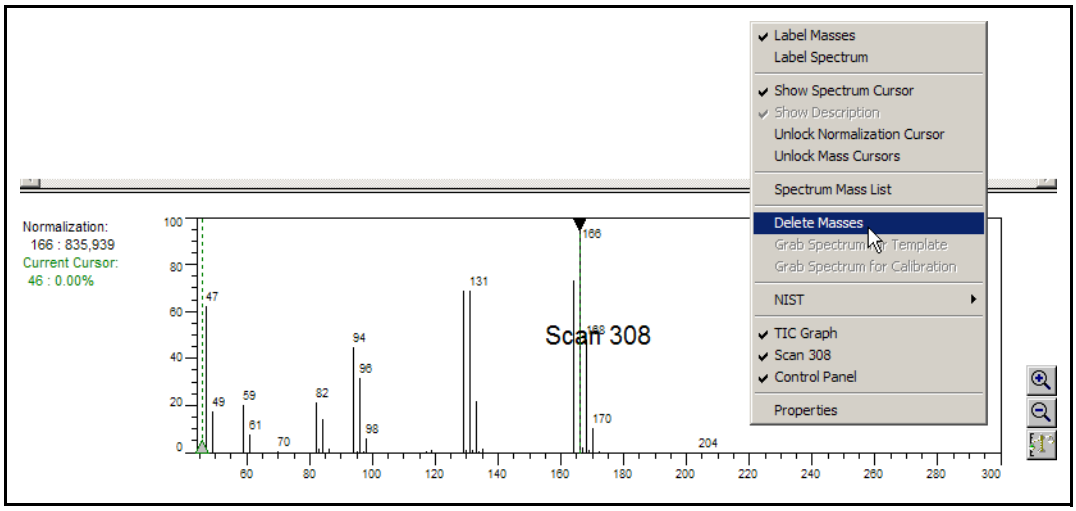
Figure 8-116 Properties



8.11.2 Spectrum Window

Right-clicking in the **Spectrum** window will access the menu shown in Figure 8-117.

Figure 8-117 Spectrum Display Menu



Label Masses . . . . . When checked, it will display the atomic weight of the mass fragments in the **Spectrum** window.

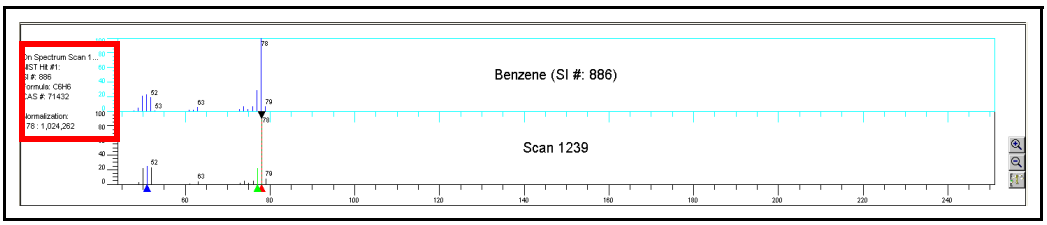
Label Spectrum . . . . . Displays a text box in order to manually label the spectrum.

Show Spectrum Cursor . . . . . Displays the spectrum cursor in the spectrum window.

Show Description . . . . . This will display the SI number, the NIST hit number, the formula, CAS number and the normalization number next to the spectrum. (See Figure 8-118.)

NOTE: Show description is only active if **Search NIST/User** is selected.

Figure 8-118 Show Description



Unlock Normalization Cursor . . . . Must be unlocked to move the normalization cursor to a mass other than the largest mass fragment.

Unlock Mass Cursors . . . . . Unlocks the mass cursors to reassign a new color to the mass fragment when using RIC plots.

Spectrum Mass List . . . . . Displays a report of all the masses in the spectrum.

Delete Masses . . . . . Deletes masses from the mass spectrum display to manually subtract the background. (Does not delete data.)

Grab Spectrum for Template . . . . . Used for Quantitative methods. See Chapter 11, Calibration.

Grab Spectrum for Calibration . . . Used for Quantitative methods. See Chapter 11, Calibration.

NIST . . . . . Allows the analyst to utilize the NIST database for qualitative identification of the displayed spectrum. Refer to Analyzing Data Using NIST, see section 8.11.3 on page 8-59.

TIC Graph . . . . . When checked, displays **TIC** window.

Spectrum Scan ### . . . . . When checked, displays the **Spectrum** window.

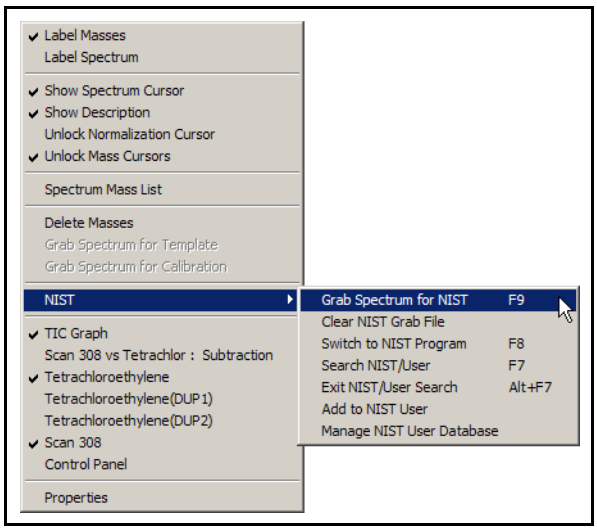
Control Panel . . . . . When checked, displays the **Control Panel**.

Properties . . . . . Accesses display properties.

8.11.3 Analyzing Data Using NIST

By right-clicking on the **Spectrum** window, the NIST menu is displayed. (See Figure 8-119.)

Figure 8-119 NIST Menu



Grab Spectrum for NIST (F9). . . . . This function will select a file to be exported into the NIST database program.

Clear NIST Grab file . . . . . Clears the list of previously selected files.

Switch to NIST Program (F8). . . . . Starts the NIST database program and will export any selected files to NIST database program.

Search NIST/User (F7) . . . . . Starts the NIST Library search. Refer to NIST Library Searches, see section 8.6 on page 8-24.

Exit Search NIST/User (Alt+F7). . . Exits the **Search NIST/User** Library search function.

Add to NIST User . . . . . Adds selected spectrum to the **Search NIST/User** Library.

Manage NIST User Database. . . . . Displays, deletes or plots entries in a **Search NIST/User** Library.

8.11.4 NIST Database Program

The NIST database program is third-party software that is included with the HAPSITE ER. Instructions for using the software are located by selecting **HELP** from the Menu selection in either the AMDIS or NIST program. (See Figure 8-120 and Figure 8-121.)

Figure 8-120 Help in AMDIS

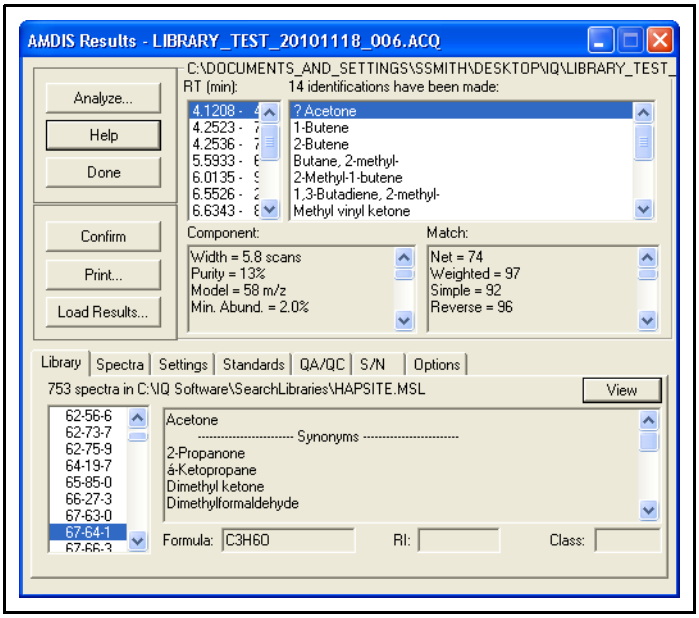
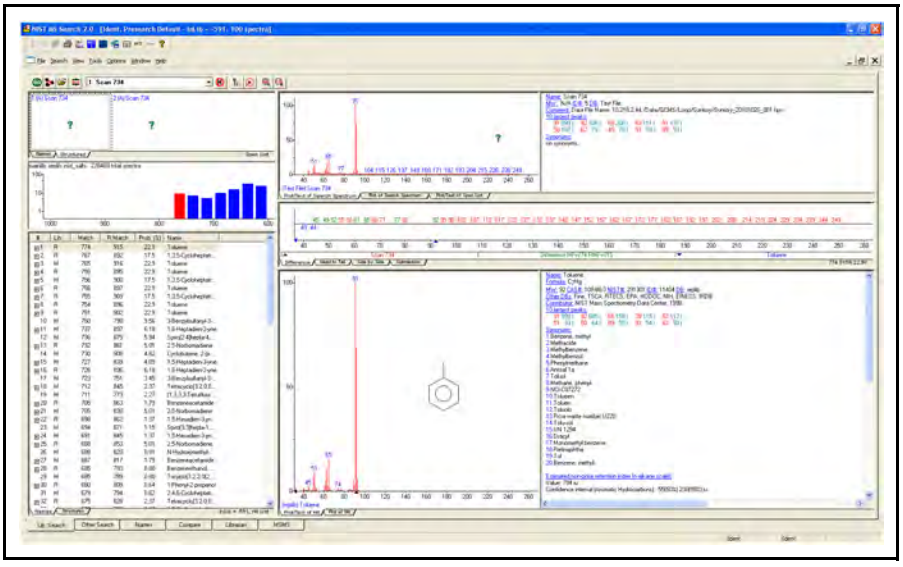


Figure 8-121 Help in NIST

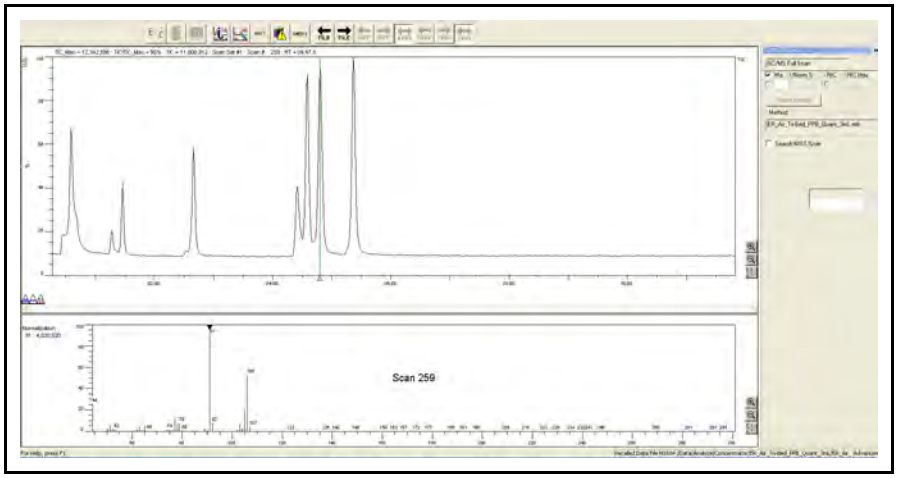


8.11.5 Grab Spectra for NIST

To export the spectrum to the NIST database:

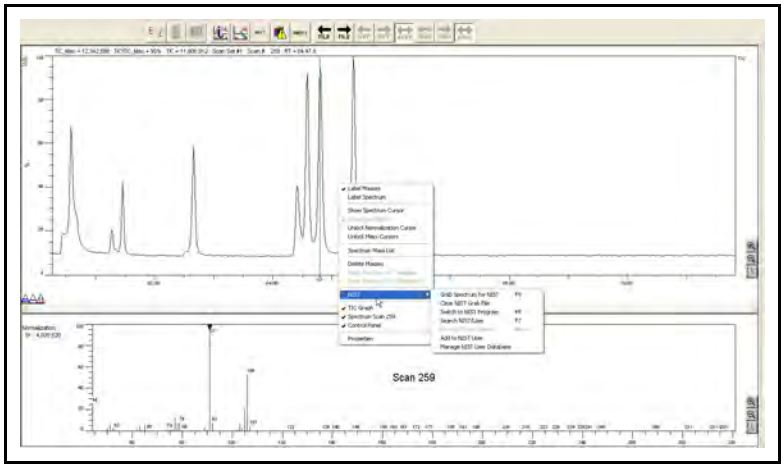
1 Double-click on the desired peak in the **TIC/RIC** window. (See Figure 8-122.)

Figure 8-122 TIC/RIC Window



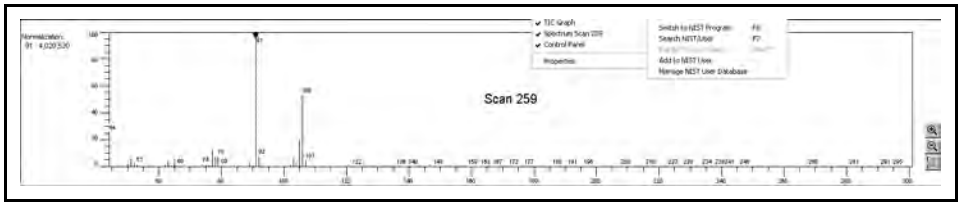
2 Place the cursor in the **Spectrum** window and right-click. (See Figure 8-123.)

Figure 8-123 Spectrum



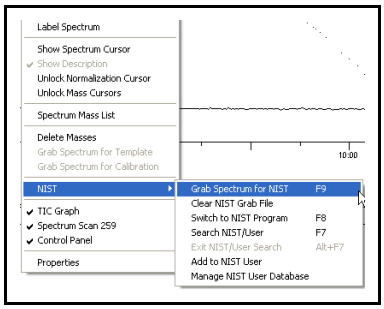
3 Select **NIST**. **(**See Figure 8-124.)

Figure 8-124 NIST



4 Click **Grab Spectrum for NIST**. (See Figure 8-125.)

Figure 8-125 Grab Spectrum for NIST

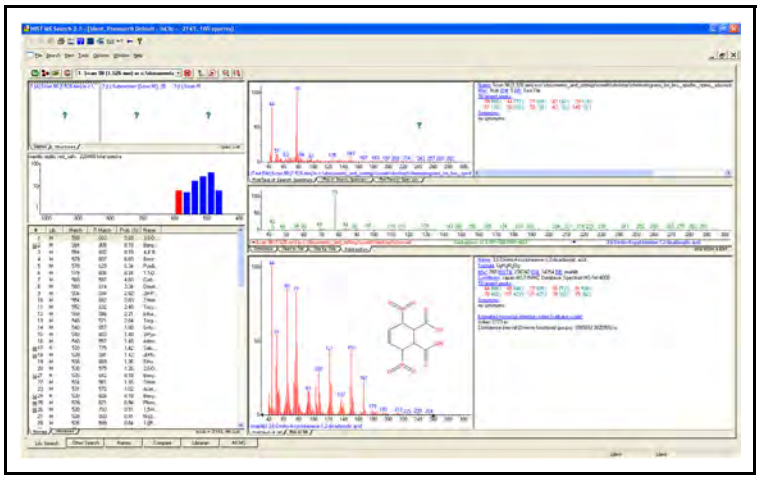


5 Click **Switch to NIST Program**. (See Figure 8-126.)

Figure 8-126 Switch to NIST Program

6 The identification will be displayed on the screen. (See Figure 8-127.)

Figure 8-127 NIST Database



Chapter 9
Tune

9.1 Introduction to AutoTune and Manual Tune

The tune of a Mass Spectrometer (MS) determines the quality of the mass spectrum produced by the system. The MS performance will run an autotune upon start-up and after 12 hours of continuous operation. Tuning is normally accomplished by the AutoTune program, which automatically sets and adjust all parameters, however, user can set the parameters by manual tuning.

HAPSITE ER uses two gas internal standards which contain mass fragments that span the mass range of interest. The internal standards are:

- 1,3,5-Tris (trifluoromethyl) benzene
- Bromopentafluorobenzene

9.2 AutoTune

AutoTune can be started from the front panel or from the laptop.

For front panel instructions, refer to section 4.7.1.5, TUNE STATUS Icon, on page 4-53.

9.2.1 Starting AutoTune from the Manual Tune Screen on Laptop Computer

1 Double-click on the **ER IQ** icon. (See Figure 9-1.)

Figure 9-1 ER IQ icon

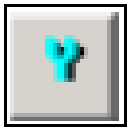
2 Double-click on the **Tune** icon. (See Figure 9-2.)

NOTE: Manual Tune is an advanced user function. Refer to section 7.3.4.1, Set Access Level, on page 7-13 for instructions on changing access levels.

Figure 9-2 Manual Tune icon

3 Wait until the **EM and Emission** buttons on the **Control Panel** turns green. Click the **Tune** icon. (See Figure 9-3.)

Figure 9-3 Tune icon

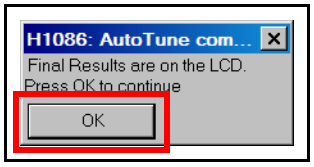


CAUTION

Adjusting other parameters without proper training may damage the instrument.

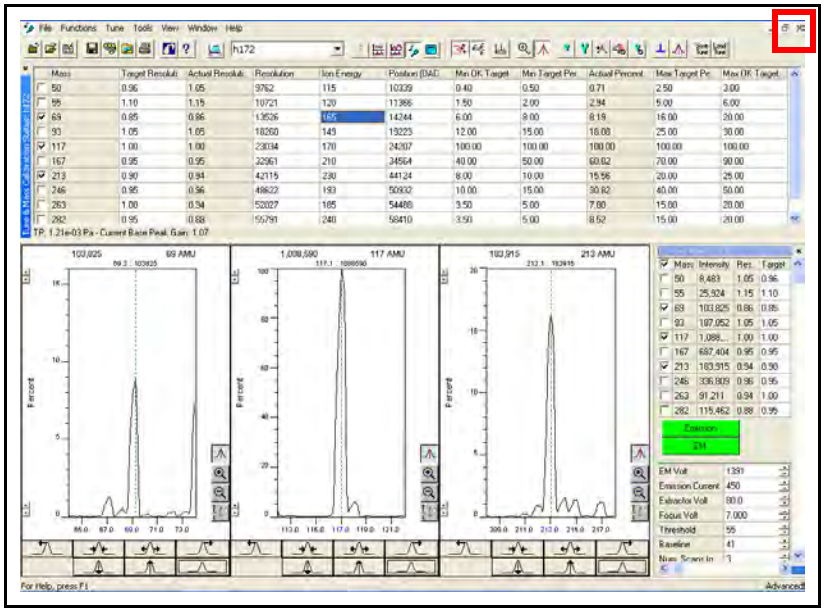
4 Allow HAPSITE ER to AutoTune. When AutoTune is finished, the message **Final Results are on the LCD** will be displayed. Click **OK**. (See Figure 9-4.)

Figure 9-4 AutoTune complete



5 Close the manual tune screen by clicking the **X** on the top right corner.

Figure 9-5 Close the manual tune screen

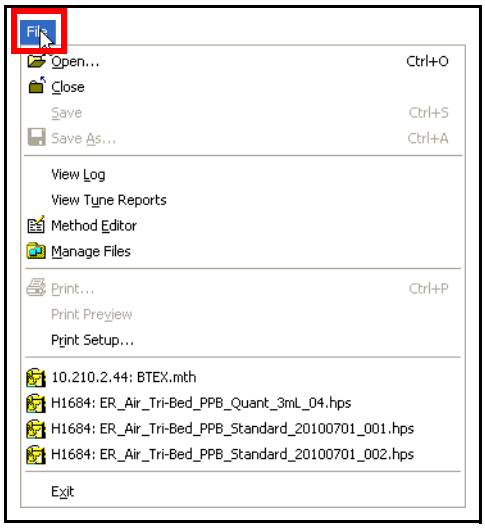


9.3 Viewing a Tune Report

The most current tune report can be viewed from the front panel display or from the laptop. Past tune reports can be viewed from the laptop.

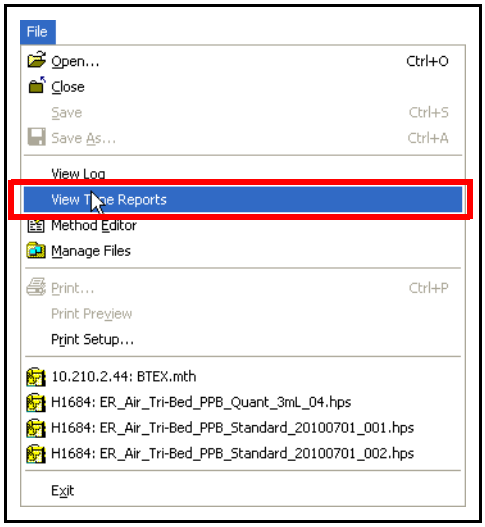
1 To view the report from the laptop computer, select **File**. (See Figure 9-6.)

Figure 9-6 File menu



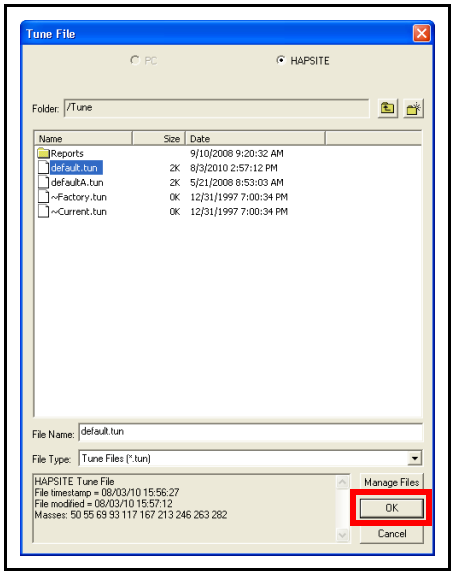
2 Select **View Tune Reports** from the drop-down menu. (See Figure 9-7.)

Figure 9-7 View Tune reports



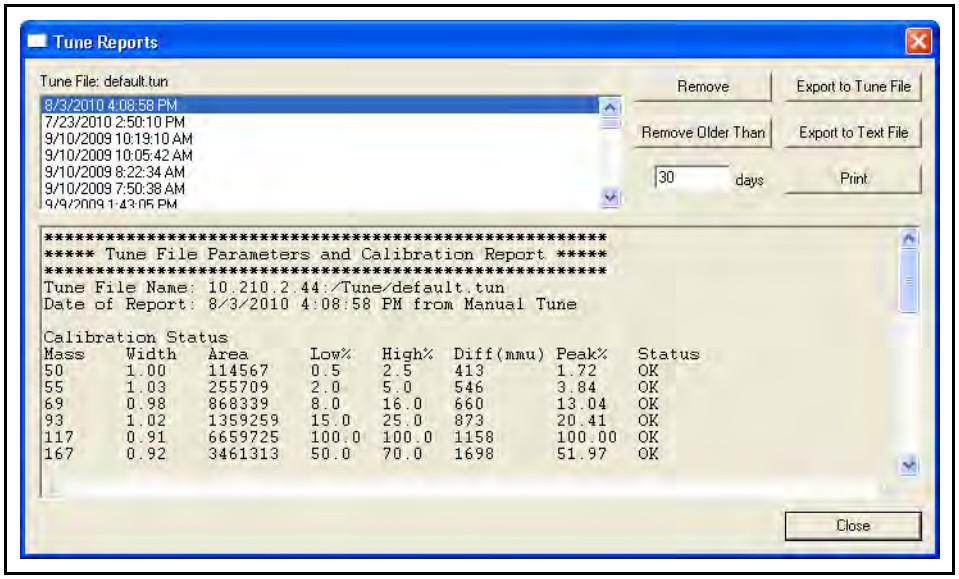
3 Highlight the **`default.tun`** file and press **OK**. (See Figure 9-8.)

Figure 9-8 Highlighting *default.tun*



4 The **Tune Reports** will be displayed. **Tune Reports** are stored, by default, for 30 days. (See Figure 9-9.)

Figure 9-9 Tune Reports



9.3.1 Tune Reports Options:

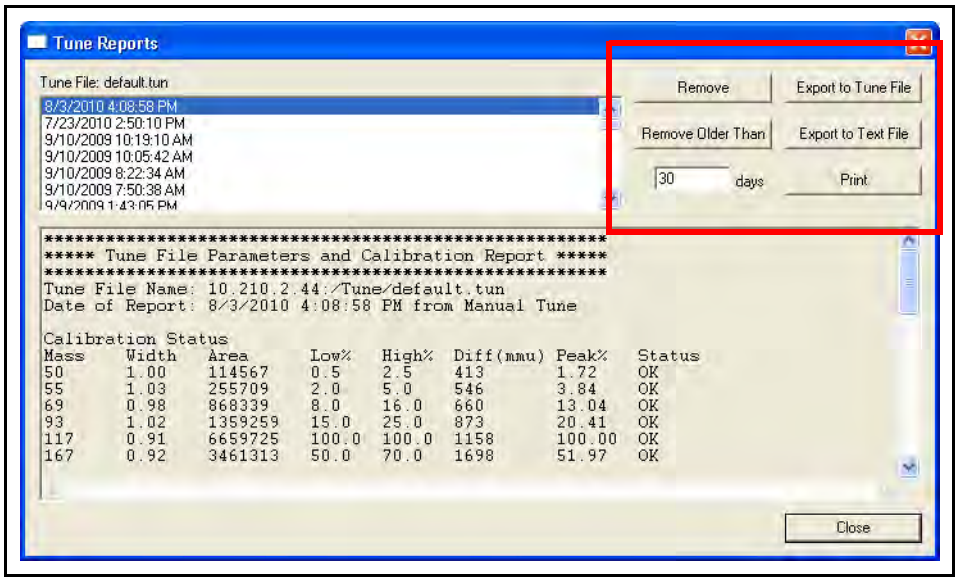
Remove . . . . . Deletes the selected report. **No confirmation is requested**.

Remove Older Than . . . . . Deletes files older than the number of days specified. Confirmation is requested before the files are deleted.

Export to text file . . . . . Creates a text file of the tune report.

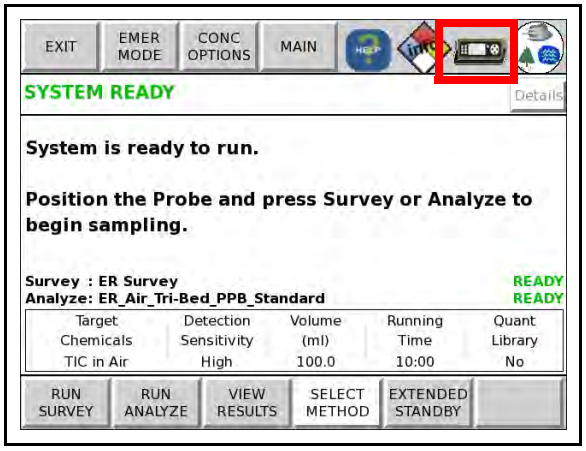
Print . . . . . Prints the selected tune report.

Figure 9-10 Tune Reports Screen from Laptop Computer



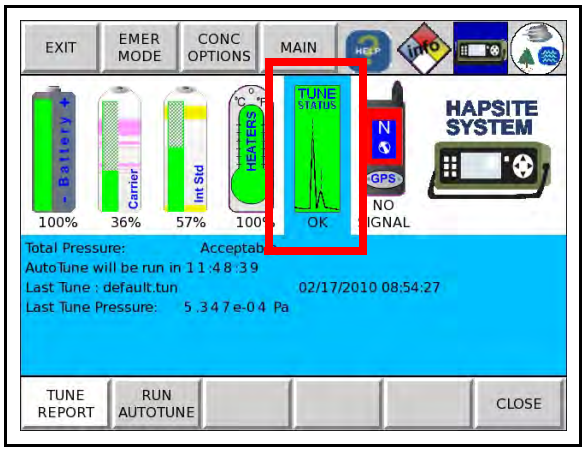
1 To view the **Tune Report** from the front panel display, touch the **HAPSITE ER** icon or push the **SYSTEM STAT** button until the **HAPSITE ER** icon is highlighted. (See Figure 9-11.)

Figure 9-11 Accessing Tune report



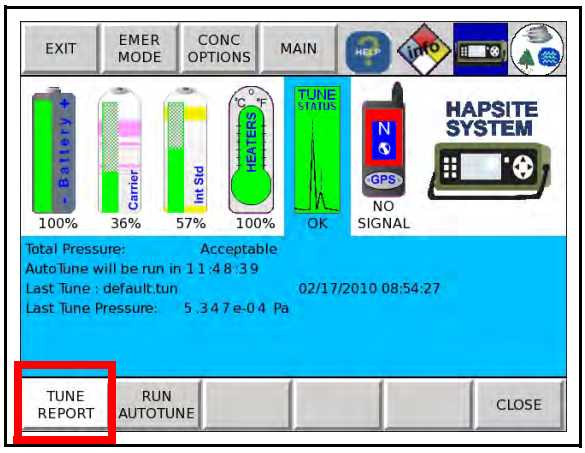
2 Touch the **TUNE** icon. (See Figure 9-12.)

Figure 9-12 Tune report



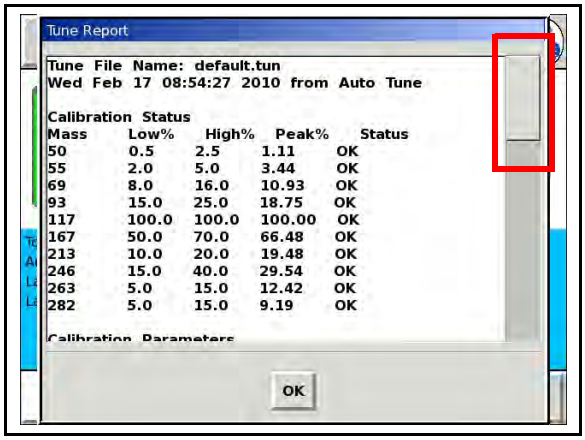
3 Touch the **TUNE REPORT** button or use the arrow keys to highlight the **TUNE REPORT** button. The last tune report will be displayed. (See Figure 9-13.)

Figure 9-13 Tune Report



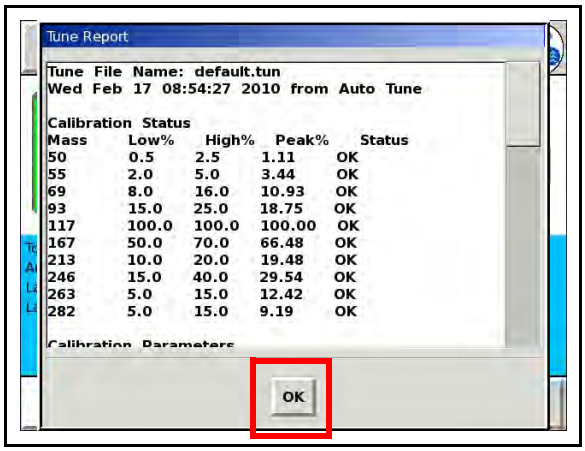
4 To scroll through the tune report, use up or down arrows keys. (See Figure 9-14.)

Figure 9-14 Tune Report



5 Touch **OK** or push **OK SEL** to exit the screen. (See Figure 9-15.)

Figure 9-15 Tune report



9.4 Performing Manual Tune

Manual tunes are a standard routine maintenance practice for HAPSITE ER and HAPSITE SmartPlus, and should be performed once every 4 to 6 months to maintain optimal performance of the unit's mass spectrometer.

Routine manual tunes will improve the accuracy of compound identifications, and provide indications of the health of the mass spectrometer.

The following procedure outlines the steps in manually tuning HAPSITE ER. If performing this task for the first time, we recommend contacting INFICON directly for support.

9.4.1 Manual Tune Variables

The goal of Manual Tune is to adjust the inputs, such that the outputs fall within appropriate ranges.

Instrument Outputs:

- Base Peak Gain (BPG)
- Ion Percentages
- Status Column

Primary User Inputs/Editables:

- Ion Resolutions
- Ion Energies
- EM Voltage

Secondary Inputs/Editables:

- Focus Voltage
- Emission Current
- Baseline + Threshold

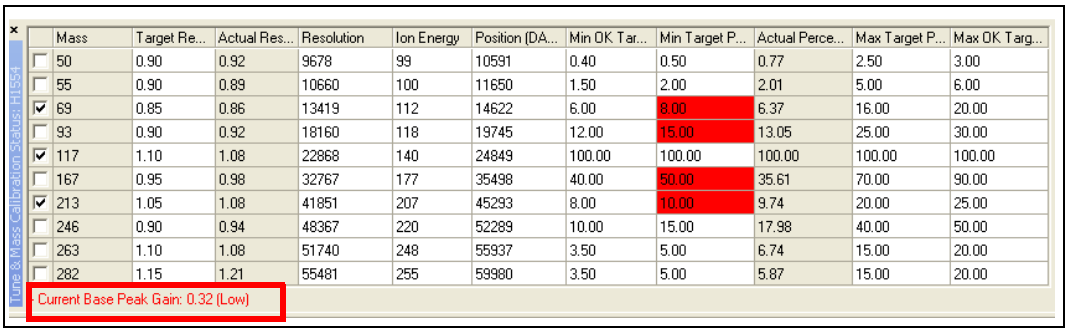
9.4.2 Outputs

Base Peak Gain (BPG)

BPG influences sensitivity. (See Figure 9-16.)

- ER ideal setting is 0.5 (range is 0.4 to 0.6)
- Smart Plus ideal setting is 1.0 (range is 0.8 to 2.0)

Figure 9-16 Base Peak Gain



	Mass	Target Re...	Actual Res...	Resolution	Ion Energy	Position (DA...	Min OK Tar...	Min Target P...	Actual Perce...	Max Target P...	Max OK Targ...
☐	50	0.90	0.92	9678	99	10591	0.40	0.50	0.77	2.50	3.00
☐	55	0.90	0.89	10660	100	11650	1.50	2.00	2.01	5.00	6.00
☑	69	0.85	0.86	13419	112	14622	6.00	8.00	6.37	16.00	20.00
☐	93	0.90	0.92	18160	118	19745	12.00	15.00	13.05	25.00	30.00
☑	117	1.10	1.08	22868	140	24849	100.00	100.00	100.00	100.00	100.00
☐	167	0.95	0.98	32767	177	35498	40.00	50.00	35.61	70.00	90.00
☑	213	1.05	1.08	41851	207	45293	8.00	10.00	9.74	20.00	25.00
☐	246	0.90	0.94	48367	220	52289	10.00	15.00	17.98	40.00	50.00
☐	263	1.10	1.08	51740	248	55937	3.50	5.00	6.74	15.00	20.00
☐	282	1.15	1.21	55481	255	59980	3.50	5.00	5.87	15.00	20.00

Tune & Mass Calibration Status: Hi Res

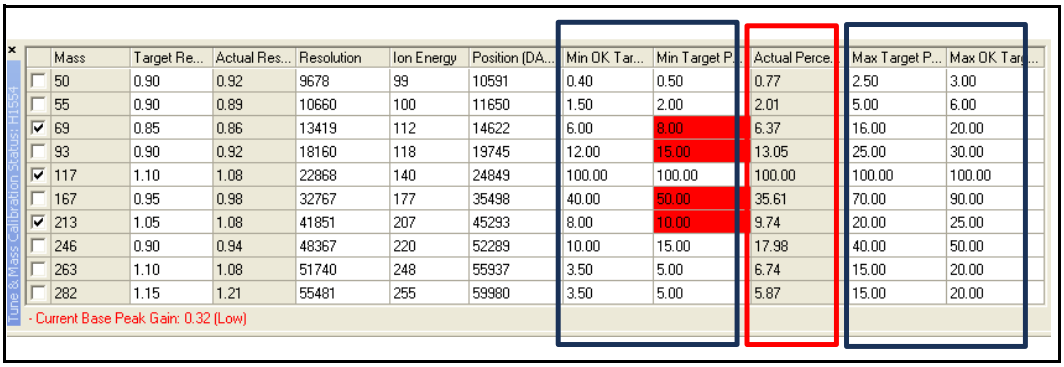
Current Base Peak Gain: 0.32 (Low)

Ion Percentages

Actual Percentages are listed in the Mass Calibration table, outlined in red. The range of acceptable values is presented in the 4 adjacent columns, outlined in blue.

Example: The percentage of mass 50, first row, should fall within 0.5 to 2.5%, and must fall within 0.4 to 3.0%, for the mass spec to be properly calibrated.

Figure 9-17 Ion Percentages



	Mass	Target Re...	Actual Res...	Resolution	Ion Energy	Position (DA...	Min OK Tar...	Min Target P...	Actual Perce...	Max Target P...	Max OK Targ...
☐	50	0.90	0.92	9678	99	10591	0.40	0.50	0.77	2.50	3.00
☐	55	0.90	0.89	10660	100	11650	1.50	2.00	2.01	5.00	6.00
☑	69	0.85	0.86	13419	112	14622	6.00	8.00	6.37	16.00	20.00
☐	93	0.90	0.92	18160	118	19745	12.00	15.00	13.05	25.00	30.00
☑	117	1.10	1.08	22868	140	24849	100.00	100.00	100.00	100.00	100.00
☐	167	0.95	0.98	32767	177	35498	40.00	50.00	35.61	70.00	90.00
☑	213	1.05	1.08	41851	207	45293	8.00	10.00	9.74	20.00	25.00
☐	246	0.90	0.94	48367	220	52289	10.00	15.00	17.98	40.00	50.00
☐	263	1.10	1.08	51740	248	55937	3.50	5.00	6.74	15.00	20.00
☐	282	1.15	1.21	55481	255	59980	3.50	5.00	5.87	15.00	20.00

Tune & Mass Calibration Status: Hi Res

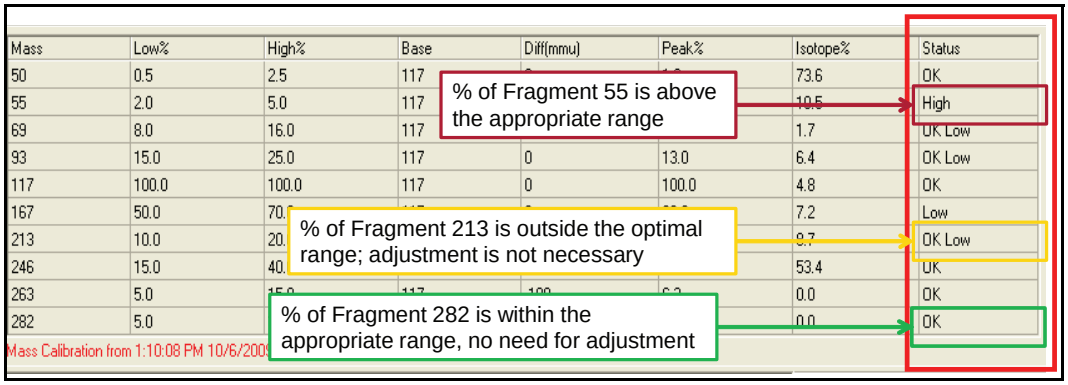
Current Base Peak Gain: 0.32 (Low)

Boxes shaded with red, like those shown in Figure 9-17, indicate that the actual percentage is outside that range for that fragment (row). For example, in the third row of the table above for mass 69, the actual percentage is 6.37 when it should fall above 8.00. Here, mass 69 requires adjustment of the Resolution and/or Ion Energy to correct the Actual Percentage.

Status Column

The Status Column provides categorical view of the actual percentages. (See Figure 9-18.) The values **OK**, **OK Low**, **OK High**, **Low** or **High** indicate whether the actual percentage for that ion are within best range (OK) or outside (Low or High). Values of High or Low are not acceptable. Adjust the corresponding mass fragments.

Figure 9-18 Status column

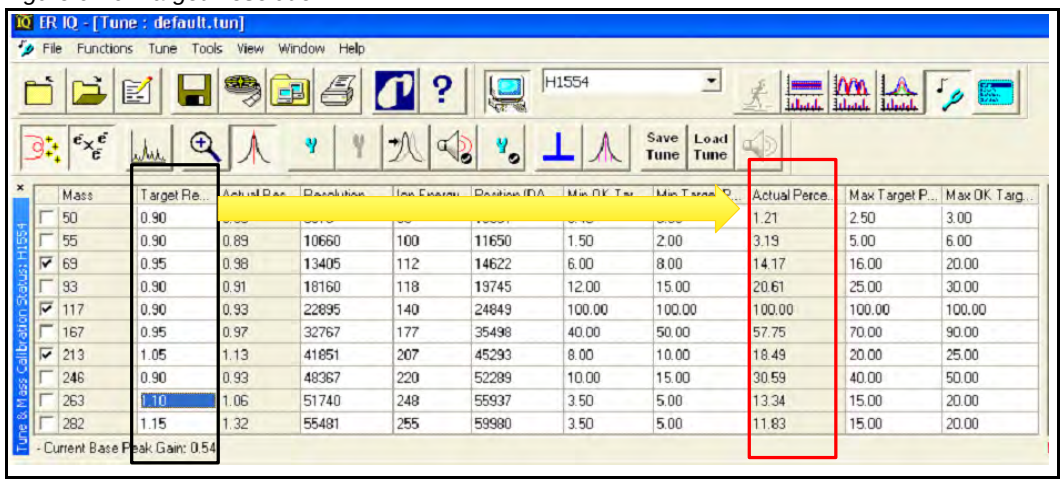


9.4.3 Inputs

Target Resolution

Resolution refers to the width of the measured mass peak in amu. The range for the Target Resolution is 0.85 and 1.10. Adjusting Resolution influences the Actual Percentages. (See Figure 9-19.)

Figure 9-19 Target Resolution

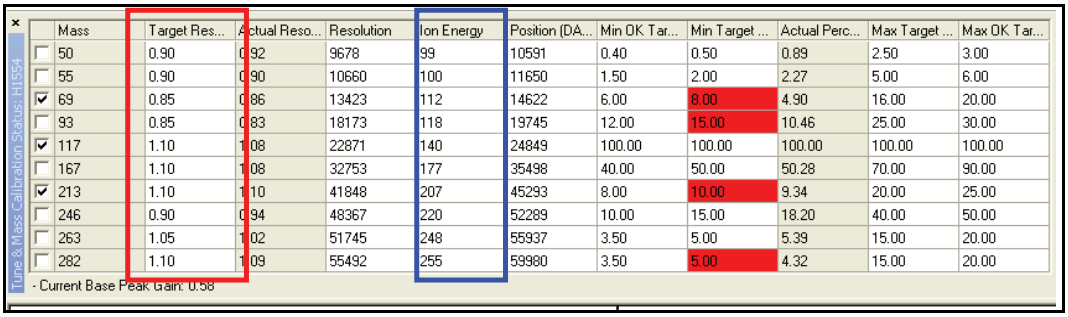


Wider resolutions mean larger percentages (measuring over a wider section of the MS window). As these are adjusted, watch and observe the changes to the percentages.

Adjusting Target Resolution

Adjustments are made in increments of 0.05. The number in the Actual Percentage column is affected by the target resolution adjustments. This should fall between the Max. Target and Min. Target. If the masses cannot be brought into range by adjusting the Target Resolution, adjust the Ion Energies. (See Figure 9-20.)

Figure 9-20 Adjusting the Target Resolution



Ion Energies

Adjusting the Ion Energy adjusts the degree of electronic amplification applied to a mass fragment, and thus the intensity (height) of the mass. Ion energies should be adjusted **after** Target Resolutions. (See Figure 9-20.)

Ideal Values

Displays the ideal values for Ion energies for each of the 10 mass fragments.

Table 9-1 Ideal Ion Energy values

Mass	IE Low	IE High
50	90	170
55	90	170
69	90	170
93	90	170
117	140	170
167	140	220
213	175	230
246	180	230
263	185	250
282	190	255

Ion Energies should generally be in ascending order, Low for the smaller masses and High for the larger masses.

Perform a Mass Alignment (press F5) after each change until **OK** is reported in the Status column.

Mass Alignment

Perform a Mass Alignment by pressing F5. This will update the Status column readings. Perform a Mass Alignment prior to and after making adjustments to the tune parameters. (See Figure 9-21.)

Figure 9-21 Mass Alignment

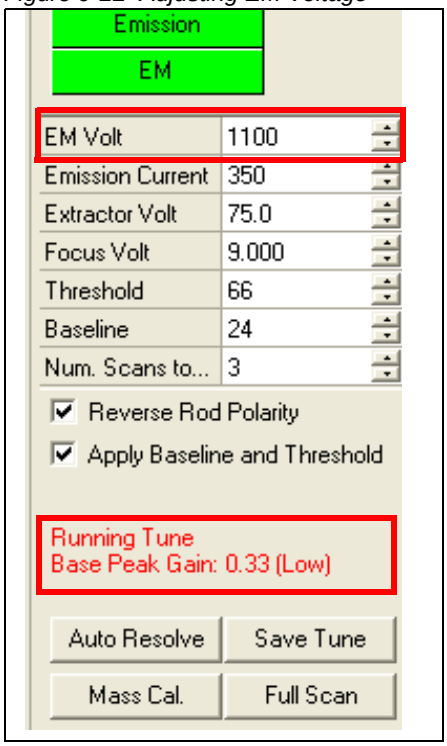
Mass	Low%	High%	Base	Diff(mmu)	Peak%	Isotope%	Status
50	0.5	2.5	117	0	1.0	73.6	OK
55	2.0	5.0	117	0	8.7	10.5	High
69	8.0	16.0	117	0	6.5	1.7	OK Low
93	15.0	25.0	117	0	13.0	6.4	OK Low
117	100.0	100.0	117	0	100.0	4.8	OK
167	50.0	70.0	117	0	36.0	7.2	Low
213	10.0	20.0	117	0	9.0	8.7	OK Low
246	15.0	40.0	117	0	17.8	53.4	OK
263	5.0	15.0	117	-100	6.2	0.0	OK
282	5.0	15.0	117	0	5.6	0.0	OK

Mass Calibration from 1:10:08 PM 10/6/2009 - Base Peak Gain: 0.34 (Low)

Adjusting EM Voltage

The BPG is adjusted using EM (Electron Multiplier) voltage. Adjustments are made using increments of 25 V. (See Figure 9-22.) The normal operating range is 1000 to 1600 V, with newer units typically showing lower values and older units showing higher values. If your unit requires an EM volt of 1600 to 2000 to reach BPG of 0.5, please contact INFICON for support, as your unit may require service.

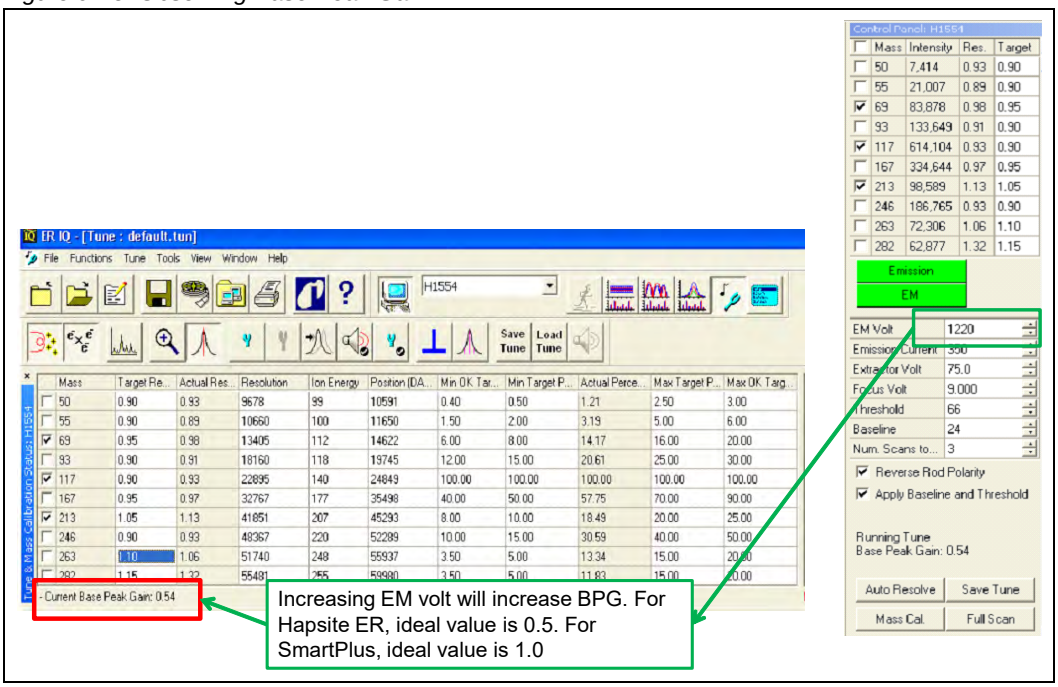
Figure 9-22 Adjusting EM Voltage



Observing Base Peak Gain (BPG)

Properly adjusted Base Peak Gain for a HAPSITE ER is between 0.4 to 0.6, ideally at 0.50. (See Figure 9-23.) Ideal value for HAPSITE SmartPlus is 1.0.

Figure 9-23 Observing Base Peak Gain



9.4.4 Other Inputs

If you are unable to attain a satisfactory tune using the Resolution, Ion Energies, and EM Volt, then further adjustments may be necessary. These should be made only after contacting INFICON.

Additional Adjustment Control

- Focus volt adjusts the relative amplification of ions larger and smaller than 117, i.e. raising amplification of larger ions and lowering smaller ions, OR raising small ions and lowering larger ions. The ideal value is between 2 to 8.
- Emission current increases the power of the ionizer. Increasing this can help raise BPG, but can also increase noise. The ideal value is 300 to 400.

Baseline and Threshold are indicative of noise, and should be less than 300 each. (Threshold will always be higher than Baseline.)

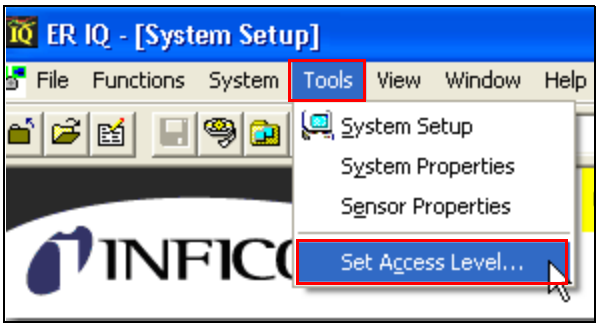
9.4.5 Set Access Level to Advanced

The **Access Level** must be set to **Advanced** to manually tune the instrument. The **Set Access Level...** is used to change ER IQ/Plus IQ user mode.

- **Normal Mode**: Allows access to default methods and data analysis
- **Advanced Mode**: Allows access to method editing, manual tuning, file transfer, and file deletion.

1 On the **System Setup** window **Tools** Menu, click **Set Access Level...**. (See Figure 9-24.)

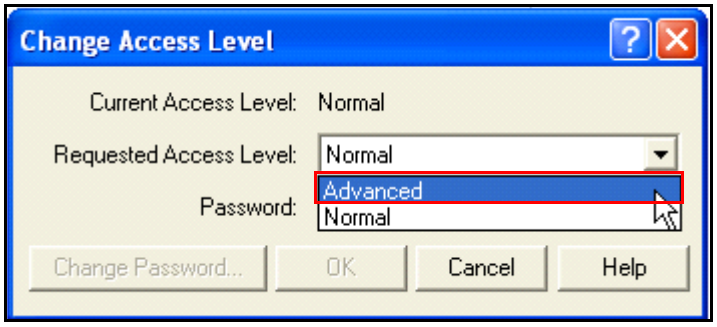
Figure 9-24 Set Access Level



2 On the Change Access Level window, select **Advanced** in the **Requested Access Level** box. (See Figure 9-25.)

NOTE: Access level is not password protected in the default settings. Advanced mode may be password protected if desired.

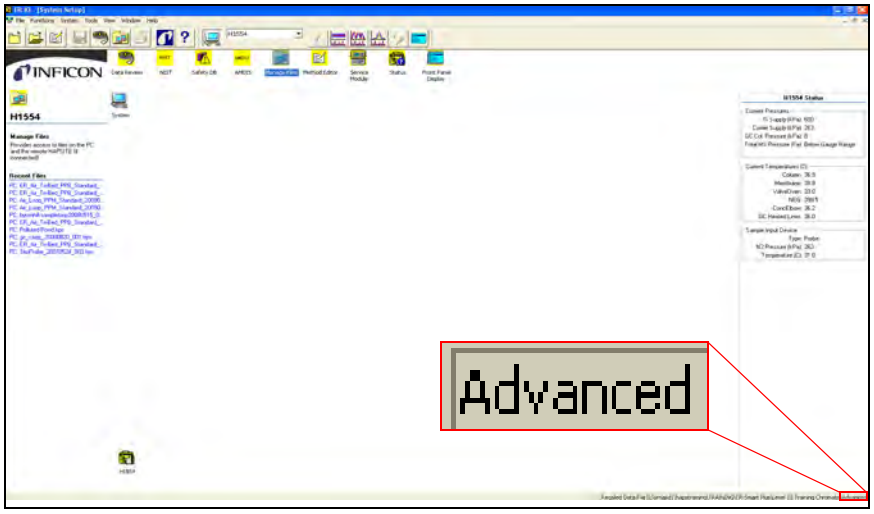
Figure 9-25 Change Access Level window



3 Click **OK**.

4 On the **System Setup** window, verify the Access Level is set to **Advanced**. (See Figure 9-26.)

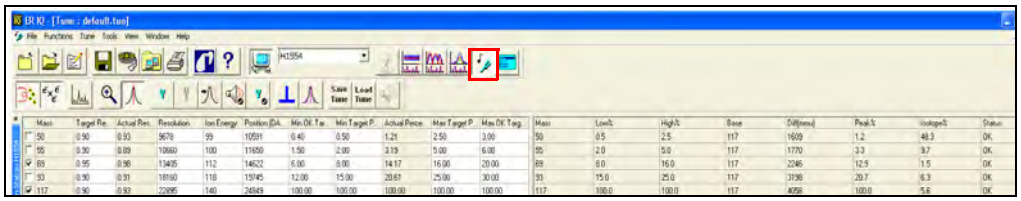
Figure 9-26 Verify access level



9.4.6 Manual Tune

1 Double click the  icon. (See Figure 9-27.)

Figure 9-27 Tune icon



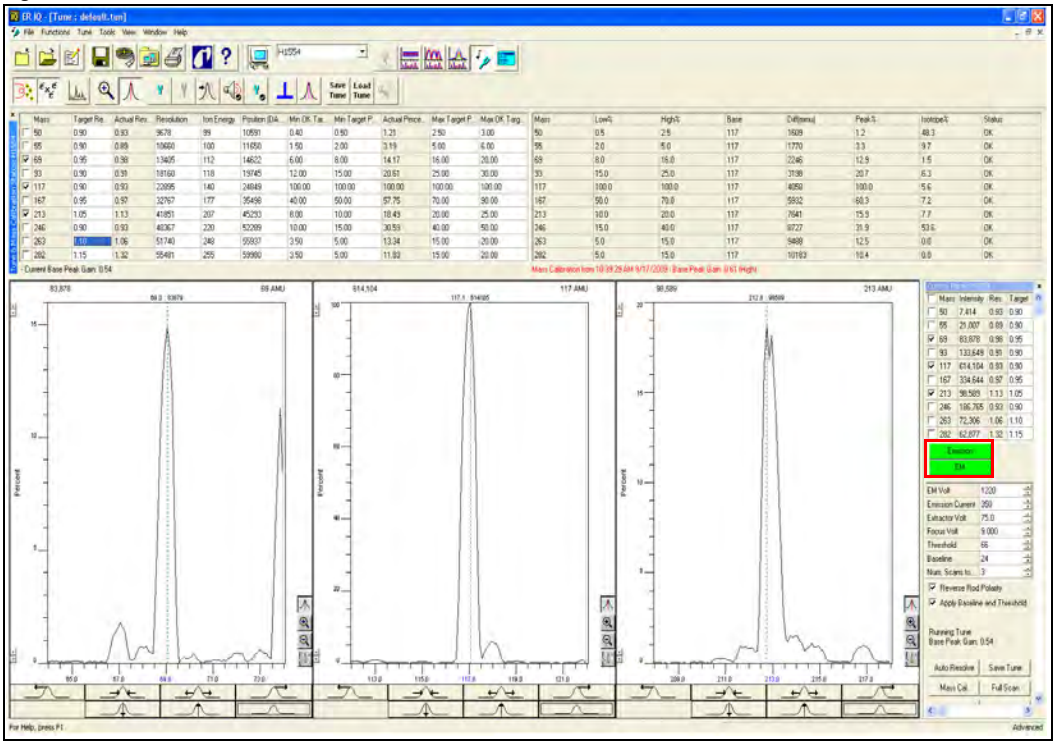
2 Select ***default.tun*** from the tuning pop-up window.

3 Click OK. It will take 10 to 20 seconds to initialize. During that time the **Emission** and **EM** boxes turn green. (See Figure 9-28.)

NOTE: The NEG (non-evaporable getters) is consumed while Manual Tune is open.

4 Adjust the tune parameters as discussed above until all values are within range.

Figure 9-28 Emission and EM boxes



9.4.7 Save Tune

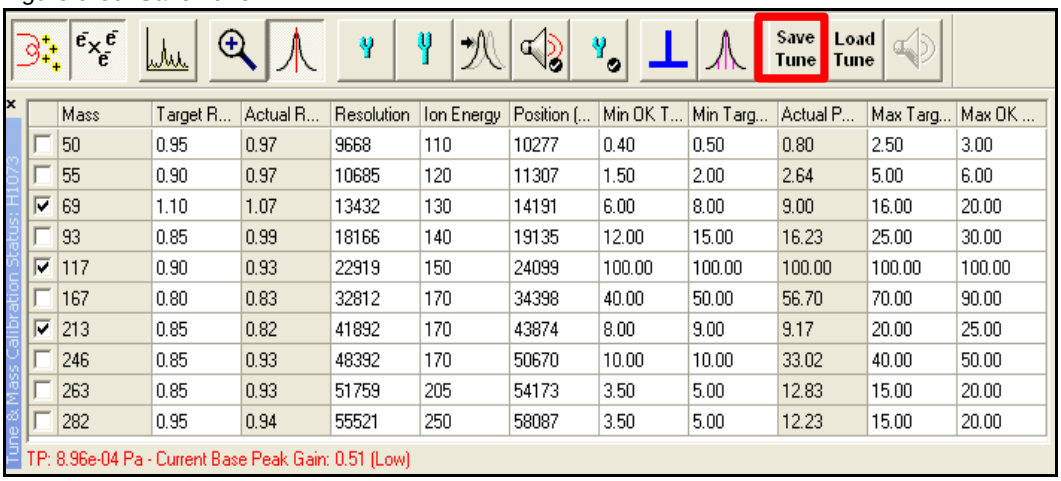
1 Verify that **OK** is displayed in the Status Column. (See Figure 9-29.)

Figure 9-29 Status Column

Mass	Low%	High%	Base	Diff(mmu)	Peak%	Isotope%	Status
50	0.5	2.5	117	1609	1.2	48.3	OK
55	2.0	5.0	117	1770	3.3	9.7	OK
69	8.0	16.0	117	2246	12.9	1.5	OK
93	15.0	25.0	117	3198	20.7	6.3	OK
117	100.0	100.0	117	4058	100.0	5.6	OK
167	50.0	70.0	117	5932	60.3	7.2	OK
213	10.0	20.0	117	7641	15.9	7.7	OK
246	15.0	40.0	117	8727	31.9	53.6	OK
263	5.0	15.0	117	9488	12.5	0.0	OK
282	5.0	15.0	117	10183	10.4	0.0	OK

2 Once you are satisfied with the quality of the tune, click Save Tune at the top right of the Percentages table. Save the tune as default.tun. (See Figure 9-30.)

Figure 9-30 Save Tune



	Mass	Target R...	Actual R...	Resolution	Ion Energy	Position (...	Min OK T...	Min Targ...	Actual P...	Max Targ...	Max OK ...
☐	50	0.95	0.97	9668	110	10277	0.40	0.50	0.80	2.50	3.00
☐	55	0.90	0.97	10685	120	11307	1.50	2.00	2.64	5.00	6.00
☑	69	1.10	1.07	13432	130	14191	6.00	8.00	9.00	16.00	20.00
☐	93	0.85	0.99	18166	140	19135	12.00	15.00	16.23	25.00	30.00
☑	117	0.90	0.93	22919	150	24099	100.00	100.00	100.00	100.00	100.00
☐	167	0.80	0.83	32812	170	34398	40.00	50.00	56.70	70.00	90.00
☑	213	0.85	0.82	41892	170	43874	8.00	9.00	9.17	20.00	25.00
☐	246	0.85	0.93	48392	170	50670	10.00	10.00	33.02	40.00	50.00
☐	263	0.85	0.93	51759	205	54173	3.50	5.00	12.83	15.00	20.00
☐	282	0.95	0.94	55521	250	58087	3.50	5.00	12.23	15.00	20.00

3 Close Manual Tune.

9.4.8 Tool Bar

Each **Manual Tune** toolbar icon is described below.

Figure 9-31 Manual Tune Tool Bar

Filament On/Off. . . . . Turns the emission on or off.

Multiplier On/Off . . . . . Turns the electron multiplier on or off.

Full Scan . . . . . Switches between displaying full scan display mode and peak scan (single peak) display mode.

Zoom . . . . . Enables the cursor to select and zoom in on a section of the screen.

Mass Adjust. . . . . Enables the cursor to select and drag a mass peak to a different position on the mass axis.

AutoTune . . . . . Starts the AutoTune function.

Mass Calibration. . . . . Verifies and corrects the ten calibration masses for correct location within the mass range.

Noise Check . . . . . Scans a **"**quiet**"** mass range (no peaks) to determine the electronic baseline and threshold noise level.

Perform Tune Checkup . . . Runs a mass calibration and noise check.

Show Target . . . . . Displays the target bar for the mass peak center and peak width at 10% peak height. Displays the target high and low percentage bars for each mass peak.

Show Bounds . . . . . Displays the peak centroid and the target peak width at 10% peak height.

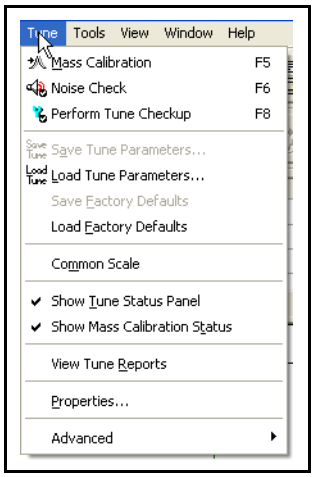
Save Tune . . . . . Saves the tune file.

Load Tune . . . . . Loads a new tune file and restarts tuning.

9.4.9 Tune Drop-Down Menu

The **Manual Tune** screen will have an additional main drop-down menu, the **Tune** menu. (See Figure 9-32.)

Figure 9-32 Tune Drop-Down menu



Mass Calibration . . . . . Verifies and corrects the ten calibration masses for correct location within the mass range.

Noise Check . . . . . Scans a **"**quiet**"** mass range (no peaks) to determine the electronic baseline and threshold noise level.

Perform Tune Checkup . . . . . Runs a mass calibration and noise check.

Save Tune Parameters... . . . . . Saves the tune file.

Load Tune Parameters... . . . . . Loads a new tune file and restarts tuning.

Load Factory Defaults . . . . . Loads the default tune settings from a factory tune file. This is intended to provide a starting point for tuning.

Common Scale . . . . . Sets all of the mass peak windows to the same common scale (Y-axis), based on Mass 117.

Show Tune Status Panel . . . . . Displays the **Tune and Mass Calibration Status** panel.

Show Mass Calibration Status . . . Displays the **Mass Calibration Status** panel.

View Tune Reports . . . . . Displays the **Tune Reports** screen.

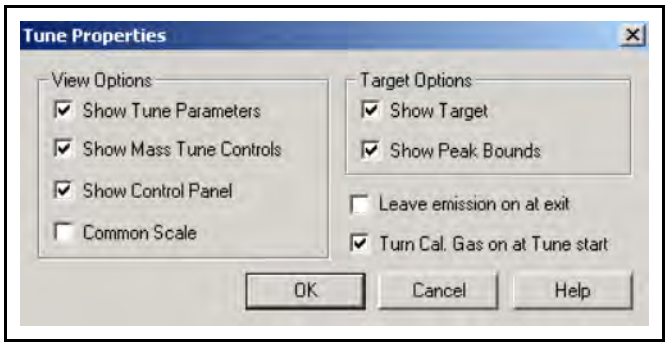
Properties . . . . . Displays the **Properties** window, which is used to set the default screen display and startup/exit conditions for **Manual Tune**. See Figure 9-23.

Advanced . . . . . Displays the **Advanced** tune functions.

- **Linearize DACS** . . . . . Repositions the mass peaks from the internal standard gas on the mass axis by linear extrapolation of the digital to analog control settings.
- **AutoTune Tolerances** . . . . . Sets the **AutoTune Tolerance** for mass resolution and mass axis position.

NOTE: The **Advanced** tune functions should only be utilized under the direction of INFICON Support personnel.

Figure 9-33 Tune Properties window



Show Tune Parameters . . . . . Displays the **EM Voltage**, **Ionizer control**, **Baseline**, **Threshold** and **Rod polarity** settings on the **Control Panel**.

Show Mass Tune Controls. . . . Displays the **Mass Tune Controls** on the **Mass Peak Scan** windows.

Show Control Panel . . . . . Displays the **Control Panel**.

Common Scale . . . . . Sets the mass peak scan windows to a common scale based on mass 117.

Show Target . . . . . Displays the target bar for the mass peak center and peak width at 10% peak height. Displays the target high and low percentage bars for each mass peak.

Show Peak Bounds . . . . . Displays the peak centroid and the target peak width at 10% peak height.

Leave emission on at exit . . . . Leaves the filament and electron multiplier on when exiting tune. This should only be used for special service procedures.

Turn Cal. Gas on at Tune start. Turns on the calibration gas, which is the internal standard gas, when the tune program is started.

9.4.10 Tune Control Panel

The **Tune Control Panel** is located on the right side of the screen and will display the individual mass peak scans, the measured intensity and the resolution. (See Figure 9-34 and Figure 9-35.)

Figure 9-34 Control Panel

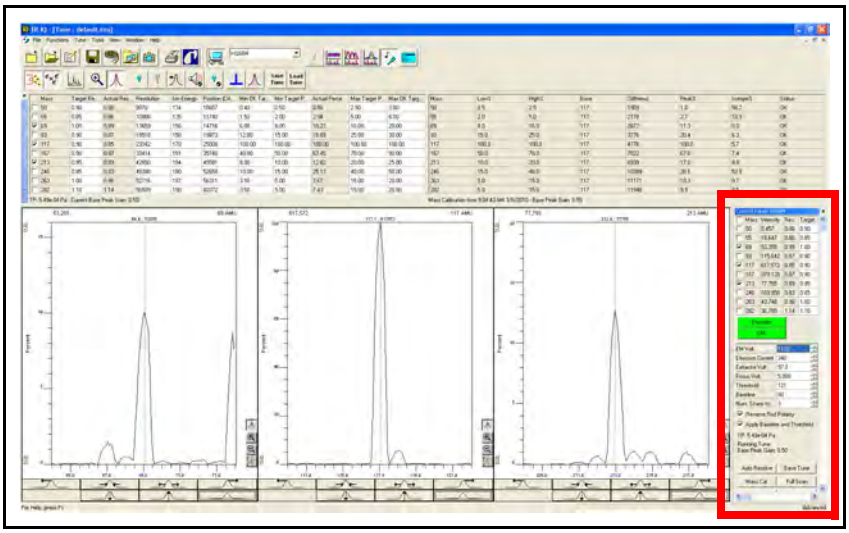
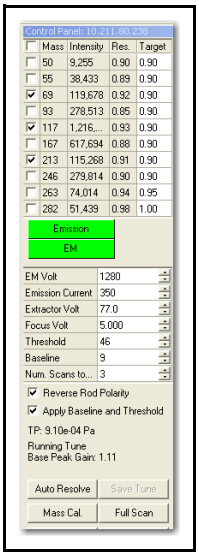


Figure 9-35 Tune Control Panel



9.4.10.1 Tune Parameters

Target Resolution . . . . . Decreasing the **Target Resolution** narrows the peak, increases the resolution and lowers the peak percentage. Increasing the **Target Resolution** will widen the peak which decreases the resolution and increases the peak percentage.

Emission . . . . . Turns the filament on and off. Green signifies that the **Emission** is on.

EM . . . . . Turns the electron multiplier on and off. Green signifies that the electron multiplier is on. Range is 1000 to 2000.

EM Volt . . . . . Increases or decreases the gain of the system. EM voltage should be set to a value that achieves a **Base Peak Gain** between 0.4 and 0.6.

Emission Current . . . . . Optimizes the ionization efficiency of the ionizer. **Emission Current** is set to achieve maximum intensity for mass 117. Range is 300 to 400. (350 is typical.)

Extractor Volt . . . . . Optimizes the ionization efficiency of the ionizer. The **Extractor Volt** setting must be set to achieve maximum intensity for mass 117. Range is 70 to 90.

Focus Volt . . . . . Optimizes the ionization efficiency of the ionizer. The **Focus Volt** setting must be set to achieve maximum intensity for mass 117. Range is 2 to 9.

Threshold . . . . . **Threshold** determines if a measured point is used in the peak area integration. If the point is used, the baseline is subtracted before use. The threshold should be set within one standard deviation of the baseline.

Baseline . . . . . The **Baseline** is the mean value of the measured noise level.

Reverse Rod Polarity . . . . . Changes the rod polarity on the mass filter and select the rod polarity that provides optimal performance at mass 117.

TP . . . . . The total MS pressure. Must be below 6E-03 for instrument to operate.

Running Tune Base Peak Gain . . . Current measured **Base Peak Gain** (BPG).

NOTE: The **Base Peak Gain** will switch to red when BPG is outside the target range.

Auto Resolve . . . . . Adjusts the resolution of all mass peaks to the target resolution.

Save Tune . . . . . Save the tune file.

Mass Cal. . . . . . Verifies and corrects the ten calibration masses for correct location within the mass range.

Full Scan . . . . . Switches between full scan display mode and peak scan display mode

Short AutoTune . . . . . Starts the AutoTune function

Noise Check . . . . . Scans a **"**quiet**"** mass range (no peaks) to determine the electronic baseline and threshold noise level.

Tune Checkup . . . . . Runs a mass calibration and noise check.

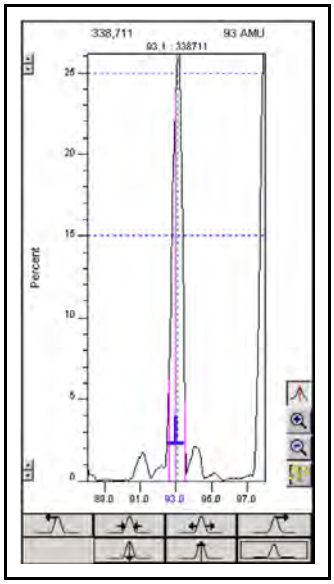
Zoom . . . . . Enables the cursor to zoom into full scan or a section of the screen.

Mass Adjust . . . . . Enables the cursor to select and drag a mass peak to a different position on the mass axis.

9.4.11 Peak Scan Window

The **Peak Scan Window**, see Figure 9-36, can be used to manually tune the mass peak.

Figure 9-36 The Peak Scan Window and Controls



9.4.11.1 Peak Scan Window Controls

Mass Adjust . . . . . Enables the cursor to select a mass peak and drag the mass peak to a different position on the mass axis.

Zoom . . . . . Enables the cursor to select and zoom into a section of the peak scan window.

Zoom Out . . . . . Returns the window to the original X axis and Y axis scale.

Zoom Out Y axis . . . . . Returns the Y axis to original scale.

Y Axis Scale . . . . . Increases or decreases the Y axis scale.

. . . . . Shifts the mass peak left.

 . . . . . Increases the peak resolution.

 . . . . . Decreases the peak resolution.

 . . . . . Shifts the mass peak right.

 . . . . . Decreases the **Ion Energy**.

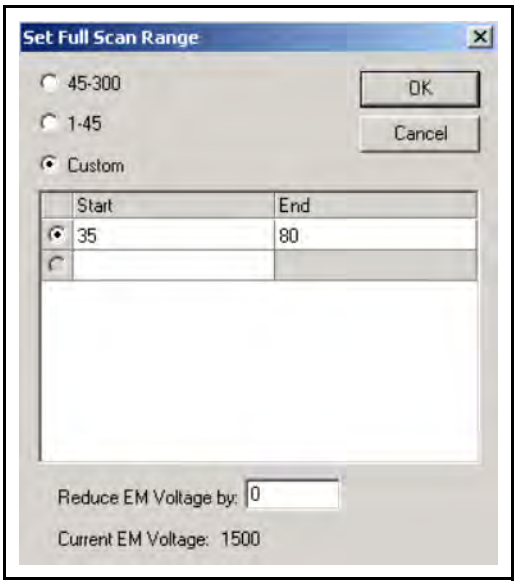
 . . . . . Increases the **Ion Energy**.

 . . . . . Zooms to a single peak scan display window.

9.4.12 Setting the Full Scan Range

Placing the mouse cursor on the x axis of the full scan window and right-clicking will display the **Set Full Scan Range** window, see Figure 9-37. This allows a custom scan range to be entered. The scan ranges of 45 to 300 amu or 1 - 45 amu can also be selected.

Figure 9-37 Setting the Full Scan Range

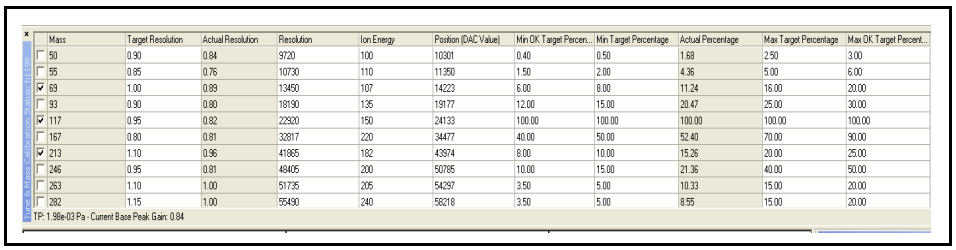


NOTE: The EM voltage will automatically be decreased by 500 volts (default) whenever a range below mass 45 is scanned.

9.4.13 Tune and Mass Calibration Status

The **Tune & Mass Calibration Status Panel** is shown in Figure 9-38.

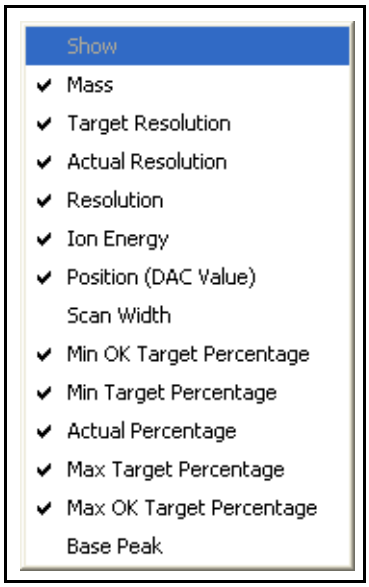
Figure 9-38 Tune and Mass Calibration Status Panel



Mass	Target Resolution	Actual Resolution	Resolution	Ion Energy	Position (DAC Value)	Min OK Target Percen...	Min Target Percentage	Actual Percentage	Max Target Percentage	Max OK Target Percent...
50	0.90	0.84	9720	100	10301	0.40	0.50	1.68	2.50	3.00
55	0.85	0.76	10730	110	11350	1.50	2.00	4.36	5.00	6.00
69	1.00	0.89	13450	107	14223	6.00	8.00	11.24	16.00	20.00
93	0.90	0.80	18190	135	19177	12.00	15.00	20.47	25.00	30.00
117	0.95	0.82	22920	150	24133	100.00	100.00	100.00	100.00	100.00
167	0.80	0.81	32817	220	34477	40.00	50.00	52.40	70.00	90.00
213	1.10	0.96	41865	182	43974	8.00	10.00	15.26	20.00	25.00
246	0.95	0.81	48405	200	50785	10.00	15.00	21.36	40.00	50.00
263	1.10	1.00	51735	205	54257	3.50	5.00	10.33	15.00	20.00
282	1.15	1.00	55490	240	58218	3.50	5.00	8.55	15.00	20.00

TP: 1.98e-03 Pa - Current Base Peak Gain: 0.84

Figure 9-39 Tune and Mass Calibration Status Menu



Mass . . . . . The mass number of the peak.

Target Resolution. . . . . **Target Resolution** at 10% peak height.

Actual Resolution. . . . . Measured resolution at 10% peak height.

Resolution. . . . . **Resolution** value; can be used to input a change in **Resolution** value.

Ion Energy. . . . . **Ion Energy** value; can be used to input a change in **Ion Energy** value.

Position (DAC Value) . . . . . Current DAC setting for mass position.

Scan Width . . . . . Displays the points measured per amu.

Min OK Target Percentage . . . . . Displays the minimum target percentage required for the mass peak to meet the **OK LOW** criteria.

Min Target Percentage . . . . . Displays the minimum target percentage required for the mass peak to meet **OK** criteria. If the actual percentage is below the minimum percentage, the box will turn red.

Actual Percentage . . . . . Displays the actual measured target percentage.

Max Target Percentage . . . . . Displays the maximum target percentage required for the mass peak to meet **OK** criteria. If the actual percentage is above the minimum percentage, the box will turn red.

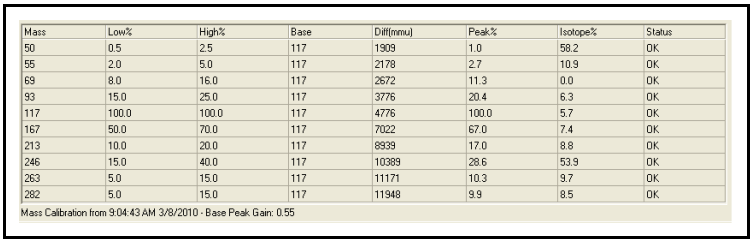
Max OK Target Percentage . . . . . Displays the maximum percentage required for the mass peak to meet the **OK High** criteria.

Base Peak . . . . . Displays the base peak, which is used to measure the mass peak percentage.

9.4.14 Mass Calibration Status

The dark gray **Mass Calibration Status** table displays the status of the last **Mass Calibration**. (See Figure 9-40.) If the **Mass Calibration** is not displayed, select **Mass Calibration** from the **Tune** drop-down menu.

Figure 9-40 Mass Calibration Status



Mass	Low%	High%	Base	Diff(mmu)	Peak%	Isotope%	Status
50	0.5	2.5	117	1909	1.0	58.2	OK
55	2.0	5.0	117	2178	2.7	10.9	OK
69	8.0	16.0	117	2672	11.3	0.0	OK
93	15.0	25.0	117	3776	20.4	6.3	OK
117	100.0	100.0	117	4776	100.0	5.7	OK
167	50.0	70.0	117	7022	67.0	7.4	OK
213	10.0	20.0	117	8939	17.0	8.8	OK
246	15.0	40.0	117	10389	28.6	53.9	OK
263	5.0	15.0	117	11171	10.3	9.7	OK
282	5.0	15.0	117	11948	9.9	8.5	OK

Mass Calibration from 9:04:43 AM 3/8/2010 - Base Peak Gain: 0.55

Mass . . . . . Mass number.

Low% . . . . . Minimum percentage for peak status to be displayed as OK.

High% . . . . . Maximum percentage for peak status to be displayed as OK.

Base . . . . . Reference mass for peak percentage calculations.

Diff(mmu) . . . . . Provides an adjustment to DAC value for mass peak alignment when necessary. 100 mmu = 0.1 amu.

Peak% . . . . . Actual peak percentage of reference mass.

Isotope% . . . . . Percentage of the Carbon 13 isotope peak as measured against the mass fragment.

Status . . . . . Status of the mass peak.

OK . . . . . Within minimum and maximum values.

OK LOW. . . . . Outside of minimum value but within acceptable tolerance.

OK HIGH . . . . . Outside of maximum value but within acceptable tolerance.

LOW. . . . . Below minimum value; needs adjustment.

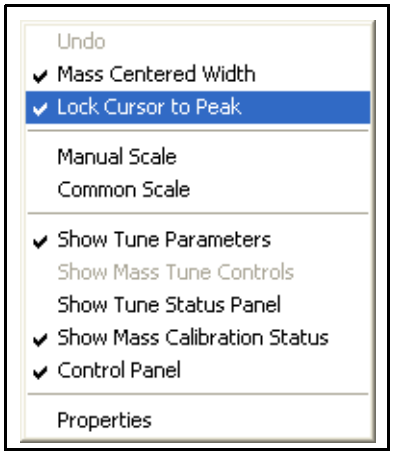
HIGH . . . . . Above maximum value; needs adjustment.

FAILED . . . . . Cannot located mass peak within window.

9.4.15 Scan Window Menu

Place the mouse cursor in the **Peak Scan** or **Full Scan** window and right-click to display the menu shown in Figure 9-41.

Figure 9-41 Scan Window Options



Undo . . . . . Returns the screen to its previous state.

Mass Centered Width. . . . . Width in amu that correctly aligns the calibration peak on the mass axis.

Lock Cursor to Peak . . . . . Locks the cursor to the mass peak to adjust the mass position.

Manual Scale . . . . . Allows the mass peak windows to be set to a user defined scale.

Common Scale . . . . . Sets the mass peak scan windows to a common scale based on mass 117.

Show Tune Parameters . . . . . Displays the **EM voltage**, **Ionizer Control**, **Baseline**, **Threshold** and **Rod Polarity** settings on the **Control Panel**.

Show Mass Tune Controls . . . . . Displays the mass tune controls on the mass peak scan windows.

Show Tune Status Panel . . . . . Displays the **Tune Status** panel.

Show Mass Calibration Status . . . Displays the **Mass Calibration Status** control panel.

Control Panel . . . . . Displays the **Control Panel**.

Properties . . . . . Displays the **Properties** window.

9.4.16 Tune Status Window Menu

Place the mouse cursor in the **Tune Status** panel or the **Mass Calibration Status** panel and right-click to display the menu shown in Figure 9-42.

Figure 9-42 Menu in Tune Status Panel

Print... . . . . . Prints the **Tune Status** panel or the **Mass Calibration Status** panel.

Show Tune Status Panel . . . . . Displays the **Tune Status** panel.

Show Mass Calibration Status . . . Displays the **Mass Calibration Status** panel.

Tile Grids Horizontally . . . . . Tiles the **Status and Calibration Status** panels horizontally.

Tile Grids Vertically . . . . . Tiles the **Status and Calibration Status** panels vertically.

Size Columns To Grid . . . . . Resets the column size to the current grid.

Dock. . . . . Locks the display position to a fixed position.

Properties.... . . . . Displays the **Properties** window.

Chapter 10
Method Editor

10.1 The Method Editor

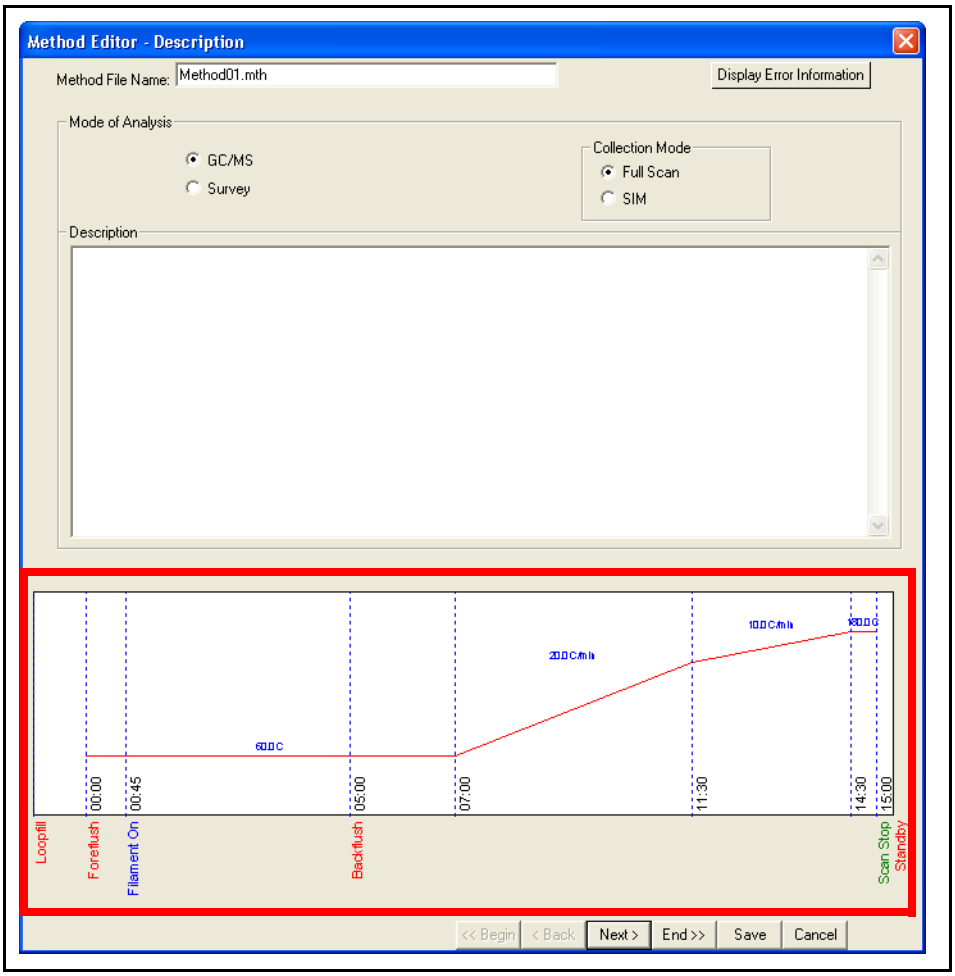
The **Method Editor** function in **ER IQ** creates methods to identify and quantify volatile organic compounds. The **Method Editor** function is composed of the following pages:

- The **Description** page for entering a description of the method.
- The **Startup** page for selecting the type of method, such as **Probe**, **Headspace**, **SituProbe** or **SPME**, to be created. Temperature settings are also selected on this page.
- The **Inlet** page defines the temperatures, timing, inlet and valve states.
- The **Search** page designates the calibration library for the method. This page also sets the **Library Search Parameters.**
- The **Data** page sets the **Data File (file extension.hps)** component and specifies where the data will be stored. By default, the data file pathway uses the pathway of IQ Software\H###\Data\method name\file name.file extension.
- A **Summary** page is provided, at the end of the **Method Editor**, to review and print the method parameters.

  NOTE: Methods cannot be viewed, created or changed when the access level is set to **Normal**.

Each page of the **Method Editor** shows a profile at the bottom of the **Inlet States** and **Temperature**. See Figure 10-1. For questions relating to method development, please contact INFICON for application support.

Figure 10-1 Method Profile



Newly created methods start with a default set of **Inlet States** and a default **Temperature Profile**, which can be modified as required by the application.

NOTE: The bottom of each page will display the inlet states, see section 10.6.1, Inlet States, on page 10-14 for more information, and the temperature profile, see section 10.6.2, GC Temperature Profile, on page 10-18 for more information.

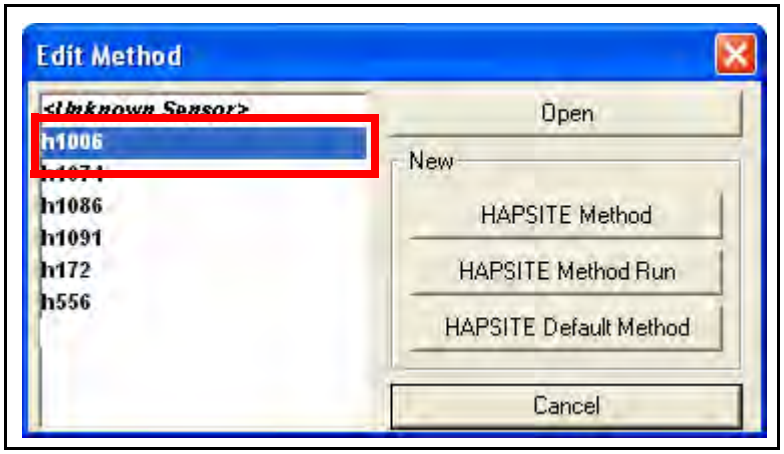
To access Method Editor:

1 On the **System Setup** screen, double-click on the **Method Editor** icon. See Figure 10-2.

Figure 10-2 Method Editor Icon

2 If more than one unit is connected to the laptop, click on the name of the desired HAPSITE ER. See Figure 10-3.

Figure 10-3 Method Editor Open Window



There are four options for accessing a method:

Open . . . . . Opens an existing HAPSITE method for modification.

Method . . . . . Opens a blank method template to modify as necessary.

Method Sequence . . . . . Allows a method to be automatically repeated or a series of methods to be run together. See Method Sequence, see section 10.13 on page 10-64.

Default Method . . . . . Selects a default method. See Loading Default Methods, see section 10.2.1 on page 10-3.

Cancel . . . . . Closes the **Edit Method** window.

10.2 Reloading Default HAPSITE Methods

Default methods can be loaded onto the laptop in case the methods have been deleted or modified.

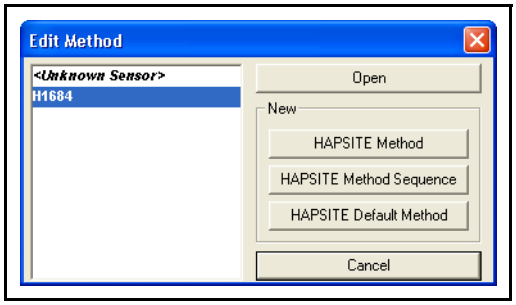
10.2.1 Loading Default Methods

1 Double-click the **Method Editor** icon.

Figure 10-4 Method Editor

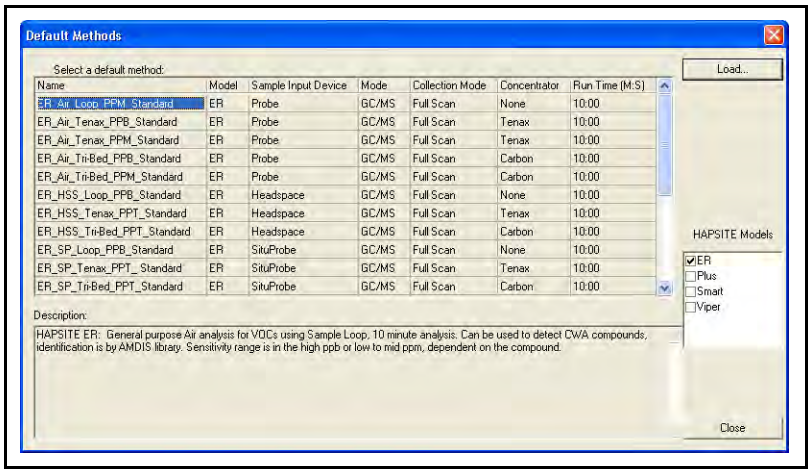
2 Select **HAPSITE Default Method** to access the default methods. See Figure 10-5.

Figure 10-5 Method Editor



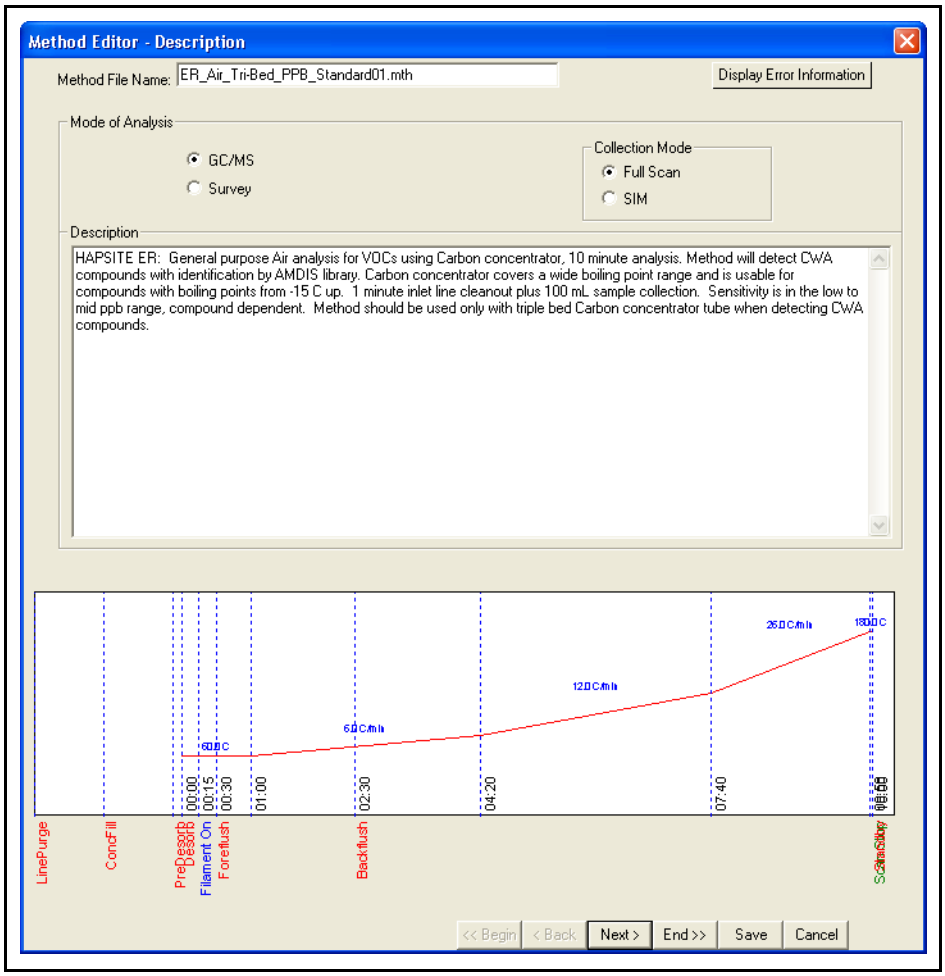
3 Verify that **ER** is checked on the right side of the window. Highlight the desired method and click **Load.** See Figure 10-6. See Default Methods, see section 10.3 on page 10-6 for a description of the methods.

Figure 10-6 HAPSITE Default Methods



4 The **Description** page will be displayed.

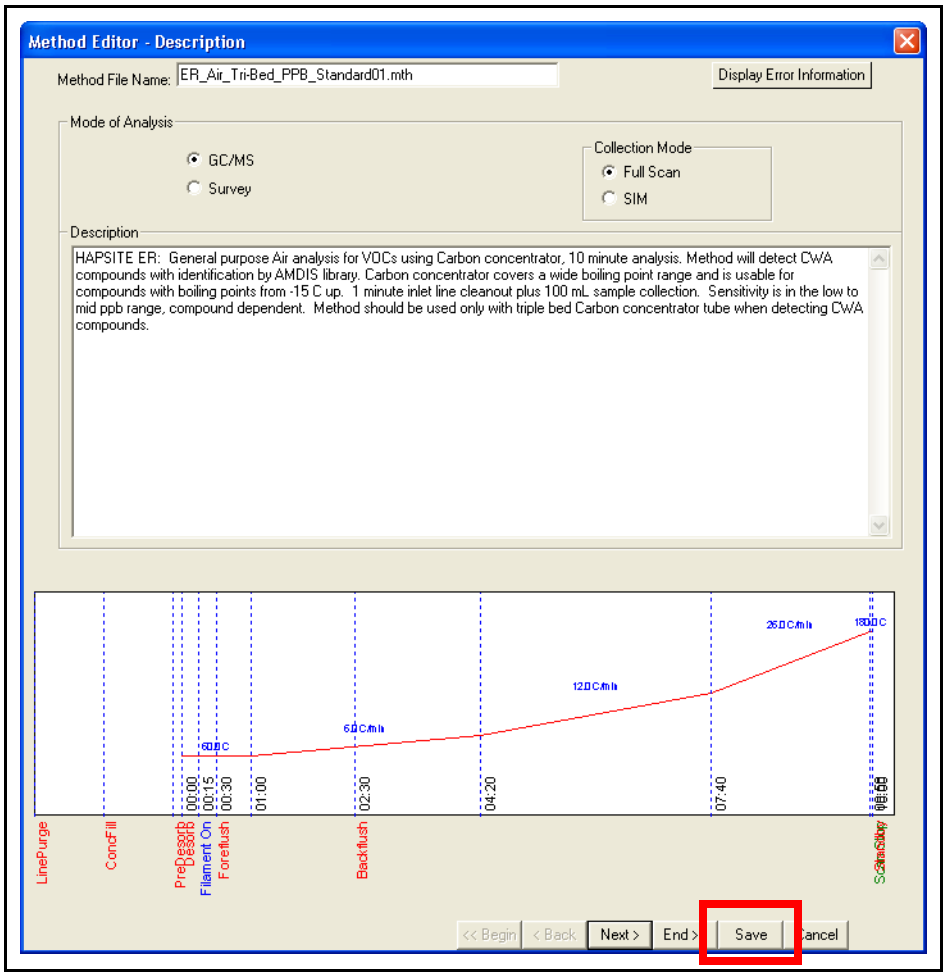
Figure 10-7 Description Page



5 Click the **Save** button at the bottom of the **Method Editor-Description** page. See Figure 10-8.

NOTE: Two digits will be appended to the method file name (i.e., 01). If the two digits are not desired, remove them before clicking the **Save** button.

Figure 10-8 Saving the Method



10.3 Default Methods

The methods found in the **Default Methods** window are general purpose methods for each of the HAPSITE configurations.

ER_Air_Tri-Bed_PPB_Standard . . Carbon concentrator method (10 minute analysis time)

ER_Air_Tri-Bed_PPM_Standard . . Carbon concentrator method to be used in lieu of ER_Air_Loop_PPM_Standard (10 minute analysis time)

ER_Air_Tenax_PPM_Standard . . . Tenax concentrator method to be used in lieu of ER_Air_Loop_PPM_Standard (10 minute analysis time)

ER_Air_Tenax_PPB_Standard . . . VOC and Chemical Warfare Agent Air Analysis using Tenax Concentrator (10 minute analysis sample time. Consists of 1 minute inlet purge plus one minute sample collection.)

ER_Air_Loop_PPM_Standard . . . . VOC and Chemical Warfare Agent analysis using Sample Loop (10 minute analysis time)

ER_HSS_Tri-Bed_PPT_Standard . VOC and Chemical Warfare Agent Headspace solid/liquid analysis using the Tri-Bed concentrator (10 minute analysis time)

ER_HSS_Loop_PPB_Standard . . . VOC and Chemical Warfare Agent Headspace solid/liquid analysis using the Sample Loop(10 minute analysis time)

ER_HSS_Tenax_PPT_Standard . . VOC and Chemical Warfare Agent Headspace solid/liquid analysis using the Tenax concentrator (10 minute analysis time)

ER_SP_Tri-Bed_PPT_Standard . . VOC water analysis using the Tri-Bed concentrator (10 minute analysis time)

ER_SP_Loop_PPB_Standard . . . . VOC water analysis using the Loop concentrator (10 minute analysis time)

ER_SP_Tenax_PPT_Standard. . . . VOC water analysis using the Tenax concentrator (10 minute analysis time)

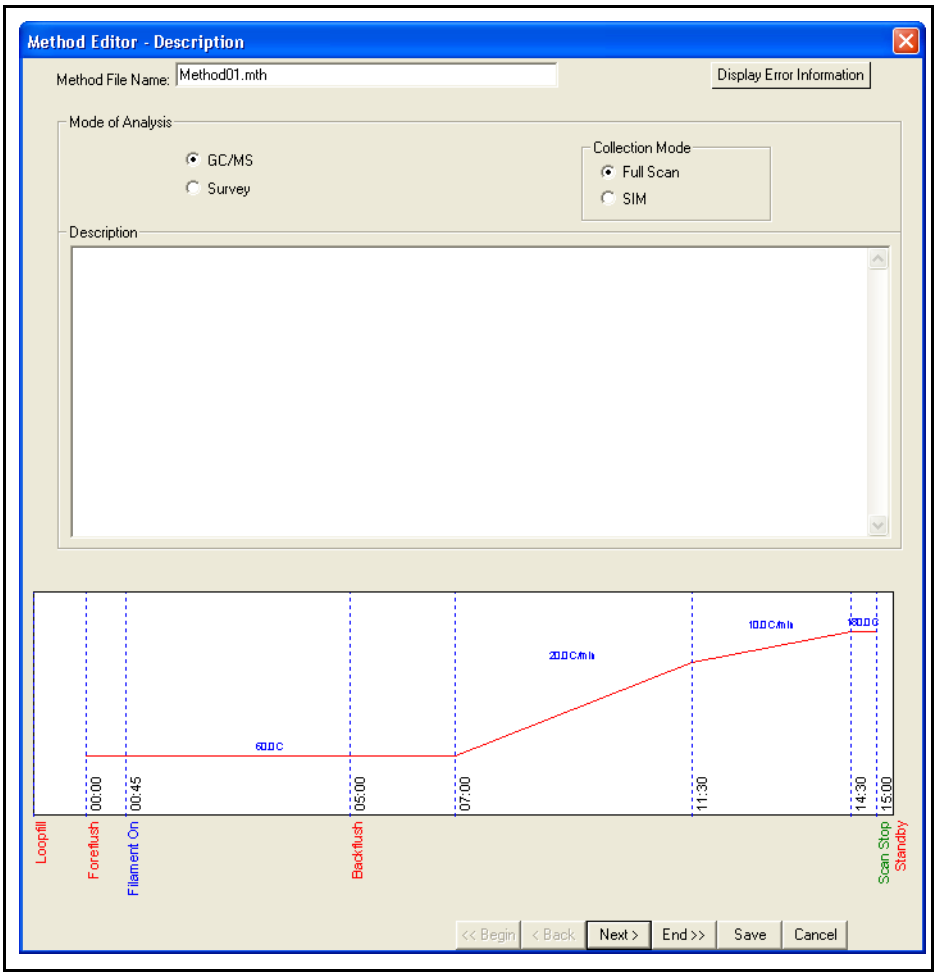
ER Survey . . . . . Quick screening method for VOCs. (Analysis time is determined by the user. Method will turn off after 5 minutes.)

10.4 Description Page

The first page displayed in the **Method Editor** is the **Description** page (Figure 10-9). This page will appear after clicking **Open**, **HAPSITE Method** and **HAPSITE Default Method**. A description of the method and the method name can be entered into this screen. A temperature profile with the inlet states is displayed at the bottom of all of the method pages.

NOTE: A method file ends with a file extension of .mth.

Figure 10-9 Method Editor Description Page



Mode of Analysis

Analyze (GC/MS) . . . . . This analysis uses both the Gas Chromatograph (GC) and Mass Spectrometer (MS) to separate and analyze compounds. Compounds are identified using a library search.

Survey . . . . . This mode uses only the Mass Spectrometer to provide a near real-time response. Samples flow directly to the Mass Spectrometer and are not separated by the GC.

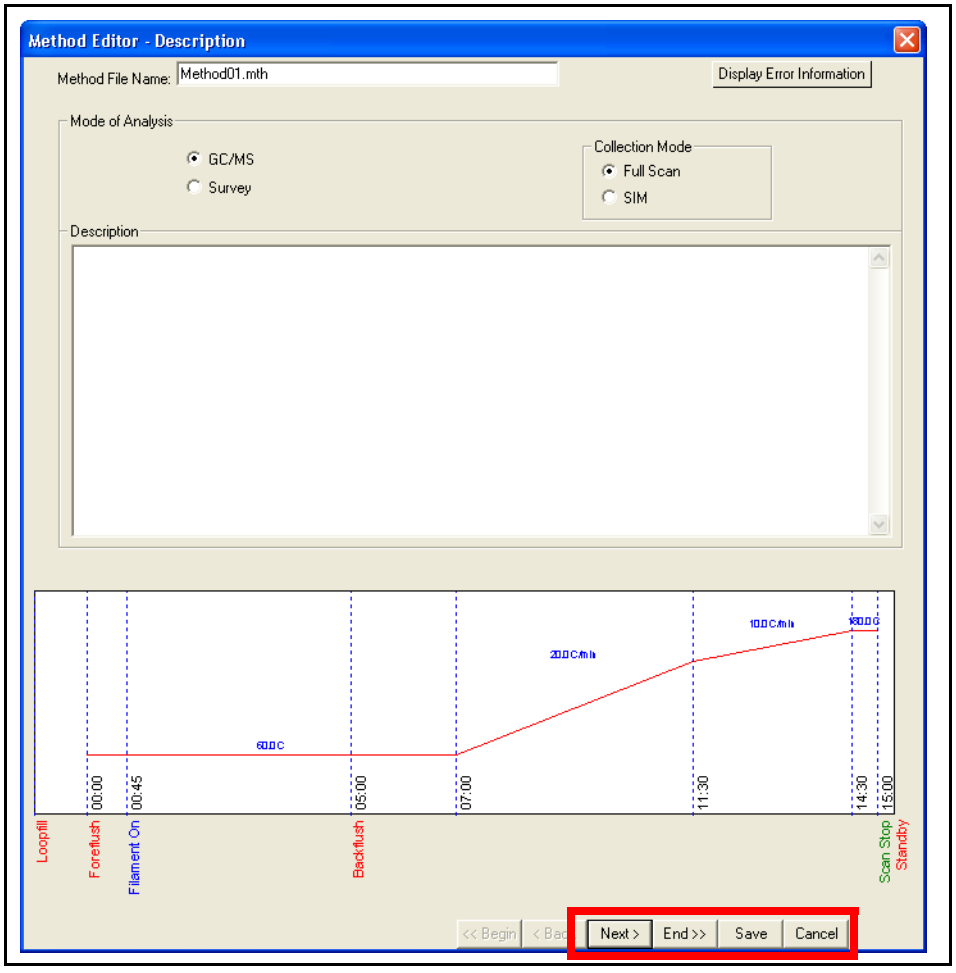
Collection Mode

Full Scan . . . . . This mode scans all the masses across a given range, which is 42-300 for default methods. It is used to identify unknown samples. Full Scan is available for both Analyze (GC/MS) and Survey modes.

SIM . . . . . This stands for Selected Ion Monitoring. This collection mode is more sensitive than a full scan method, because it only scans for user selected mass fragments. Prior to creating a SIM method, the sample components must be identified and their retention times must be known. SIM mode is available in both Analyze (GC/MS) and Survey modes.

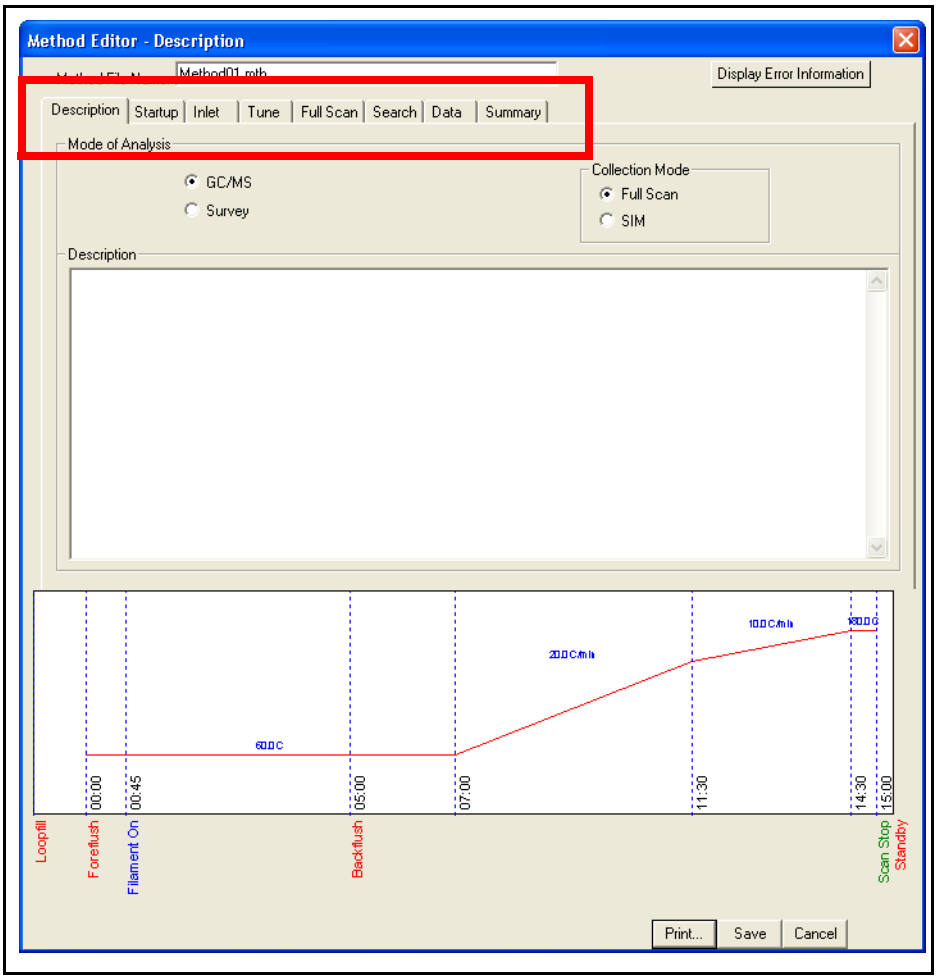
The **Method Editor** can be run in **Wizard Mode**, which moves through the method creation in a logical sequence. Adjustments can be made using the **Back** and **Next** buttons. Figure 10-10 shows the **Wizard Mode** navigation buttons.

Figure 10-10 Method Editor Navigation Buttons



In **non-Wizard** mode, which is recommended only for experienced users, all pages are available through a tabbed window. To change the **Wizard** mode settings, refer to section 7.3.3.3, Miscellaneous Tab, on page 7-8 for instructions. See Figure 10-11.

Figure 10-11 System Properties Miscellaneous Page Wizard Setting

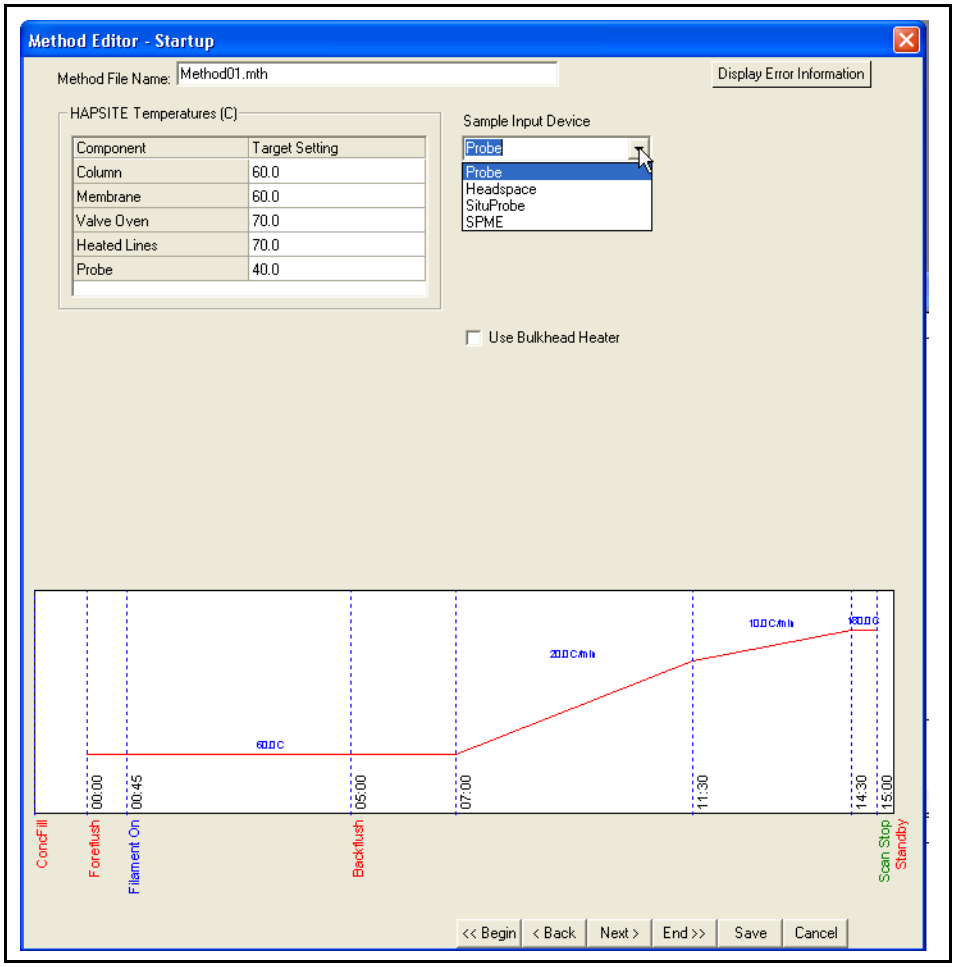


NOTE: All method parameters on each page of the **Method Editor** are checked for synchronization and correctness. The **Method Editor** function will highlight all questionable parameters in yellow, when a discrepancy occurs. The **Method Editor** permits movement from page to page, even when errors are present.

10.5 Startup Page

The **Startup** page, displayed in Figure 10-12, displays the initial settings for the **HAPSITE ER** system heaters. The initial temperature settings for the components described in **HAPSITE Temperatures (C)** can be modified on this page. The **Sample Input Device** (i.e., **Probe**, **Headspace**, **SituProbe** or **SPME**) can be selected on this page.

Figure 10-12 Method Editor Startup Page for Survey Methods



The parameters on the **Startup** page are:

HAPSITE Temperatures (C)

Column . . . . . The initial **Column** temperature setting

Membrane . . . . . The target **Membrane** temperature setting.

Valve Oven . . . . . The target **Valve Oven** temperature setting.

Probe . . . . . The target **Probe** temperature setting. This setting is not available when the **Headspace** or **SituProbe** is enabled.

Sample Input Device

Probe . . . . . Select **Probe** when using the air probe to sample volatile organic compounds in the air.

Headspace . . . . . Select **Headspace** when using this accessory to analyze solids and liquids for volatile organic compounds.

SituProbe . . . . . Select **SituProbe** when using this accessory to analyze volatile organic compounds in liquid samples.

Internal Standard Box

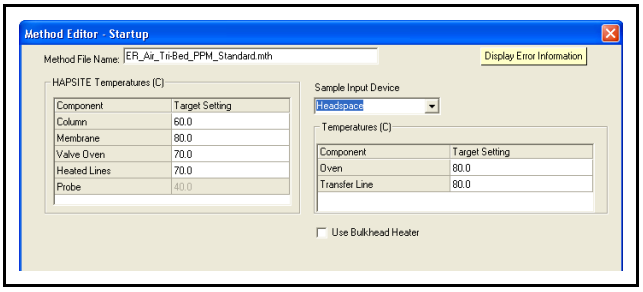
Use Internal Standard . . . . . The **Use Internal Standard** option is available when creating Survey methods. Refer to Figure 10-12.

Headspace Temperatures (C)

Oven . . . . . The target **Oven** temperature setting for the Headspace. See Figure 10-13

Transfer Line . . . . . The target **Transfer Line** temperature setting for the **Headspace**. See Figure 10-13.

Figure 10-13 Headspace Temperatures



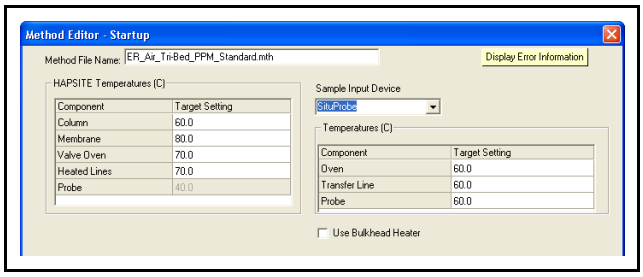
SituProbe Temperatures (C)

Oven . . . . . The target **Oven** temperature setting for the SituProbe. See Figure 10-14.

Transfer Line . . . . . The target **Transfer Line** temperature setting for the SituProbe. See Figure 10-14.

Probe . . . . . The target **Probe** temperature setting for the SituProbe sampling probe. See Figure 10-14.

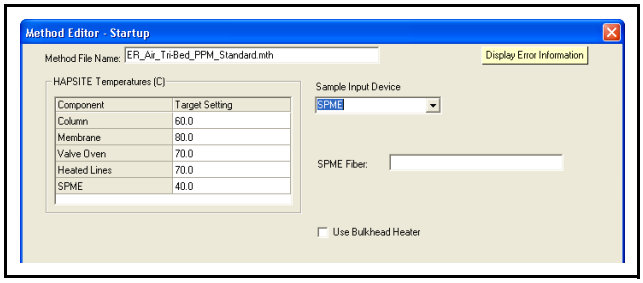
Figure 10-14 SituProbe Temperatures



SPME

SPME Fiber . . . . . Type in the color of the desired fiber into the box. See Figure 10-15.

Figure 10-15 SPME Fiber

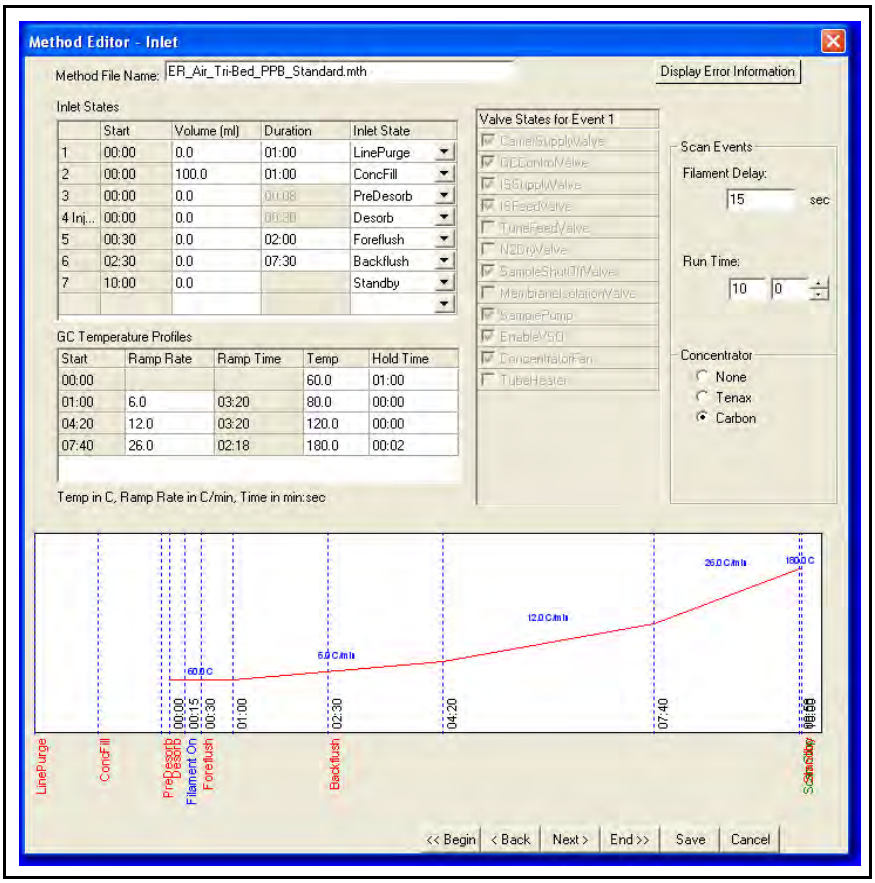


10.6 Inlet Page

NOTE: This page is only available when creating an **Analyze** (GC/MS) method.

The **Inlet** page displays the default settings for the **Inlet States**, **GC Temperature Profiles** and **Valve States**. Adjusting settings on the **Inlet** page may affect other method parameters and/or the retention time. The **Start** time of each **Inlet State** event is displayed in combination with the temperature profile at the bottom of the **Inlet** page. See Figure 10-16.

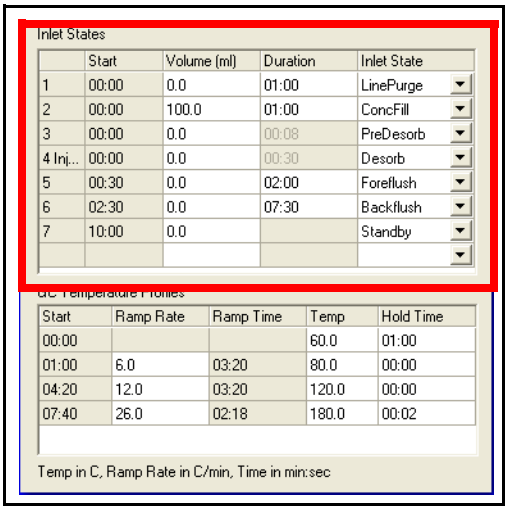
Figure 10-16 Method Editor Inlet Page for GC/MS Full Scan



10.6.1 Inlet States

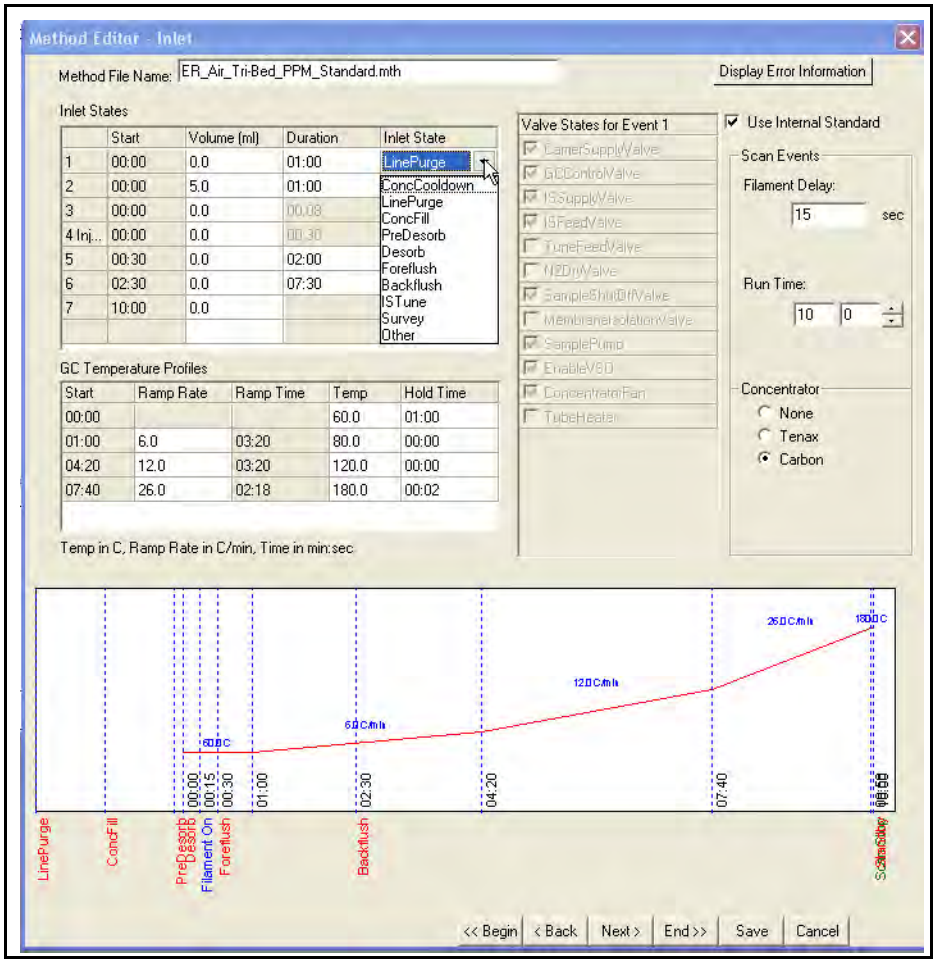
Inlet States control the **HAPSITE ER** and accessory valve settings for sampling, analysis and purging of the **HAPSITE ER**. Figure 10-17 shows the grid used to program the **Inlet States**.

Figure 10-17 Method Editor Inlet Page: Inlet States



To edit the **Inlet States** grid, select an **Inlet State** from the drop-down menu. See Figure 10-18.

Figure 10-18 Inlet States



The following choices are available for all Analyze methods in the **Inlet States** column:

Line Purge . . . . . Directs the sample throught the sample pathway and out through the exhaust vent. The sample does not pass through the concentrator.

Foreflush . . . . . Directs the carrier gas to allow the sample to flow out of the sample loop/concentrator and onto the column.

Backflush . . . . . Directs the carrier gas to the front end of the column. This state will remove non-volatile contaminants, while allowing the volatile compounds to be separated on the column.

ISTune . . . . . Directs the internal standard to the MS for tuning.

Survey . . . . . Turns on the sampling pump and directs the sample to the inlet of the MS.

Other . . . . . Customizes each specific GC valve for a custom GC valve state. Useful for GC troubleshooting.

Standby . . . . . **Standby** is the last state of every method. **Standb**y closes the **Membrane Isolation** valve and turns off the MS filament.

The following additional **Inlet States** are available in the **Inlet States** column when a sample loop is being used:

Loopfill . . . . . Controls the sample pump and directs the sample through the sample loop.

The following additional **Inlet States** are available in the **Inlet States** column when a concentrator is being used:

ConcFill . . . . . Controls the sample pump. This step directs the sample through the concentrator to allow the analytes to absorb to the concentrator bed.

ConcCooldown . . . . . The concentrator is cooled to a desired operating temperature.

PreDesorb . . . . . **PreDesorb** starts the desorption of analytes from the concentrator process.

Desorb . . . . . Completes the analyte desorption process. This state directs the analytes to the GC column.

The following **Inlet States** are only available in the **Inlet States** column when the **HSS** is enabled for use:

HSSample . . . . . Turns on the sample pump to direct sample through the transfer line to the **HAPSITE ER**. The suggested **HSSample** duration is approximately 15 seconds.

HSPurge . . . . . Directs carrier gas flow through the lines, the needle assembly and the transfer line to remove moisture and clean out the previous sample.

HSConcDry . . . . . Directs carrier gas flow through the transfer line and concentrator to remove moisture prior to sample injection. This should only be used if the **HSS** is connected to an external cylinder of carrier gas.

The following Inlet States are only available when the **SituProbe** is attached:

SPLinePurge . . . . . Directs carrier gas through the lines, **SituProbe** assembly and the transfer line to clear out carryover from a previous sample.

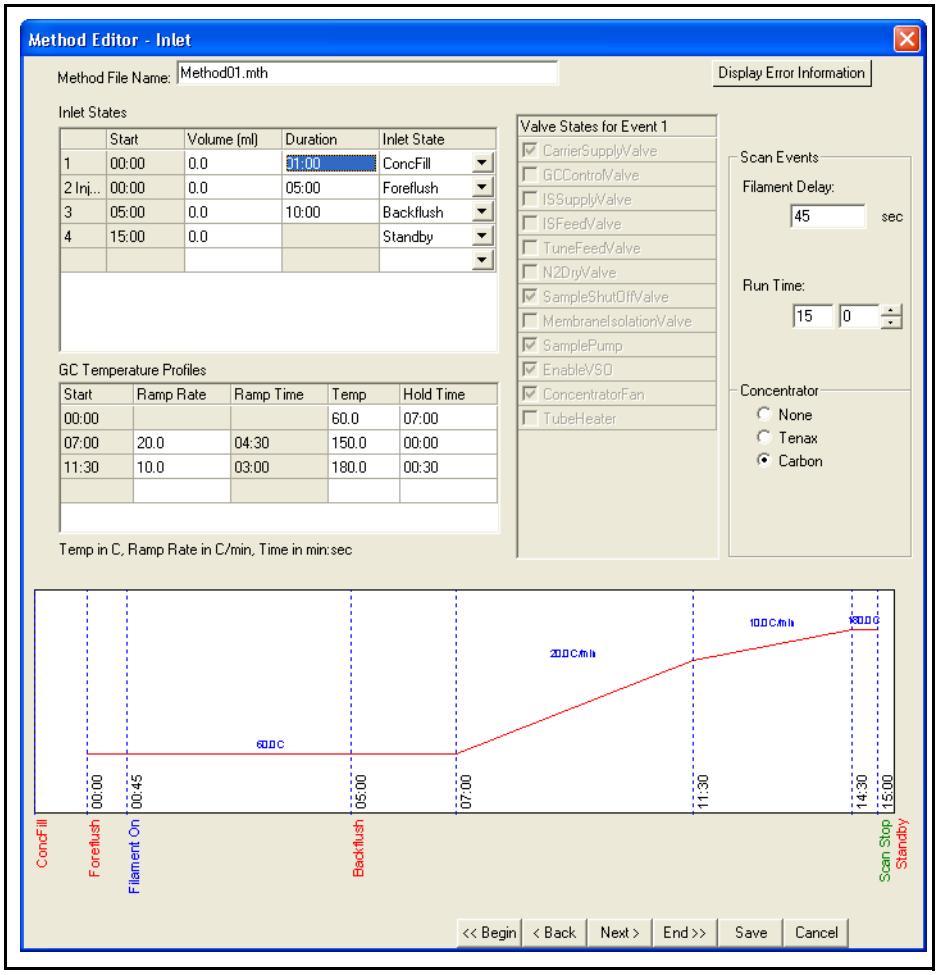
SPConcFill . . . . . Controls the sample pump and directs the sample through the concentrator

SPLoopFill . . . . . Controls the sample pump and directs the sample through the sample loop.

SPN$_2$DryPurge . . . . . Purges the transfer line and concentrator with carrier gas before sample injection to remove moisture.

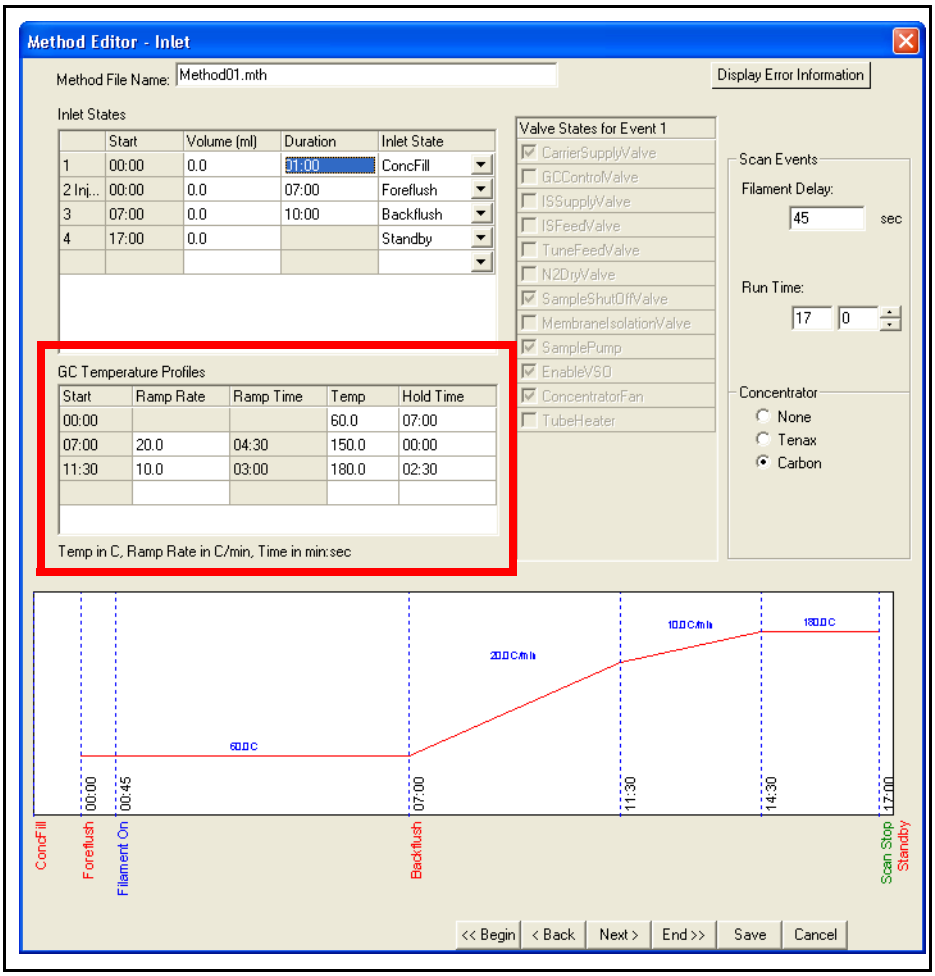
After selecting the **Inlet State**, enter the desired time period for the event in the **Duration** column. See Figure 10-19.

Figure 10-19 Inlet State



Upon entering the **Duration** settings, the **Start** time will be automatically calculated for the next **Inlet State**. See Figure 10-20.

Figure 10-20 Start Time Updating



Events can be deleted from the template. Click inside the desired cell in the grid and press the **Delete** key on the laptop keyboard.

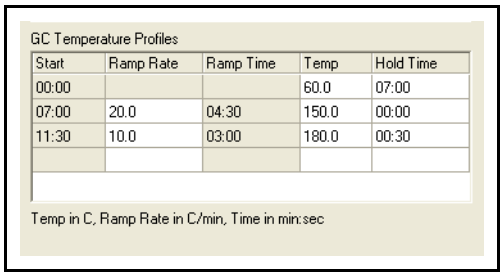
Events can be inserted into the template. Click inside the cell that will precede the desired event and press the **Insert** key on the laptop keyboard to insert a row.

NOTE: Rows cannot be inserted after the **Standby** event

10.6.2 GC Temperature Profile

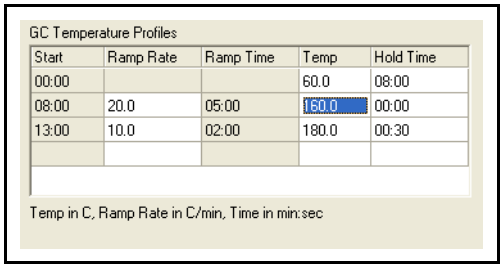
GC Temperature Profiles specify the column temperature, ramp rate and hold settings for the **HAPSITE ER** Method. Adjusting the temperature program will change the retention times of the internal standards.

Figure 10-21 Method Editor Inlet Page: GC Temperature Profiles



Adjustments to the **Hold Time**, **Ramp Rate** and **Temp** columns will automatically update dependent parameters. For example, increasing the **Temp** will increase the **Ramp Time** and increasing the **Hold Time** will adjust the **Start** time of the next parameter. See Figure 10-22.

Figure 10-22 Changing GC Temperature Profiles

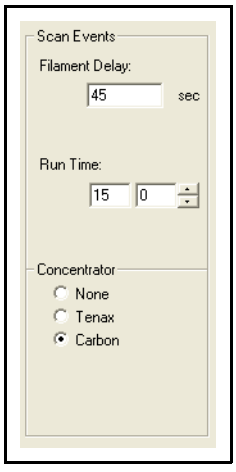


NOTE: A maximum of four lines is permitted in this section.

10.6.3 Scan Events

The items displayed in the **Scan Events** field is dependent upon the type of method.

Figure 10-23 Scan Events For Probe and SPME



The **Filament Delay** delays the turning on of the filament. This protects the filament by allowing the components of the air peak or solvents to pass through the Mass Spectrometer.

CAUTION

If the Filament delay is too short, the high pressure burst caused by a solvent peak may shut down the HAPSITE ER and stop the analysis.

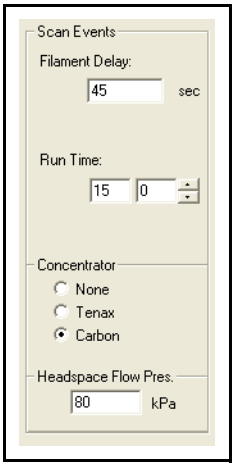
The **Run Time** is the amount of time that the method will run.

The type of concentrator being used is selected in the **Concentrator** box. The options are None, Tenax or Carbon. See section 4.4.2, Tenax Concentrator, on page 4-25 and section 4.4.1, Tri-Bed Concentrator, on page 4-25 for more information on differences between concentrators.

10.6.4 Headspace Flow Parameter

The **Scan Events** field for Headspace has an additional parameter, **Headspace Flow Pressure**. **Headspace Flow Pressure** controls the flow rate of carrier gas through the **HSS** during the **Sample** and **Purge** states. This parameter is only available when the creating **HSS** methods.

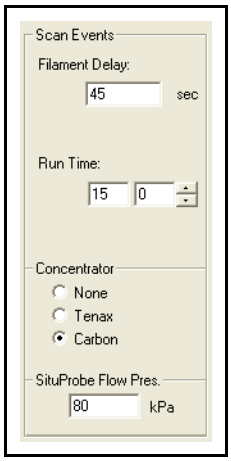
Figure 10-24 Headspace Flow Parameter



10.6.5 SituProbe Flow Parameter

The **Scan Events** field for the **SituProbe** has an additional parameter, **SituProbe Flow Pressure**. **SituProbe Flow Pressure** controls the flow rate of carrier gas through the **SituProbe** during the **Sample** and **Purge** states. This parameter is only available when creating **SituProbe** methods.

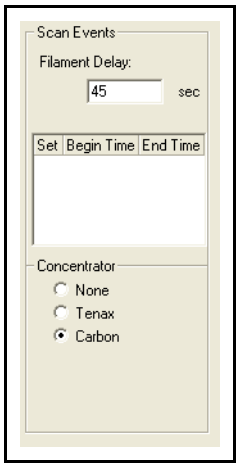
Figure 10-25 SituProbe Flow Pressure



10.6.6 Scan Events for SIM Methods

When creating SIM methods, the beginning and end time for each scan set will be displayed. See Figure 10-26. Adjustments to these times can be made on the SIM page. See section 10.9, SIM Page, on page 10-26 for more details.

Figure 10-26 SIM Methods



10.7 Tune Page

The **Tune** page contains two tabs, **Report** and **Param**. Each provide information about the **Tune** file.

10.7.1 Param Page

The **Param** tab (see Figure 10-27) displays the tune filename, which sets the MS tune parameters for the method. The default filename is **`default.tun`**. If a different tune file is desired, the **Browse** button can be used to locate and specify the desired tune for the method.

This page also has a **Show Details** checkbox (Figure 10-28), which will produce a grid of tune parameters contained in the file. These parameters cannot be edited. If editing is desired, refer to Chapter 9, Tune.

Figure 10-27 Method Editor Tune Parameter Page

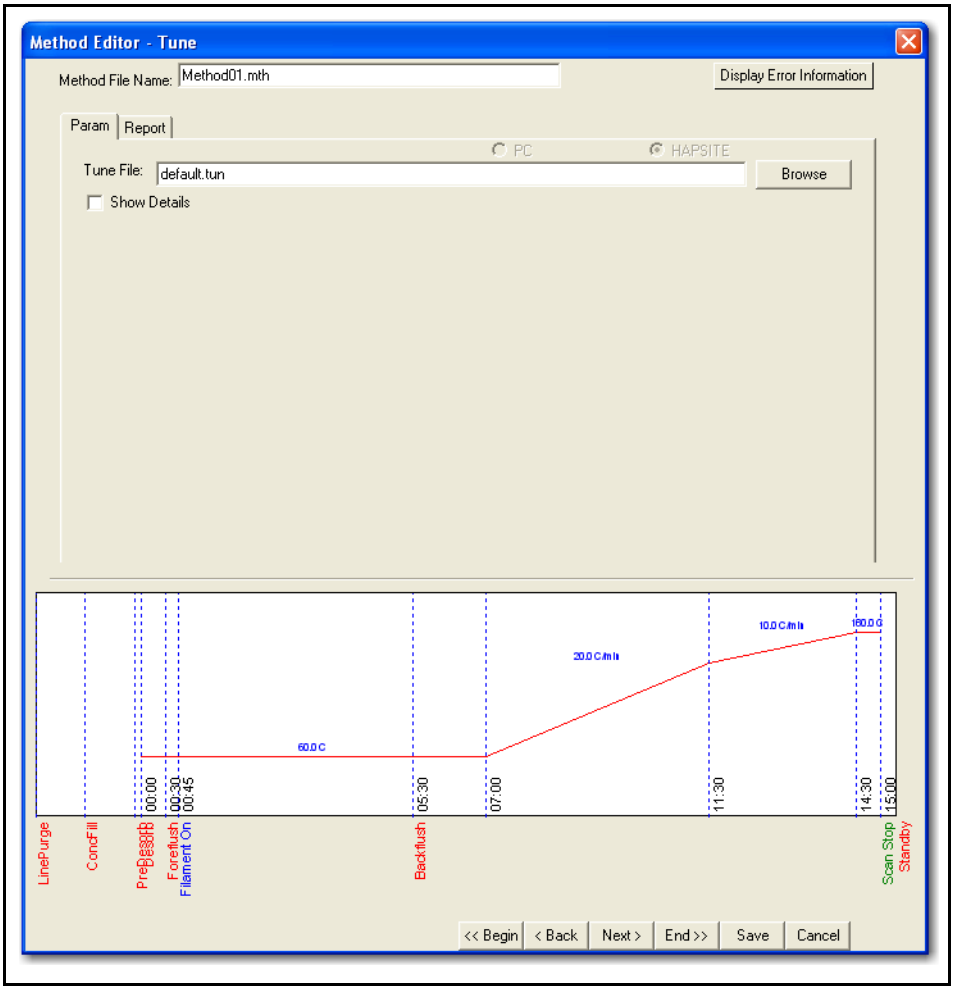
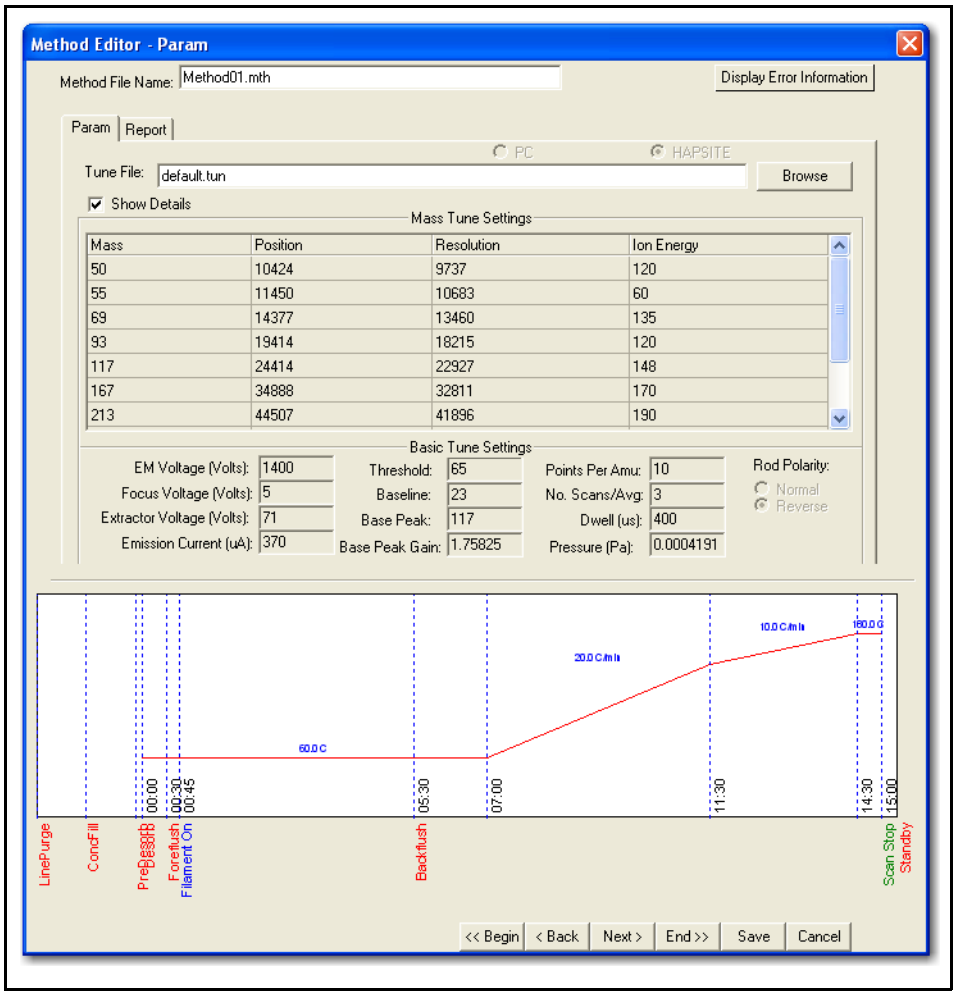


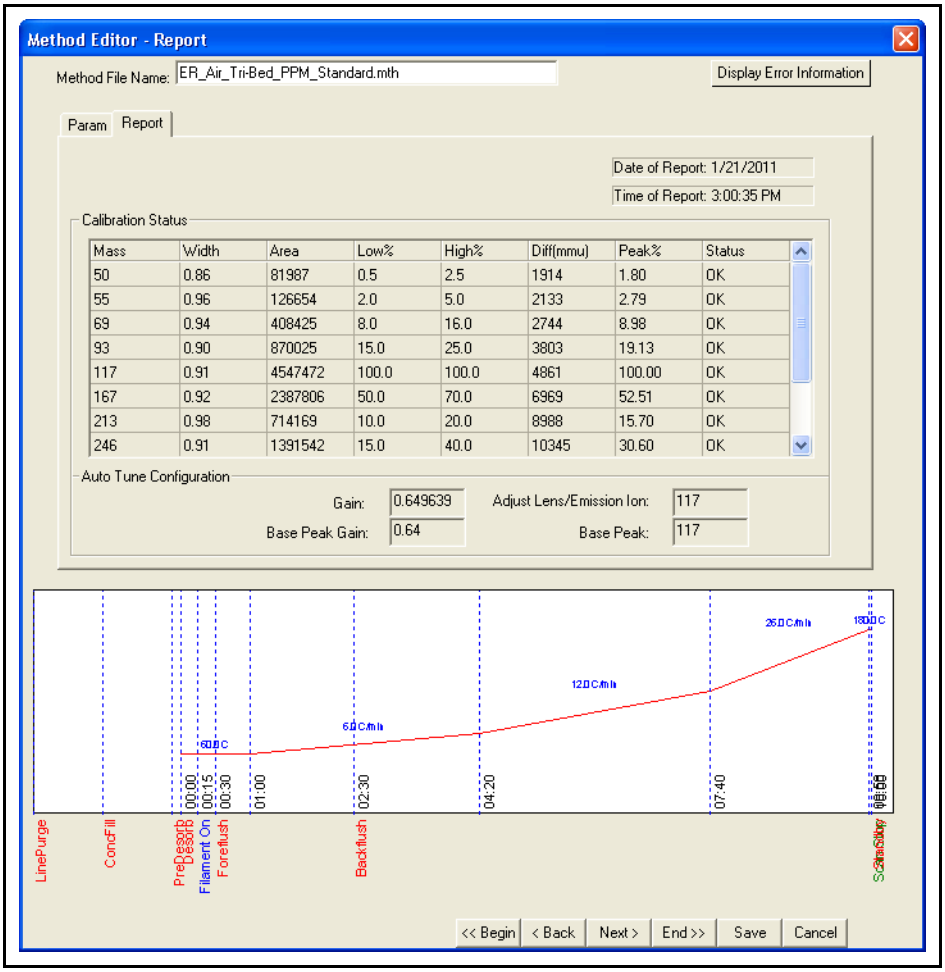
Figure 10-28 Method Editor Tune Parameter Page - Show Details



10.7.2 Report Page

The **Report** page (see Figure 10-29) displays the AutoTune report in a printable format.

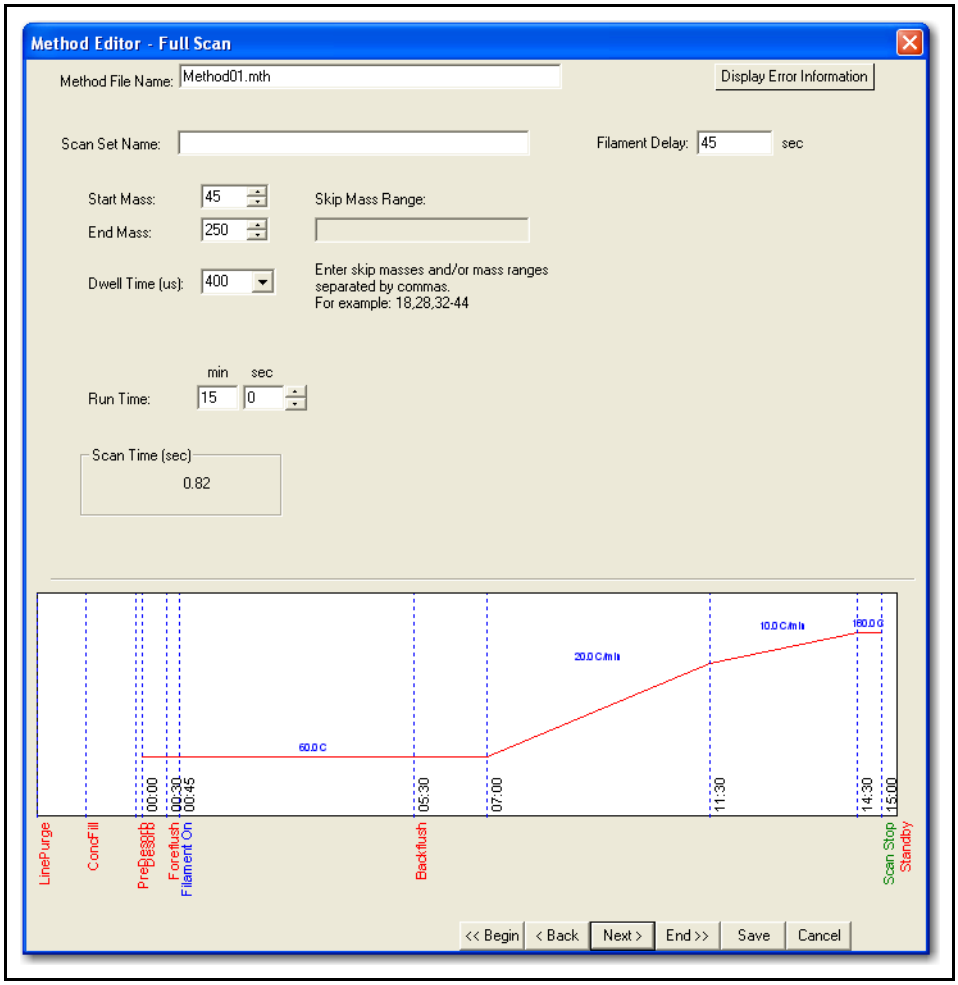
Figure 10-29 Method Editor Tune Report Page



10.8 Full Scan Page

The **Full Scan** page sets the mass ranges for the method. The set can be assigned a **Scan Set Name** for easy identification, if desired. The **Filament Delay**, from the **Inlet Page** (see section 10.6.3, Scan Events, on page 10-19), is also shown on the **Full Scan** page. Changing the **Filament Delay** on this page may require changes to the **Inlet Page**.

Figure 10-30 Method Editor Full Scan Page



The following Mass Spectrometer parameters can be programmed:

Start Mass . . . . . The mass at which the Mass Spectrometer will start to scan. The starting mass can be set from 1 to 300 amu, however values between 40-50 are recommended to avoid detection of high-volatility interferences

End Mass . . . . . The mass at which the Mass Spectrometer will end a scan. The end mass can be set from 1-300 amu. This value must be larger than the start mass.

NOTE: End the scan at least 2 amu above any mass used for compound identification. However, do not increase the end mass higher than necessary, as this will increase the scan time and a lower number of scans will be collected.

Dwell Time . . . . . The **Dwell Time** is the length of time the Mass Spectrometer will sample data at each sampling point. The longer the **Dwell Time**, the better the signal to noise ratio of the analyte.

Run Time . . . . . The time span of the method from start to finish.

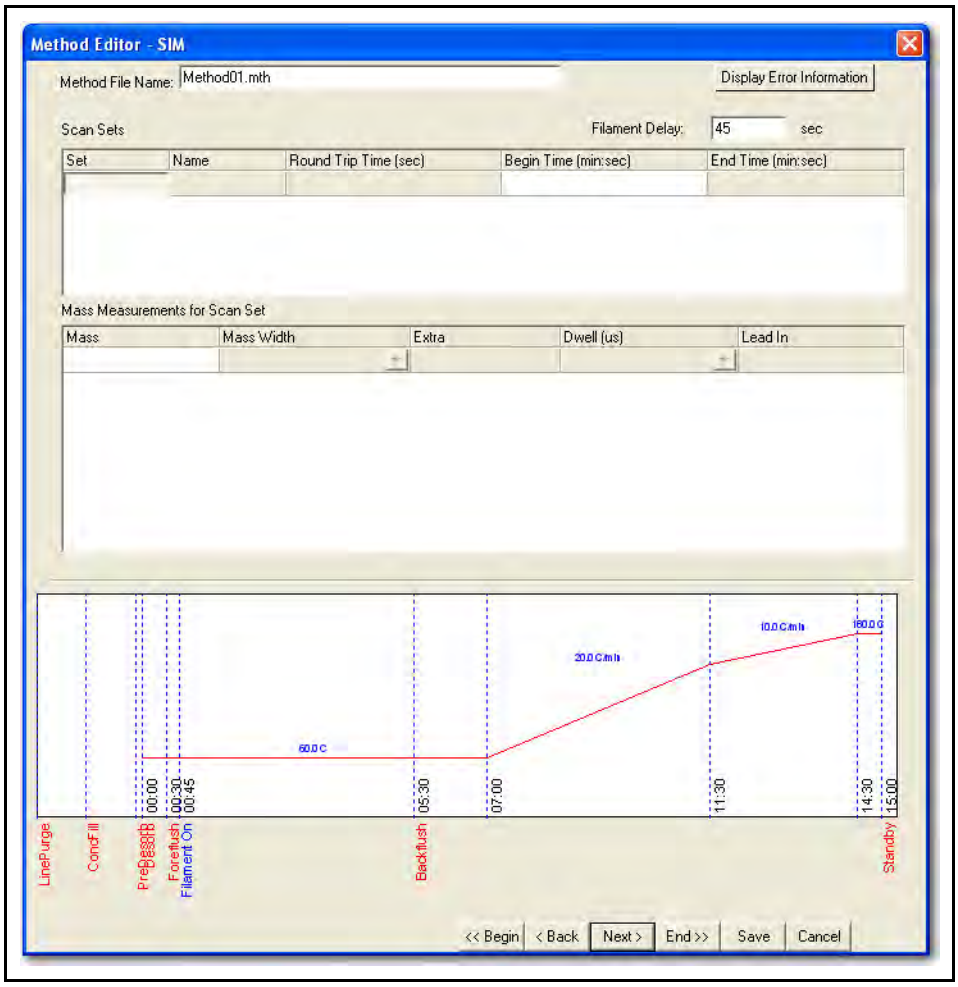
10.9 SIM Page

Selected Ion Monitoring (**SIM**) scans a set of specific masses to increase the sensitivity for known compounds. Figure 10-31 displays the **SIM** page.

10.9.1 SIM for Analyze

Each set has a **Begin Time** and an **End Time** which must be entered when programming the **Set**. An optional **Name** can also be entered at this point. After entering the times, the mass fragments for the compound can be entered into the **Mass** column. As the mass fragments are entered, the **Round Trip Time** is automatically calculated and entered in the **Scan Sets** grid.

Figure 10-31 Method Editor SIM Page for Analyze Methods



The **Scan Sets** fields, in the order recommended for editing, are as follows:

Begin Time . . . . . The start time for mass collection.

End Time . . . . . The stop time for mass collection.

Name . . . . . Each scan set can be assigned a name for identification purposes. This entry is optional.

NOTE: One of the column entries listed above must be highlighted to enable editing of the **Mass** list for that specific **Scan Set**.

Mass . . . . . The mass fragments of each column are entered in this column.

Mass Width . . . . . The width, in tenths of an amu, around the mass which the Mass Spectrometer will scan. For example, a **Mass Width** of 0.6 will scan 0.3 amu on each side of the peak.

Extra . . . . . This sets the number of extra scans, from 0 - 10, for each mass. Extra scans lower the detection limits by increasing the intensity within the Mass Spectrometer. Extra scans should be used when scanning for compounds with concentrations of ppb or lower.

Dwell . . . . . **Dwell** is the amount of time the software will search each for the selected mass. The dwell can be set from 100 µs - 5,000 µs. 400 µs is recommended. Increasing the **Dwell** decreases the detection limit.

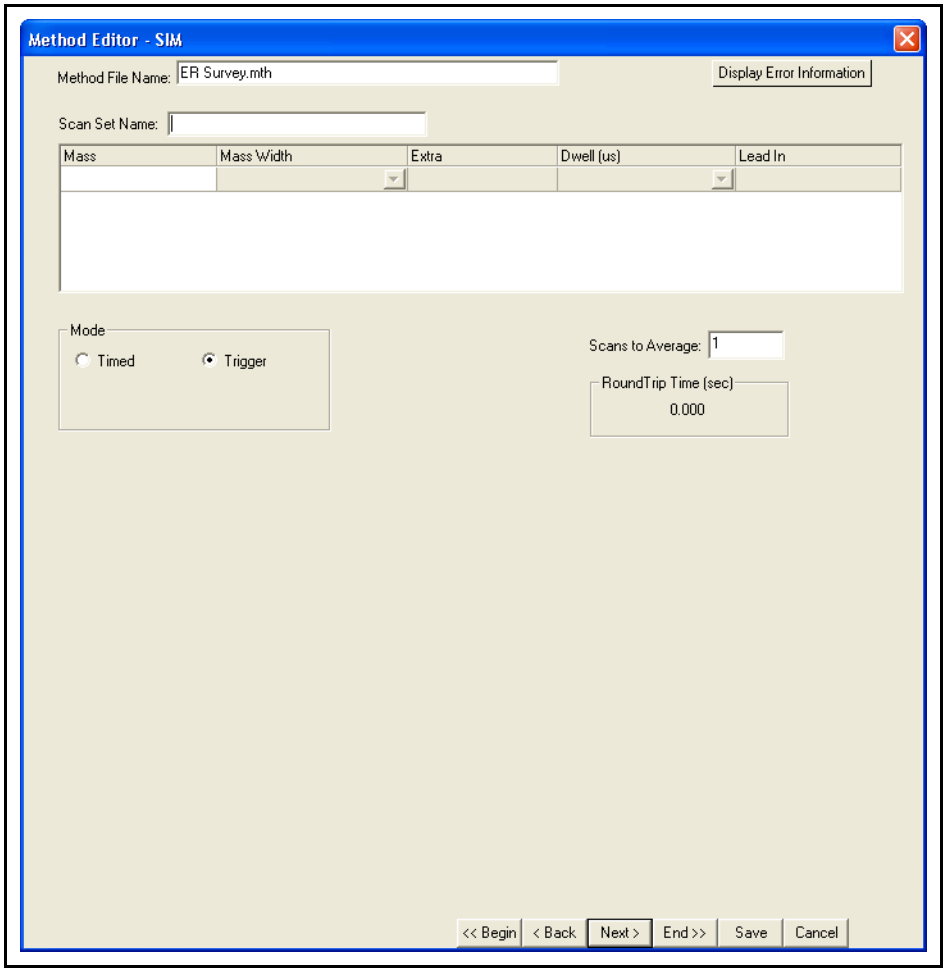
Lead In. . . . . **Lead In** determines the number of points the Mass Spectrometer will skip prior to scanning the desired mass peak. Best practice is to set the **Lead In** to at least a 1000 µs delay prior to collecting data. The delay is based on **Lead In** multiplied by the **Dwell**.

NOTE: The **Mass Width**, **Extra**, **Dwell** and **Lead In** values for a new entry are automatically populated based upon the entry listed above.

NOTE: To fill any column with the entry listed above, click in the desired cell and press Ctrl+D.

10.9.2 SIM for Survey

Figure 10-32 SIM for Survey



The SIM page for Survey mode provides the ability to create only one scan set. Refer to Figure 10-32.

Scan Set Name . . . . . References the specific set of ions being detected.

Timed Mode . . . . . The Survey method will run for a programmed amount of time.

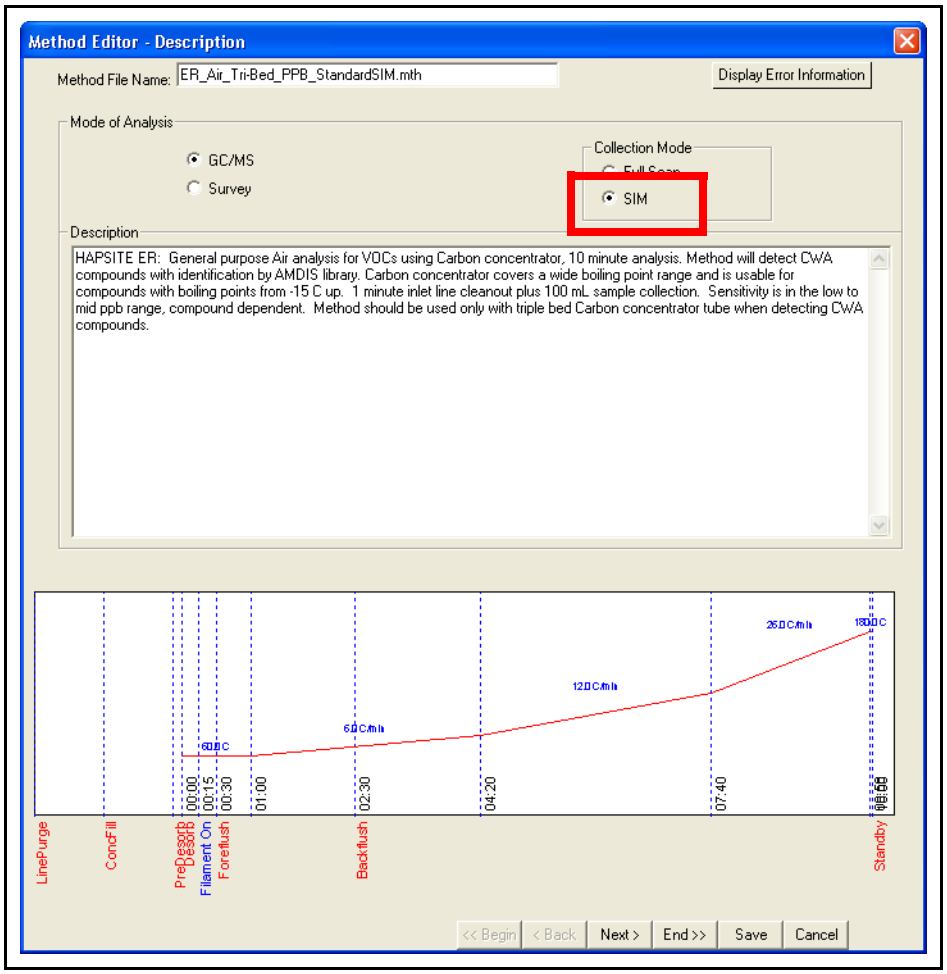
Trigger Mode. . . . . The method will stop when the **STOP** button or **SURVEY RUN** button is selected.

Scans to Average . . . . . Determines the number of scans that will be collected and averaged before the results are displayed on the chromatogram.

10.9.3 Creating a SIM Method

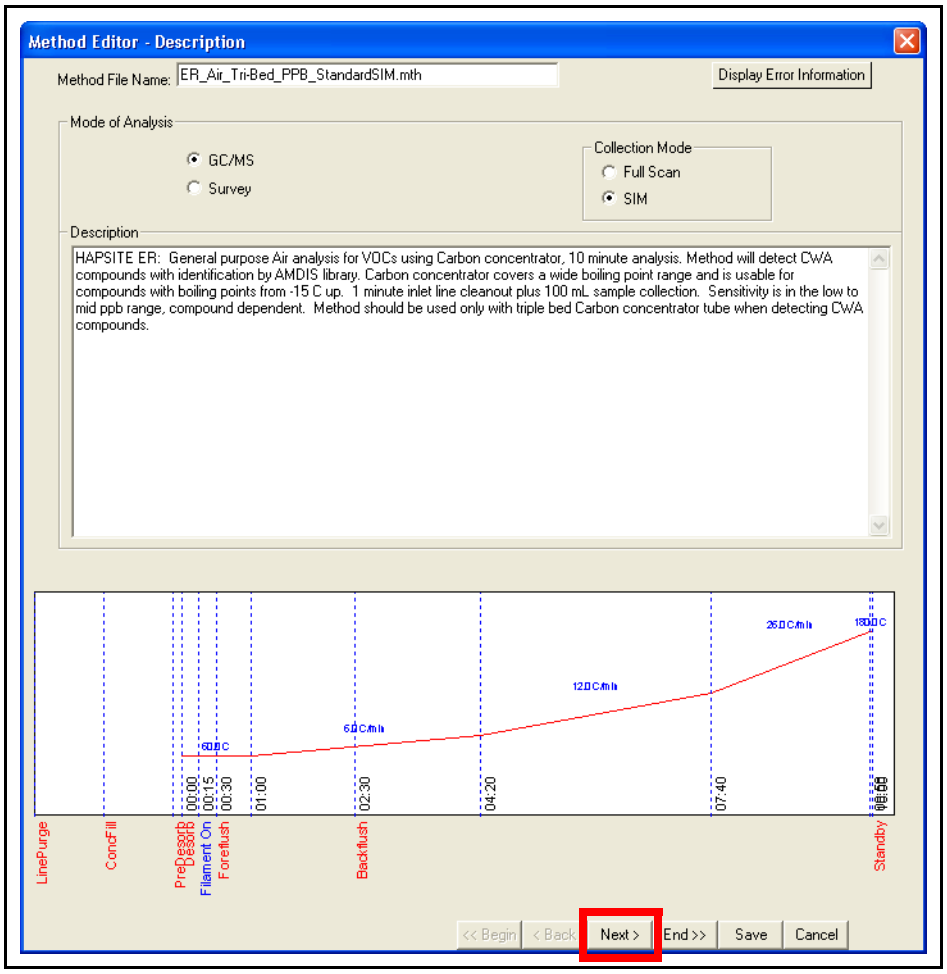
1. Follow Step 1 through Step 4 of section 10.2, Reloading Default HAPSITE Methods, on page 10-3
2. Change the **Collection Mode** to **SIM**. See Figure 10-33.

Figure 10-33 Changing Collection Mode



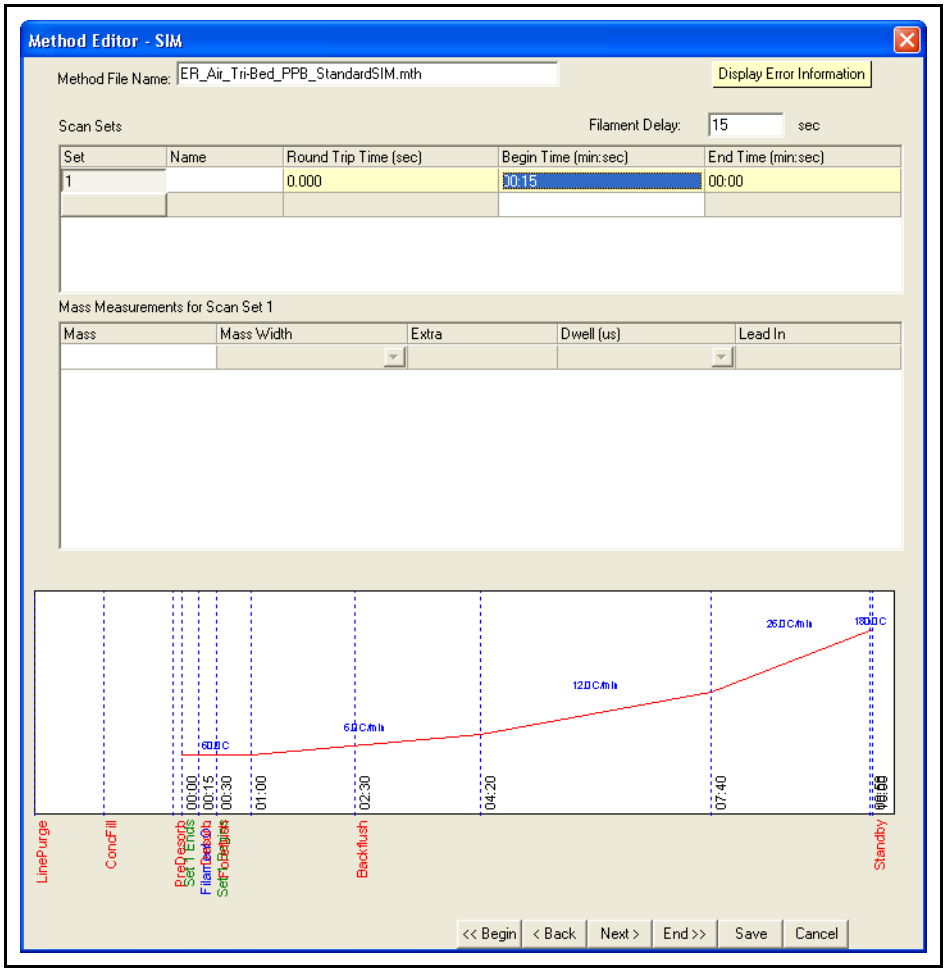
3. Select **Next** until the **SIM** page is displayed. See Figure 10-34.

Figure 10-34 Displaying the SIM Page



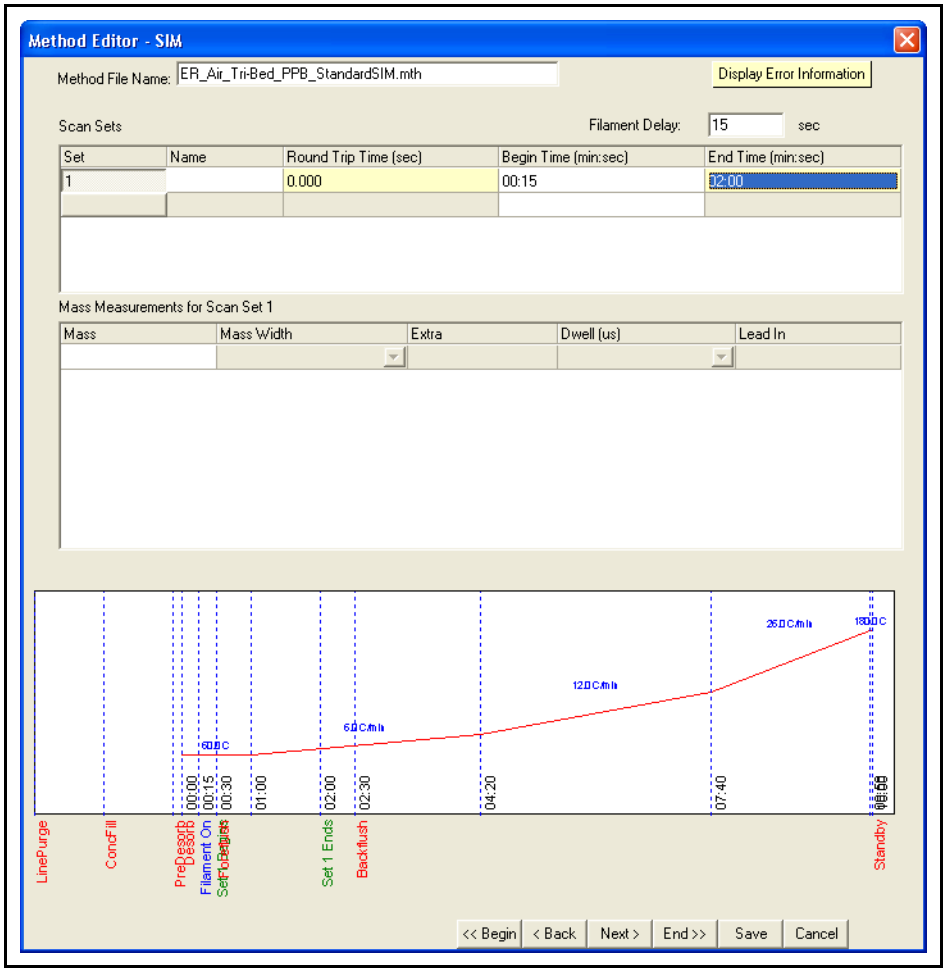
4 For the **Begin Time**, enter in the number displayed in the **Filament Delay**. For default ER methods, this is 15 seconds. See Figure 10-35.

Figure 10-35 Begin Time



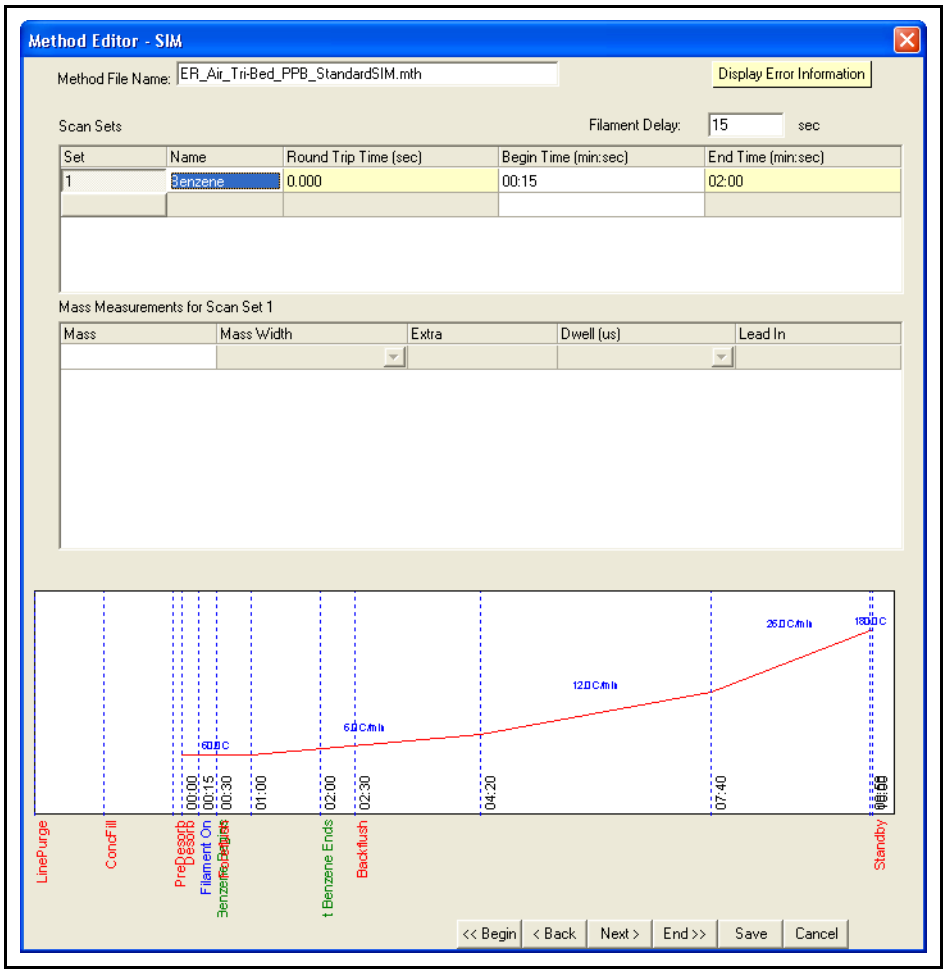
5 Enter the desired the **End Time** so that the **Begin Time** and the **End Time** surround the expected retention time of the compound. See Figure 10-36.

Figure 10-36 End Time



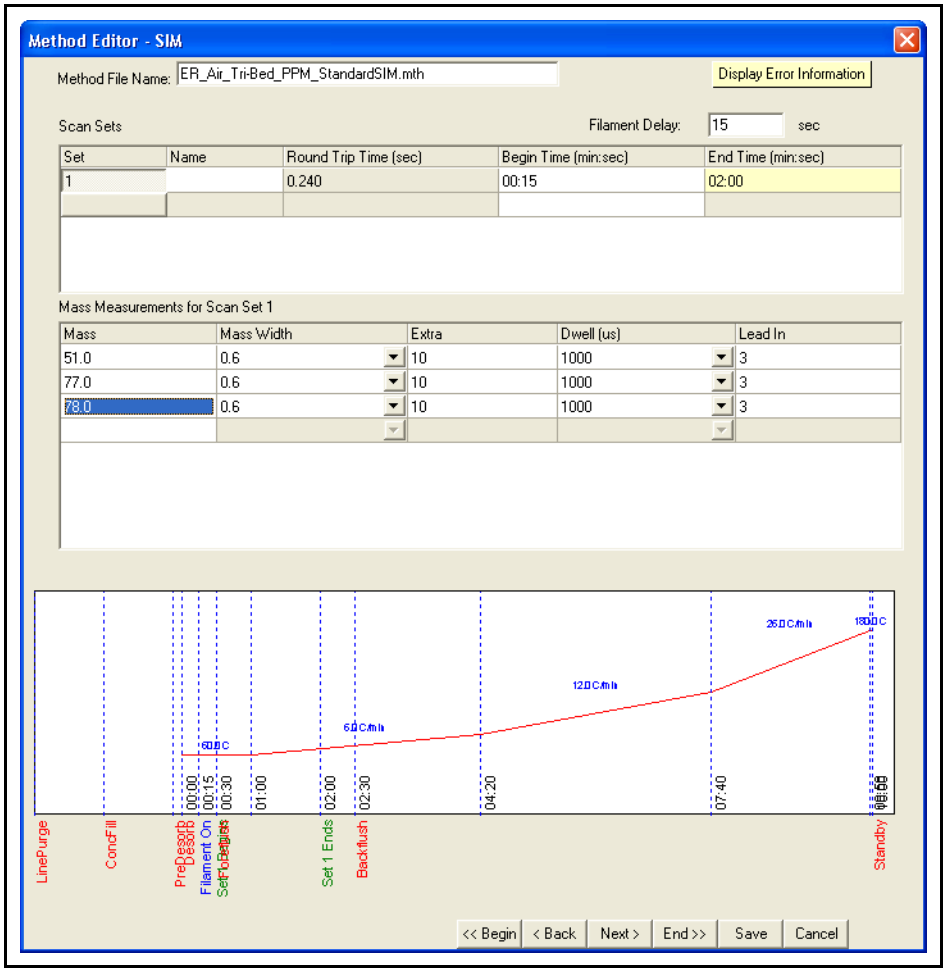
6 Enter the name of the chemical of interest. (See Figure 10-37.)

Figure 10-37 Entering the Chemical of Interest



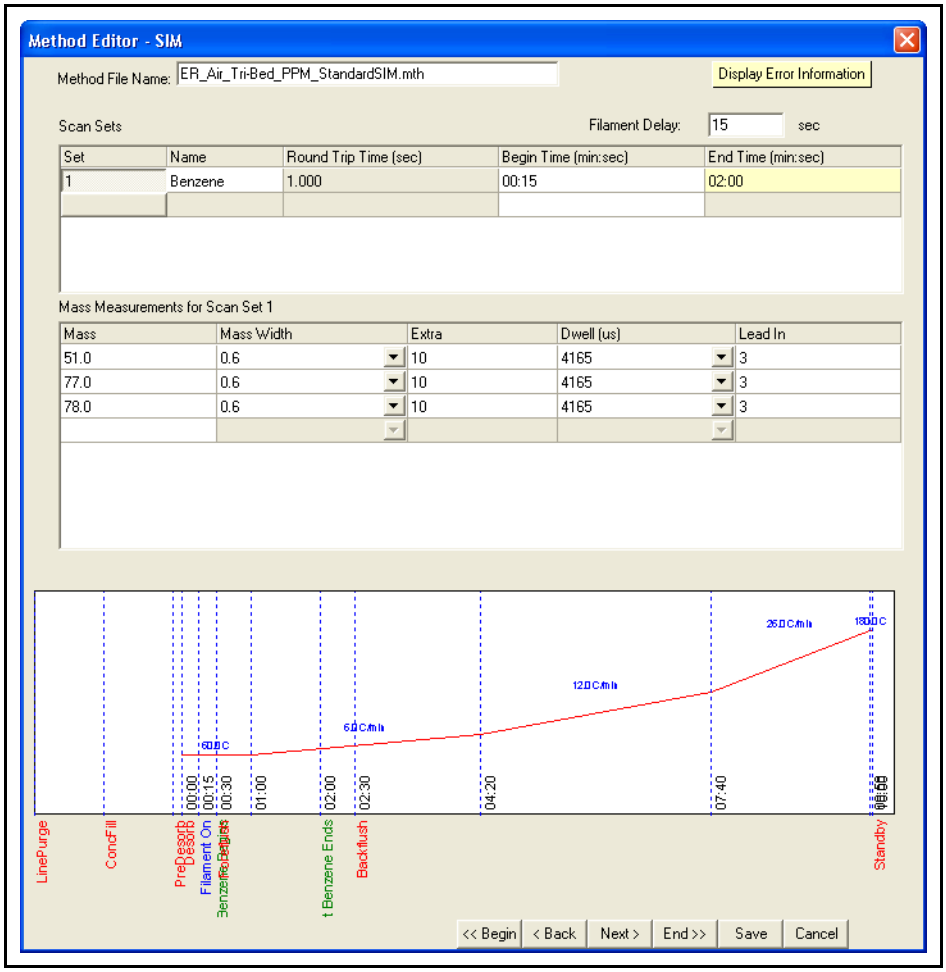
7 Enter at least three mass fragments for the selected chemical of interest. (See Figure 10-38.)

Figure 10-38 Entering Mass Fragments



8 It is recommended that the **Dwell Time** is adjusted until the **Round Trip** is approximately one second. (See Figure 10-39.)

Figure 10-39 Adjusting Dwell Time



9 Repeat Step 4 through Step 8 if successive chemicals are desired.

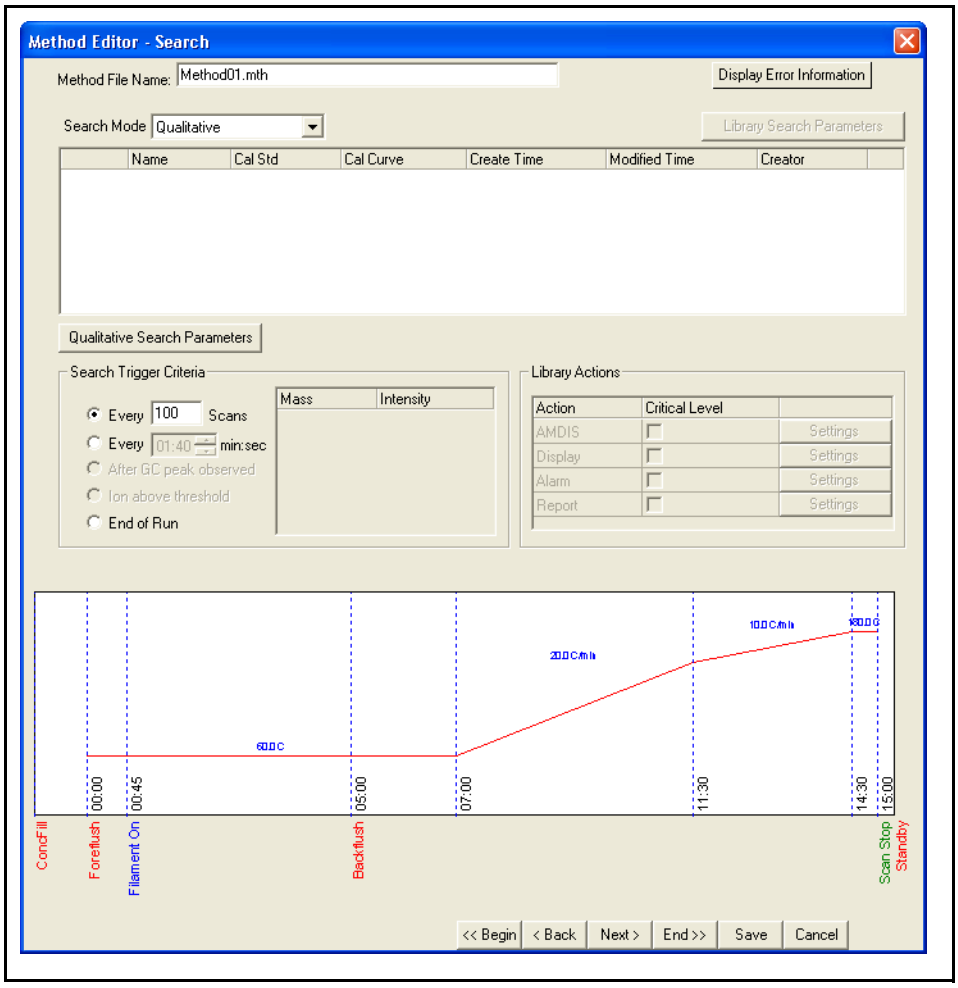
NOTE: The **End Time** for the final SIM compound must be the same as the end run time for the method.

NOTE: **AMDIS** and the **SearchNIST/User** libraries are not available when using a SIM method.

10.10 Search Page

The **Search Page** sets the necessary parameters to qualify and quantify data. To quantify data, a calibration library must be created. See Figure 10-40. See Chapter 11, Calibration for instructions on creating a calibration library.

Figure 10-40 Method Editor Search Page



There are four choices in the **Search Mode** drop down menu.

No Search . . . . . If this option is selected, a library search will not be conducted and a report will not be displayed on the front panel at the end of the run.

NOTE: SIM Methods only allow **No Search** as the search option.

Qualitative . . . . . Searches AMDIS during a run to provide near real-time identifications. A report will be generated at the end of the run and can be viewed on the front panel display.

Quantitative . . . . . Generates a **Quantitative (Quant)** report at the end of the run by referencing the designated library.

Qualitative/Quantitative . . . . . Searches AMDIS to provide identifications during a run and generates a **Quantitative** report.

10.10.1 Setting Up a Qualitative Search

CAUTION

Only trained users should modify methods. Changing parameters may result in incorrect data.

To set up a qualitative search, the drop-down menu for the Search Mode must be set to **Qualitative**. AMDIS will be used to identify the sample components. The search parameters can be modified using the **Qualitative Search Settings** button. (See Figure 10-41.)

Figure 10-41 AMDIS Search Settings

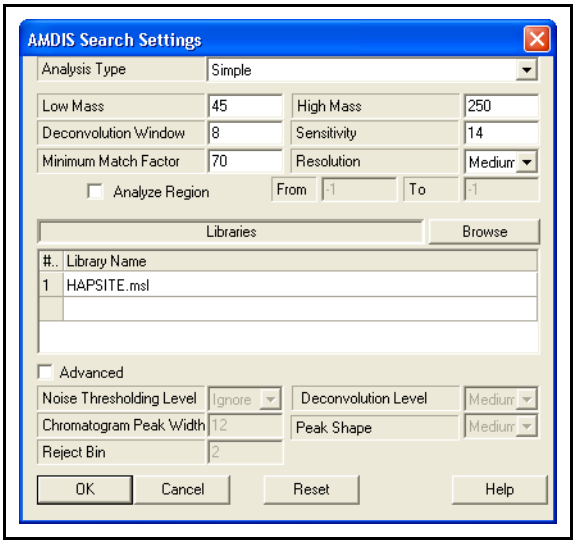
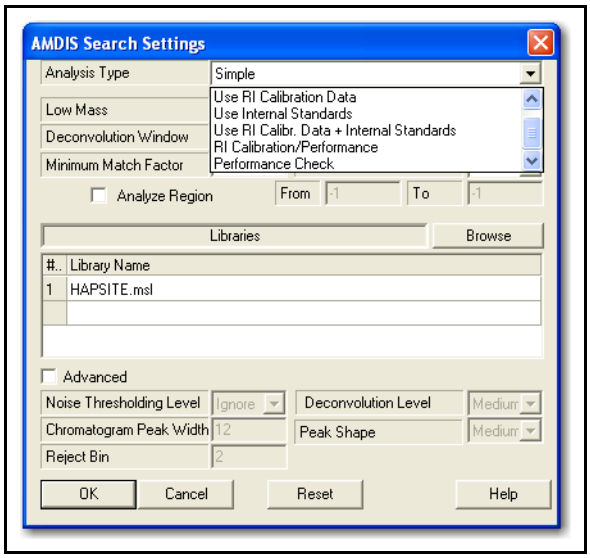


Figure 10-42 lists the different analysis types available for the search.

Figure 10-42 Type of Analysis



Analysis Type

Simple . . . . . The mass spectral data is used to identify the compounds. The calculated match factor is only based upon the quality of the match between the deconvoluted component spectra and the target library spectra.

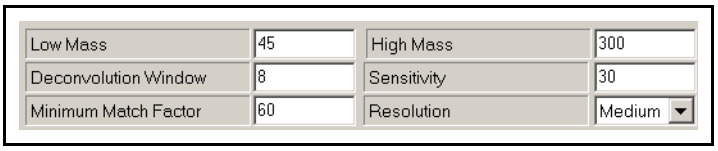
RI Calibration Data . . . . . This type of analysis uses an external calibration file. If the identified compound is not within a specified retention window, the program will penalize the match factor by a specified amount.

RI Calibr. Data + Internal Std. . . . . In this mode, the retention indices are calculated from the external calibration file. The internal standards are used to ensure that the instrument is functioning properly and that the samples were prepared properly. The internal standards are not used to calculate retention indices.

RI Calibration/Performance . . . . . This analysis establishes the correlation between the retention time of a component and the retention index using the set of standards specified in the calibration library.

Performance Check . . . . . This analysis verifies that the **HAPSITE ER** is properly identifying performance standards. The analysis does not perform a calibration.

Figure 10-43 Performance Window



Low Mass . . . . . The lowest mass in the range of masses being considered.

Deconvolution Window . . . . . The number of adjacent peaks subtracted from the deconvoluted peak.

Minimum Match Factor . . . . . The threshold net match factor value for an identification to be reported. Values at or above 80 are good matches, 70-79 are fair and less than 70 is poor. For most cases, a match factor of 70 is the minimum that should be used if identification rather than detection is desired.

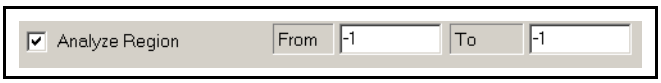
High Mass . . . . . The highest mass in the range being considered.

Sensitivity . . . . . Sets the sensitivity for the method. If the sensitivity is set too low, an increase in noise and broad peaks may result. If the sensitivity is set too high, it increases the risk of false positives.

Resolution . . . . . The resolution can be set to high, medium or low. The default setting is medium. This setting affects peak shape. Higher resolution results in sharper peaks, while lower resolution results in broader ones.

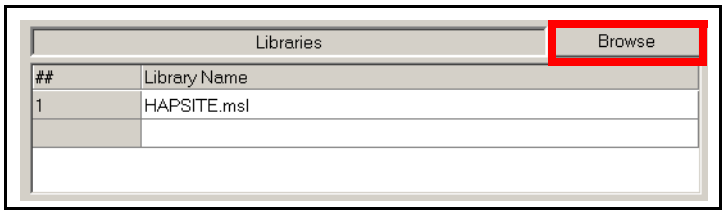
If **Analyze Region** is selected, see Figure 10-44, AMDIS will only search in the selected scan range. When **Analyze Region** is off (i.e., unchecked), the software will search the entire range specified by **Low Mass** and **High Mass**.

Figure 10-44 Analyze Region



The HAPSITE.MSL is the default AMDIS library for the system. See Figure 10-45.

Figure 10-45 The Libraries



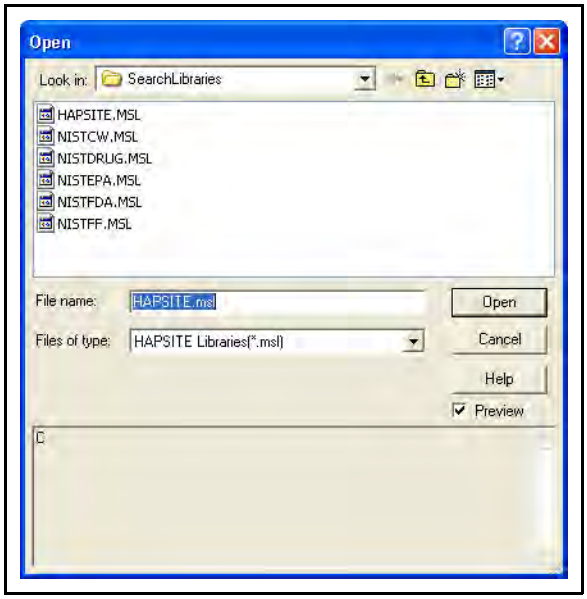
To view other library choices, select the **Browse** button, refer to Figure 10-45. There are several small and specific libraries in addition to the HAPSITE.MSL. See Figure 10-46. Many of the compounds found in these small libraries, that can be detected by the HAPSITE, are incorporated in the HAPSITE.MSL file.

NOTE: INFICON recommends using HAPSITE.MSL.

AMDIS Libraries:

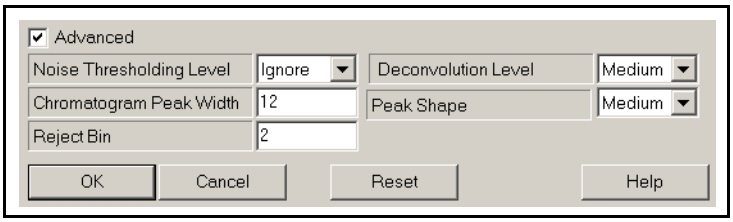
- HAPSITE.MSL
- NISTEPA.MSL
- NISTCW.MSL
- NISTFDA.MSL
- NISTFF.MSL
- NISTDRUG.MSL

Figure 10-46 Library Options



Advanced Settings

Figure 10-47 Advanced Settings



NOTE: INFICON does not recommend changing the **Advanced Settings**.

Noise Thresholding Level . . . . . Refers to the minimum signal recorded. Will filter out noise along the baseline.

Chromatogram Peak Width . . . . . Deconvoluted peaks will maintain same shape, because the width, in amus, has been specified.

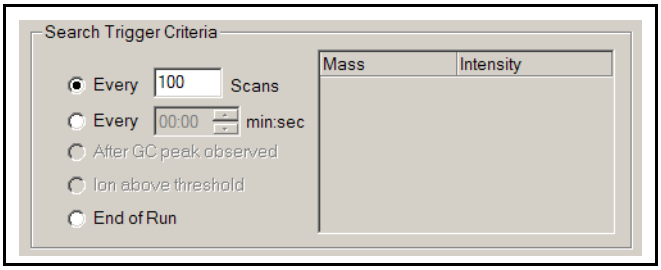
Reject Bin . . . . . Rejects peaks that have less than a set number of scans.

Deconvolution Level . . . . . As the level of deconvolution increases, the software increases the separation between peaks. The default setting is medium, but low and high options are available.

Peak Shape . . . . . The shape requirement allows all of the deconvoluted peaks to maintain the same shape. As the shape requirement increases, the shape of the individual ions will be more uniform.

The **Search Trigger Criteria** section of the **Search** page determines when an **AMDIS** search will be run. There are three choices, see Figure 10-48.

Figure 10-48 Search Trigger Criteria



Every ____ Scans . . . . . Determines the scan interval for running an AMDIS search. The default value for this is 100 scans.

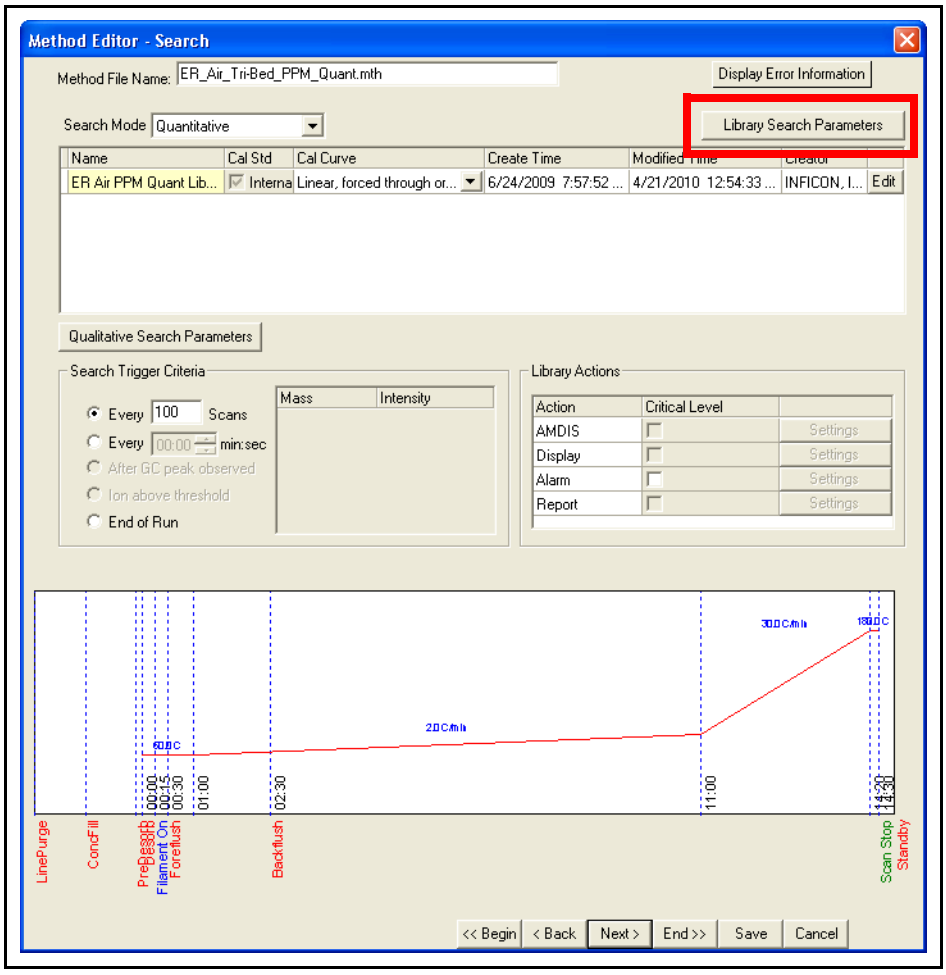
Every ____ min:sec . . . . . Determines the time intervals for running an AMDIS search.

End of Run . . . . . An AMDIS search will only be conducted at the end of a run.

10.10.2 Setting Up a Quantitative Search

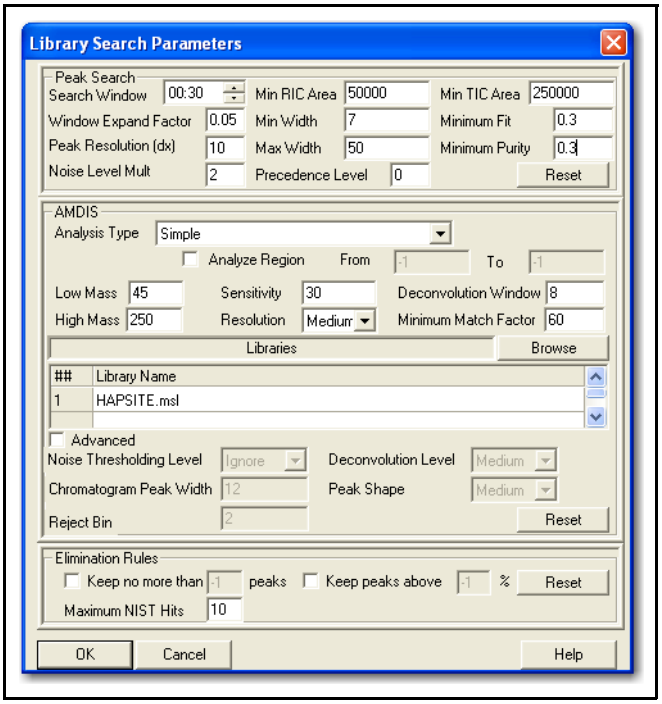
Once a calibration library has been created, the **Library Search Parameters** button will be activated. The **Library Search Parameters** functions sets the peak identification criteria of the library compounds, as well as the unknown analytes. See Figure 10-49.

Figure 10-49 Library Search Parameters Button



Clicking the **Library Search Parameters** button on the **Method Editor Search** page will display the following window. See Figure 10-50.

Figure 10-50 Library Search Parameters Window



10.10.3 Peak Search

The peak search section is compromised of the parameters that are used in distinguishing a peak from the baseline.

Search Window. . . . . This value defines the acceptable retention time range for a peak. The default value is 20 seconds. When using the default value, the window is 10 seconds on either side of the expected retention time in order for the software to make an identification

Min RIC Area . . . . . The area of the intensity of the largest mass fragment of the peak must be above this setpoint.

Min TIC . . . . . The area of the intensity of the total ion count for the peak must be above this setpoint.

Window Expand Factor . . . . . This option multiplies the retention time of the peak by the **Window Expand Factor** to give a period of time by which the search window will be expanded. For example, if the peak retention time is 10 minutes and the **Window Expand Factor** is set to its default setting of 0.05, the 10 minute retention time will be multiplied by the 0.05 **Window Expand Factor** to equal 30 seconds. Then, 30 seconds is added to the **Search Window**. If the default value of the **Search Window** is 20 seconds, adding 30 seconds from the **Window Expand Factor** to the **Search Window** would increase the search range to 50 seconds.

Min. Width . . . . . This value is the minimum number of scans per peak, which designates the area measurement for peak integration. Any peaks with fewer scans than this value will be disregarded by the software. Decreasing this number will result in the software accepting broader peaks.

Min. Fit. . . . . This compares the mass intensities of the compound to those saved in the library. Reasonable values depend on the selectivity of the calibration, but typically 0.5 to 0.9 is used. A higher **Min. Fit** number is more discriminative.

Peak Resolution (dx) . . . . . This number indicates the minimum number of scans between two peaks. It is used to determine whether a peak should be considered a single peak or if the peak should be split into two separate peaks.

Max Width . . . . . This value is the maximum number of scans per peak, which designates the area measurement for peak integration. Any peaks with more scans than this value will be disregarded by the software. Increasing this number will result in the software accepting broader peaks.

Min. Purity . . . . . This compares the purity level of the detected peak to the mass peak in the library. Reasonable values depend the selectivity of the calibration, but typically 0.5 to 0.9 is used. A higher **Min. Purity** number is more discriminative.

Noise Level Mult . . . . . The peak intensity must be greater than the product of the **Noise Level Mult** number multiplied by the baseline noise in order to be identified as an analyte.

Precedence Level . . . . . Determines if the search uses the global parameters to use or compound-specific parameters. Leaving this set to zero allows for the use of specific search parameters for individual compounds as discussed in Chapter 11.

Min. Area . . . . . This number discriminates against low responses which are usually attributed to noise rather than analyte detection. Increase this number to 10,000 or more if false positives are encountered.

Max Width . . . . . The peak must contain less scans than the setpoint number.

Low Mass . . . . . NIST will only use masses above this setpoint to make an identification.

High Mass . . . . . NIST will only use masses below this setpoint to make an identification.

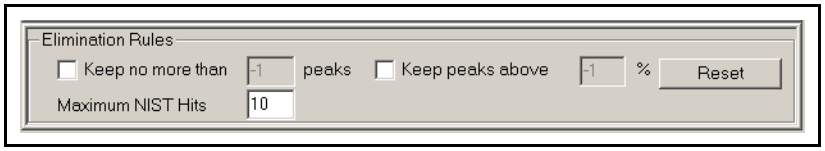
Minimum Match Factor . . . . . The net fit in AMDIS must be above this number.

The **Reset** button resets the entered values to the default settings in the **Peak Search** window. See Figure 10-51.

Figure 10-51 Resetting Default Search Parameters

The **Elimination Rules** section gives parameters for peaks to be reported. There are three options. See Figure 10-52.

Figure 10-52 Elimination Rules Window



Keep no more than . . . . . This check box determines the number of peaks that will be displayed. If ten is selected, the ten peaks with the largest areas will be displayed.

Keep peaks above . . . . . When this box is checked, only peaks above the desired percent intensity will be displayed. Fifteen is generally used as the low end for intensity.

Maximum NIST Hits . . . . . This value is the number of matches that will be reported by NIST.

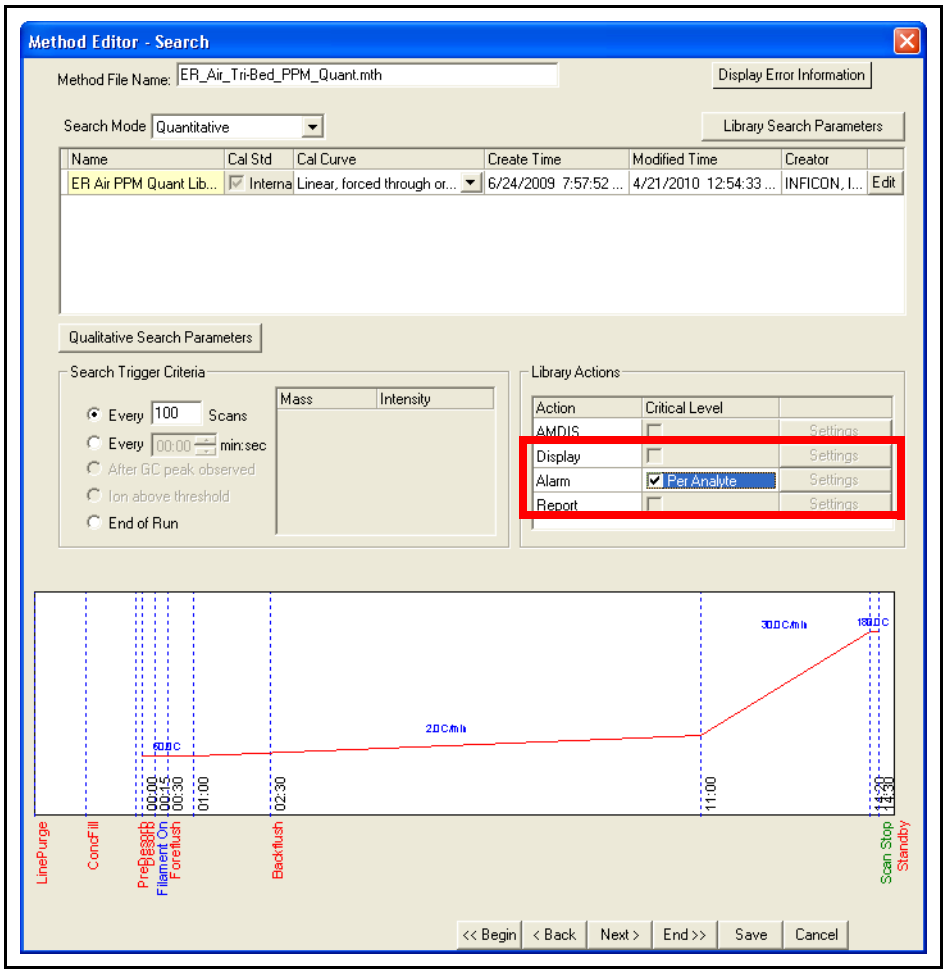
NOTE: This section has a **Reset** button which will reset the entered values to the default settings.

10.10.4 Alarm

On the main **Method Editor Search** page, the **Alarm** option in the **Library Actions** box will activate when a calibrated library has been saved to the method. To enable the **Alarm** option

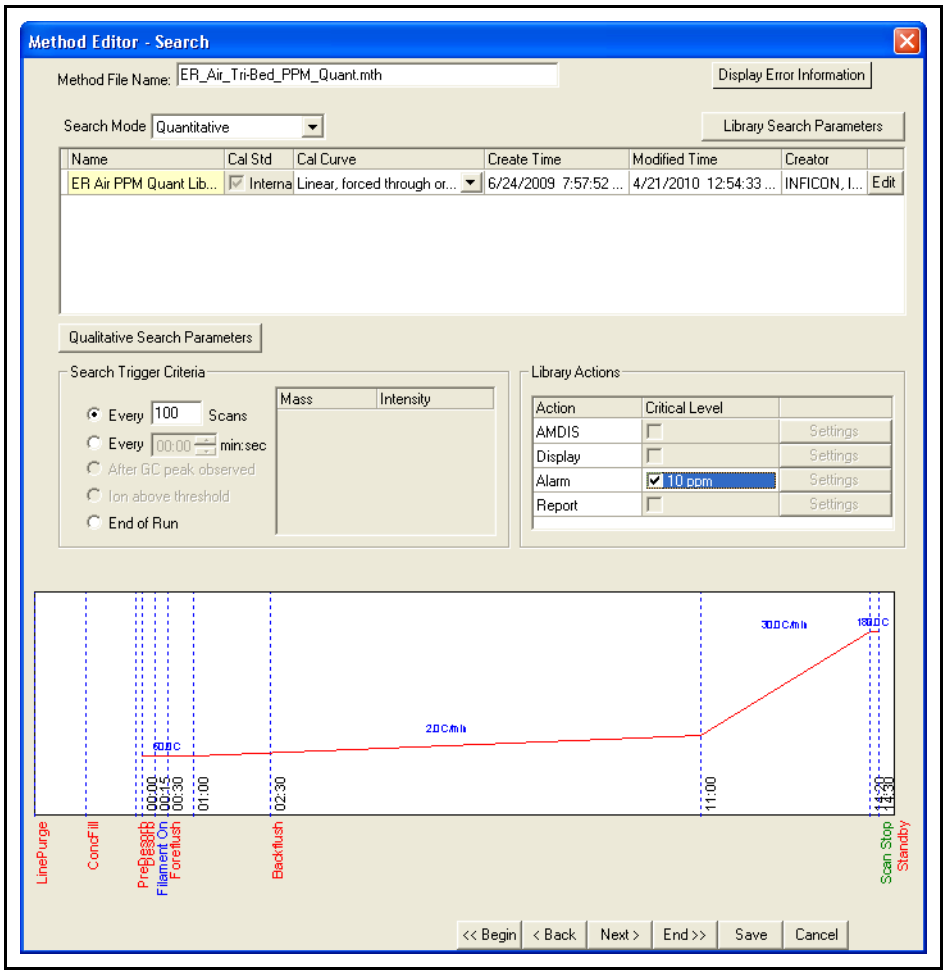
1 Check the **Alarm** box. See Figure 10-53.

Figure 10-53 Alarm Box



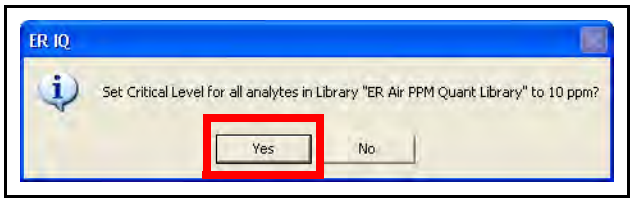
2 Enter the desired alarm level into the box with the units. The alarm will be displayed when any analyte is detected at a concentration above the alarm level. To enter in alarm levels for individual analytes, see Figure 10-54.

Figure 10-54 Entering in the Alarm Units



3 Click **Yes** to confirm that the alarm level is correct as entered. See Figure 10-55.

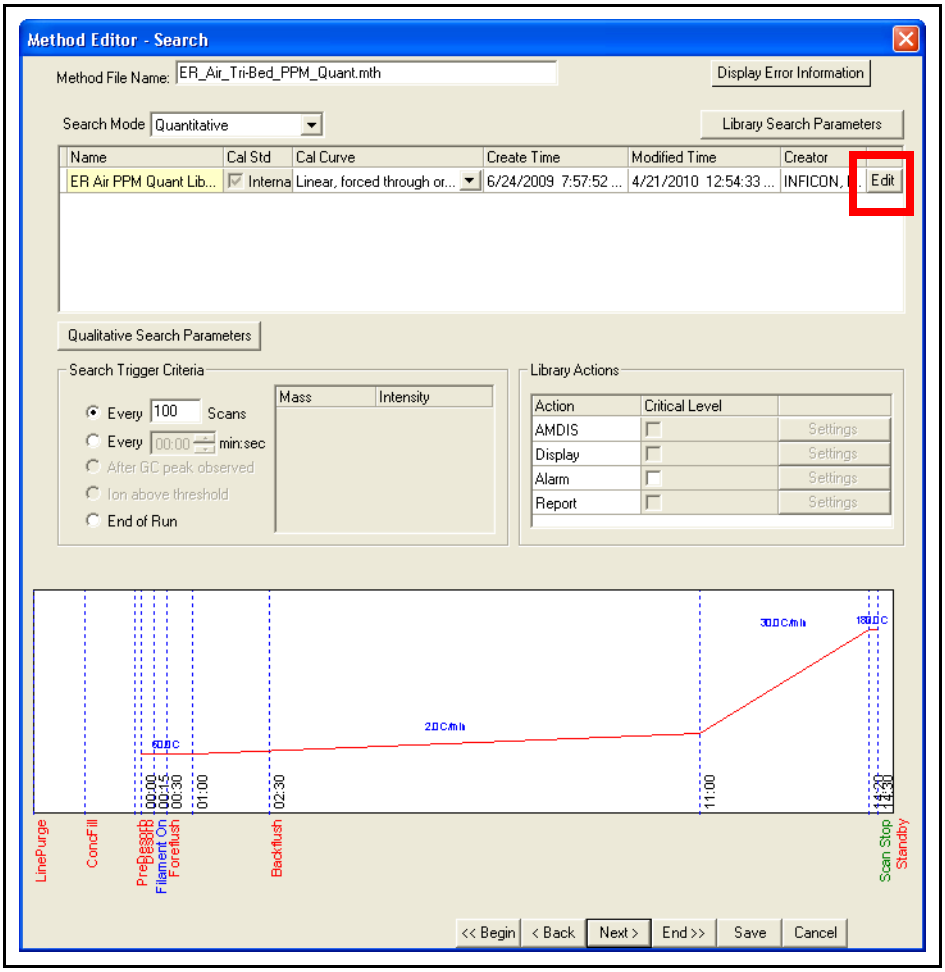
Figure 10-55 Confirming the Alarm Level



10.10.5 Edit Options

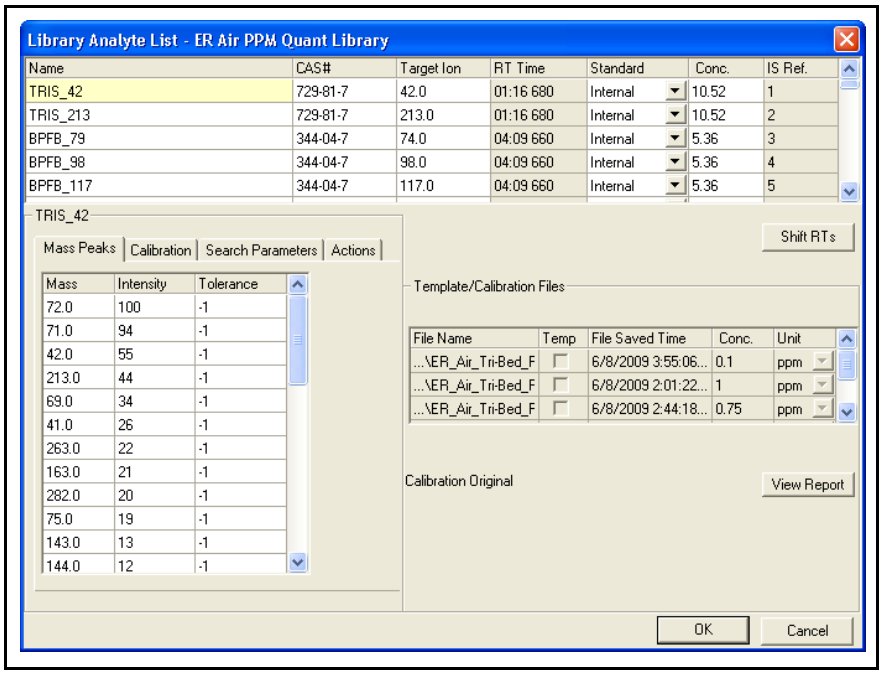
Clicking the **Edit** box will display the following information about the calibration library. See Figure 10-56.

Figure 10-56 Edit



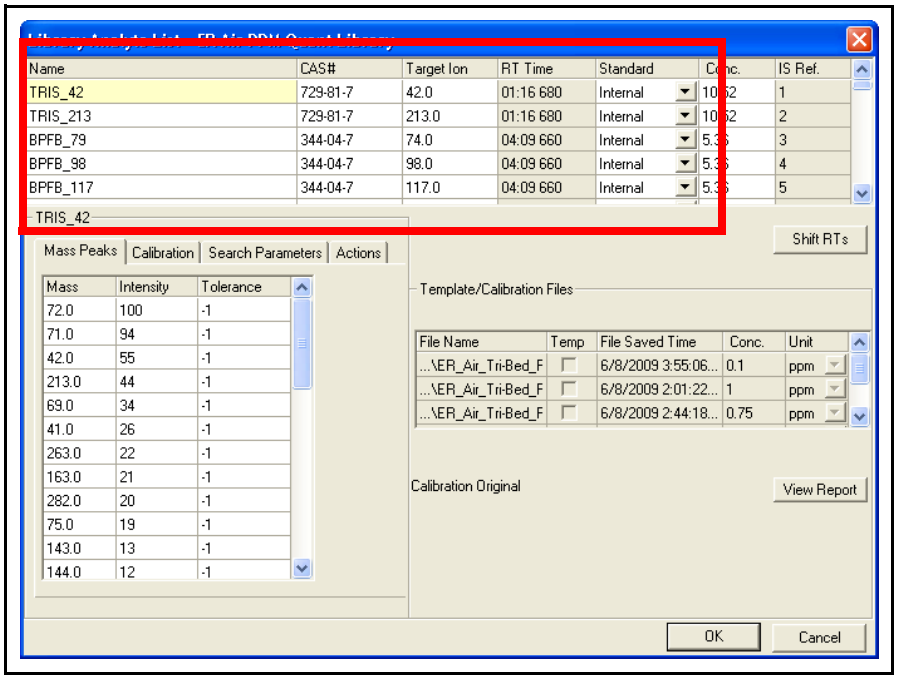
The **Analyte List** will be displayed. See Figure 10-57.

Figure 10-57 Analyte List



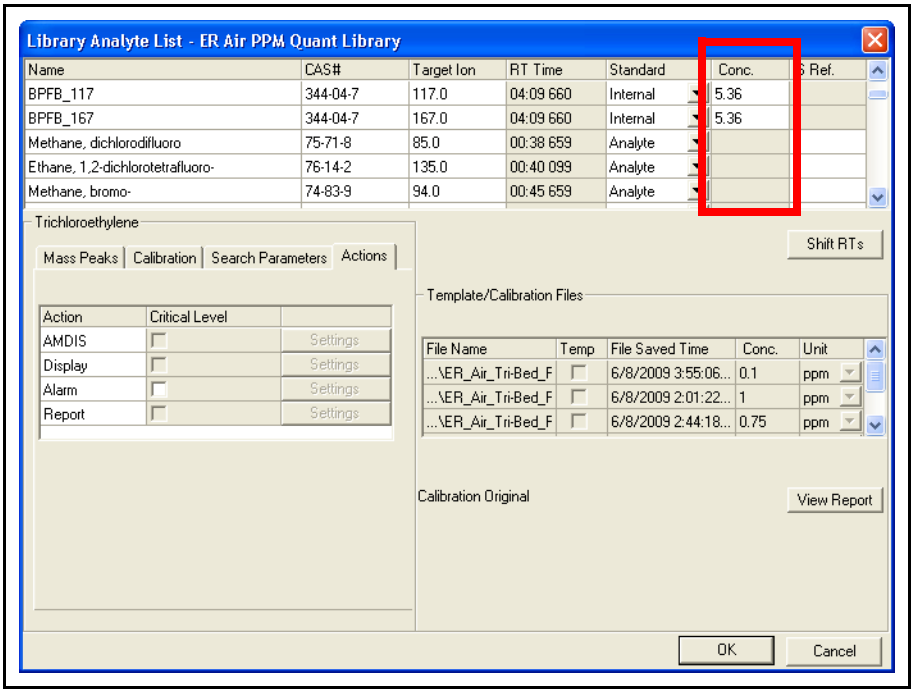
The name of the compound will be displayed in the name column, followed by the CAS number, the target ion and the predicted retention time. See
In the **Standard** column, either **Internal** or **Analyte** will be selected. If **Internal** is selected, the compound is an internal standard. If **Analyte** is selected, the compound is an analyte of interest. See Figure 10-58.

Figure 10-58 Edit Window



The **Conc.** (concentration) column will be populated for internal standards. It will be left blank if the compound is an analyte. See Figure 10-59.

Figure 10-59 Concentration



In the **IS Ref** column, all internal standards are given a number. For the air internal standards, this is 1-6. The analyst, when creating a method, will assign a number, (1-6 for the air internal standard) to each analyte. The assigned number is based upon the closeness of the target ion of the analyte to the closeness of the target ion of the internal standard. For instance, trichloroethylene has a target ion of 130. The internal standard, BPFB_117, has a target ion of 117 and was assigned the number 5. Therefore, the analyst would enter 5 into the **IS Ref** column for trichloroethylene, because BPFB_117 is the closest internal standard. See Figure 10-60 and Figure 10-61.

Figure 10-60 BPFB_117

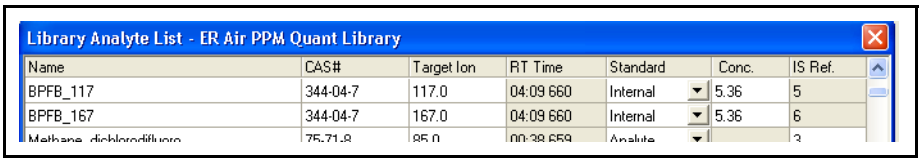
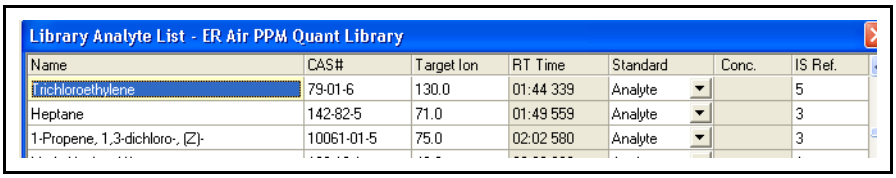
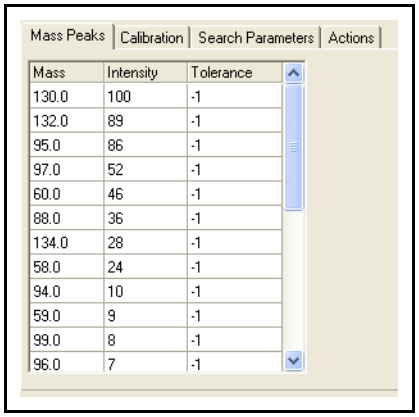


Figure 10-61 Trichloroethylene



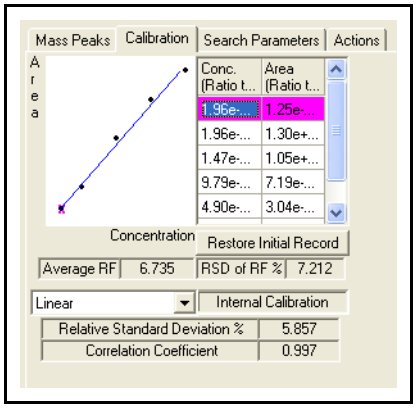
On the **Mass Peaks** tab, the mass fragments for the highlighted compound will be displayed with their intensity. See Figure 10-62.

Figure 10-62 Mass Peaks



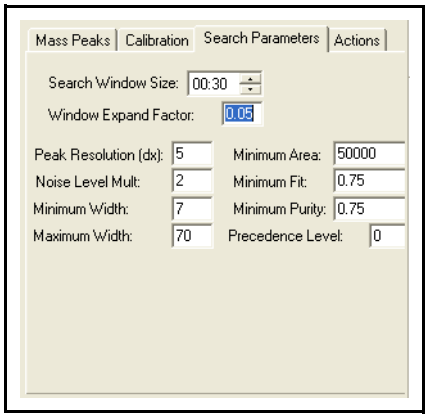
On the **Calibration** tab, the calibration curve for the analyte will be displayed. See Chapter 11, Calibration. See Figure 10-63.

Figure 10-63 Calibration



For information on the **Search Parameters** tab, refer to section 10.10.3, Peak Search, on page 10-44. See Figure 10-64.

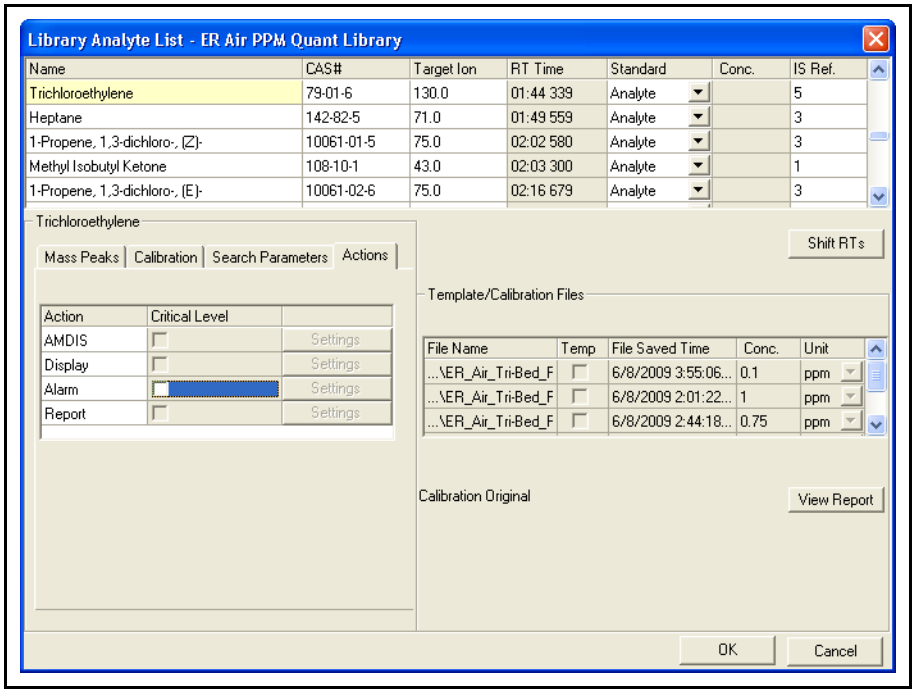
Figure 10-64 Search Parameters



The **Alarm** tab allows for an alarm level to be entered for each individual compound. To enter in an alarm:

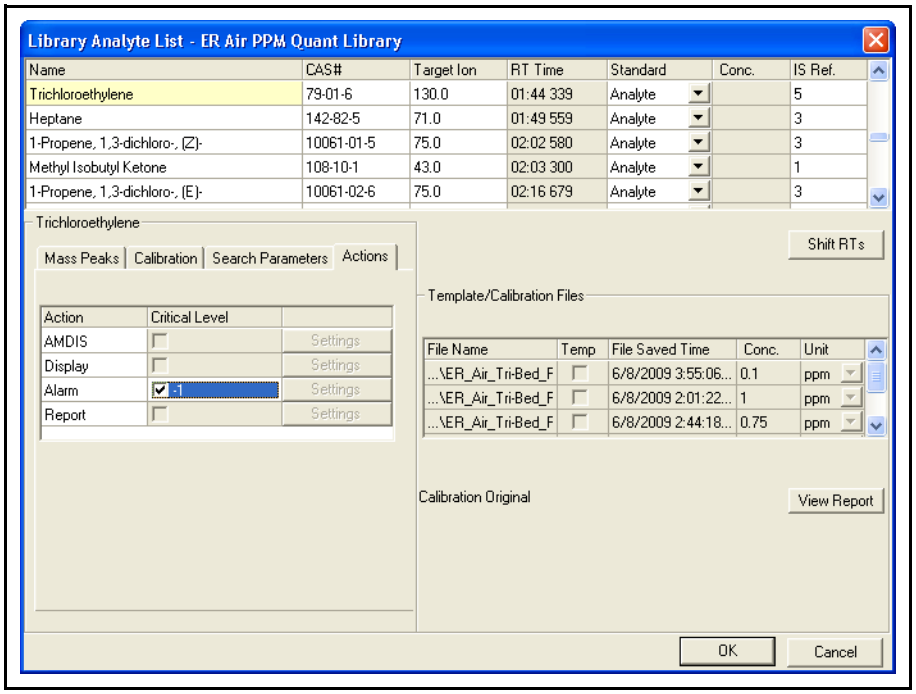
1 Highlight the desired compound. See Figure 10-65.

Figure 10-65 Highlighting Desired Compound



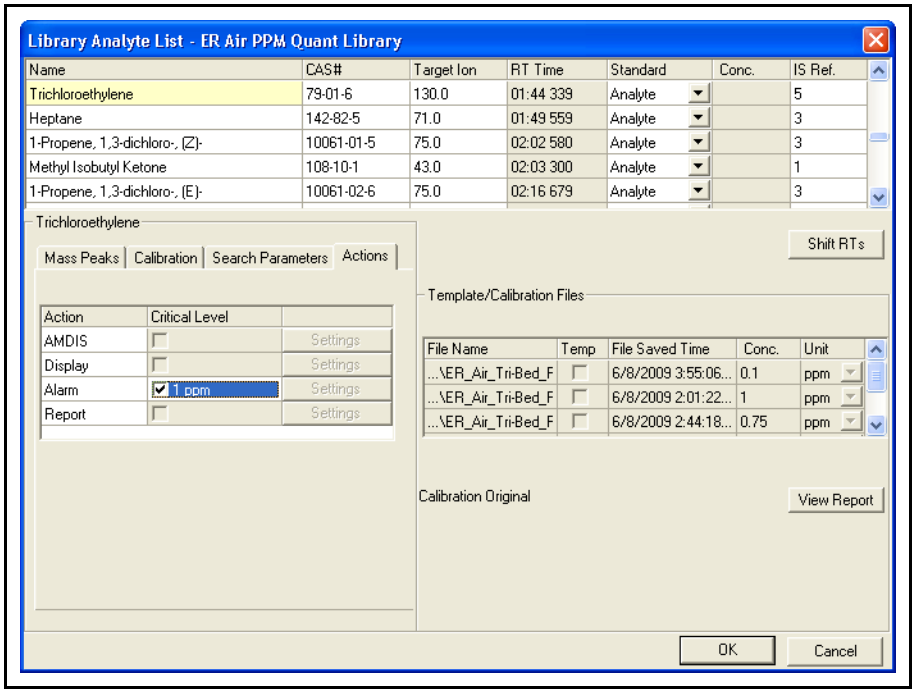
2 Check the **Alarm** box. See Figure 10-66.

Figure 10-66 Alarm



3 Enter the desired concentration followed by the desired units. See Figure 10-67.

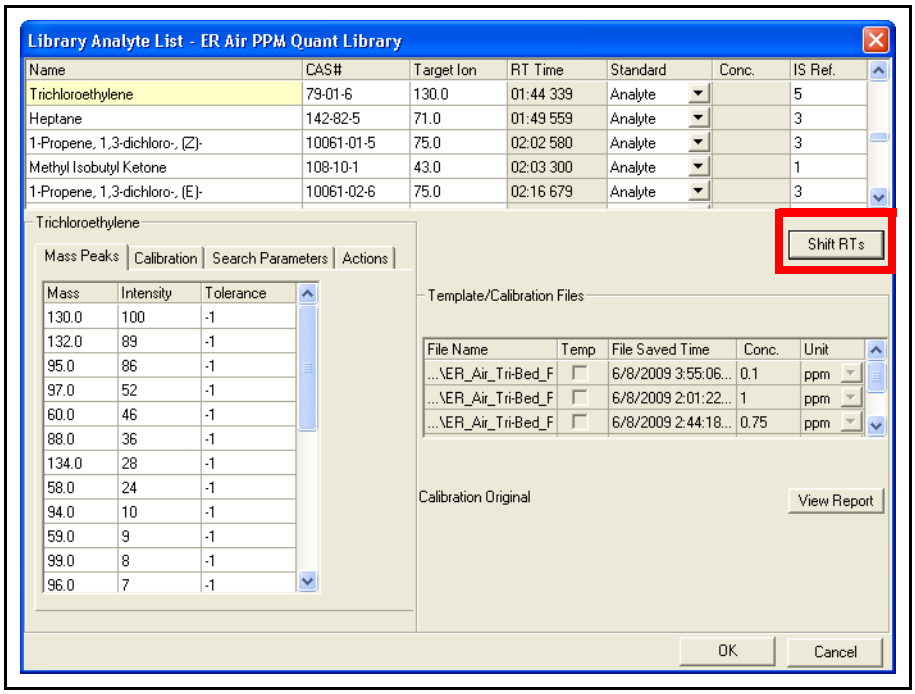
Figure 10-67 Entering Desired Concentration



The **Shift RTs** option allows the predicted retention time for the highlighted analyte to be shifted by a desired amount of time. To shift the retention time:

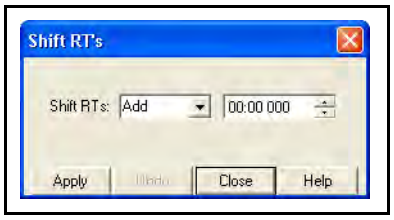
1 Click **Shift RTs**. See Figure 10-68.

Figure 10-68 Shift RTs



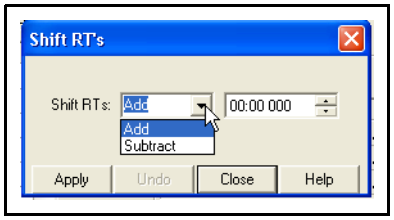
2 The **Shift RT's** window will be displayed. See Figure 10-69.

Figure 10-69 Shift RTs



3 Select **Add** or **Subtract** from the drop-down menu. See Figure 10-70.

Figure 10-70 Add or Subtract

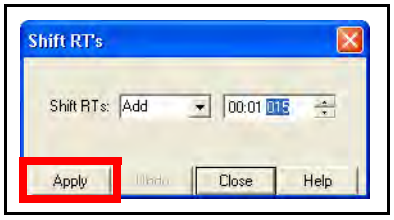


4 Type in the desired amount of time. See Figure 10-71.

Figure 10-71 Typing in the Time

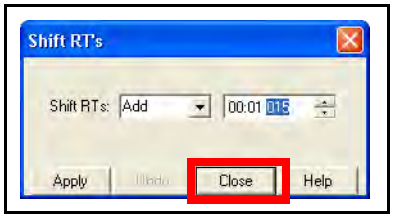
5 Click **Apply**. See Figure 10-72.

Figure 10-72 Apply



6 Click **Close**. See Figure 10-73.

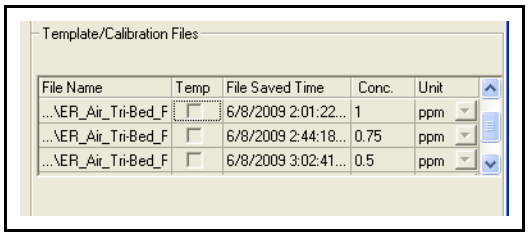
Figure 10-73 Close



10.10.6 Template/Calibration Files

The first column will display the names of the files that were used to create the calibration curve, time that the file was saved, the concentration of the file and the units. See Figure 10-74.

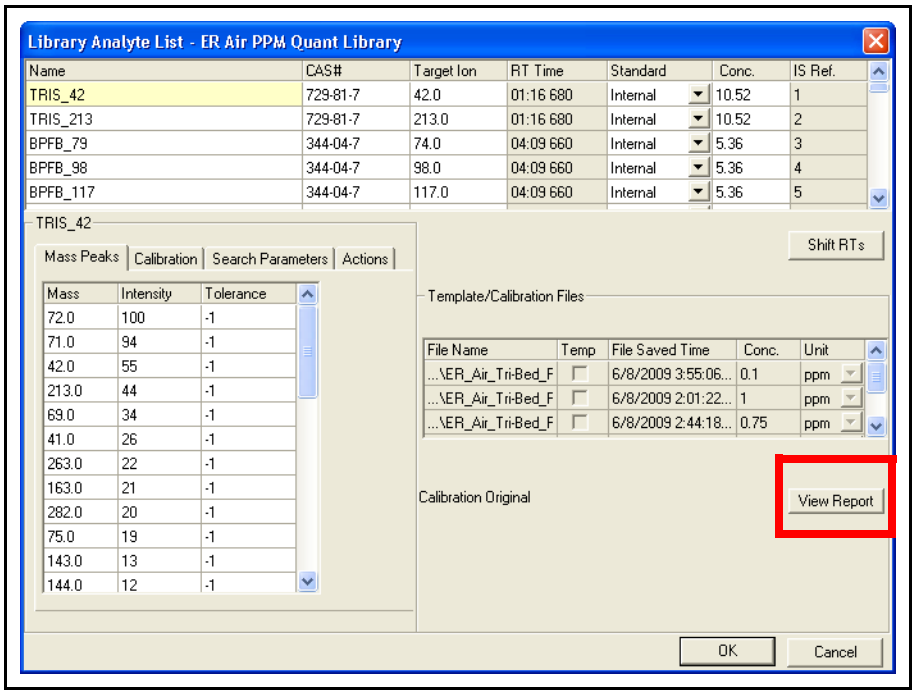
Figure 10-74 Template/Calibration Files



10.10.7 View Reports

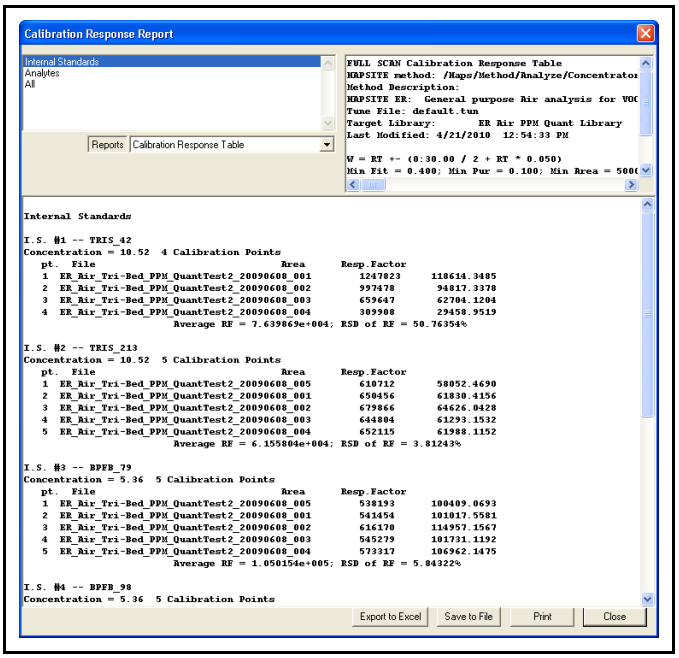
Clicking the **View Reports** button (see) will display the **Calibration Response Report**. See Figure 10-75.

Figure 10-75 View Reports



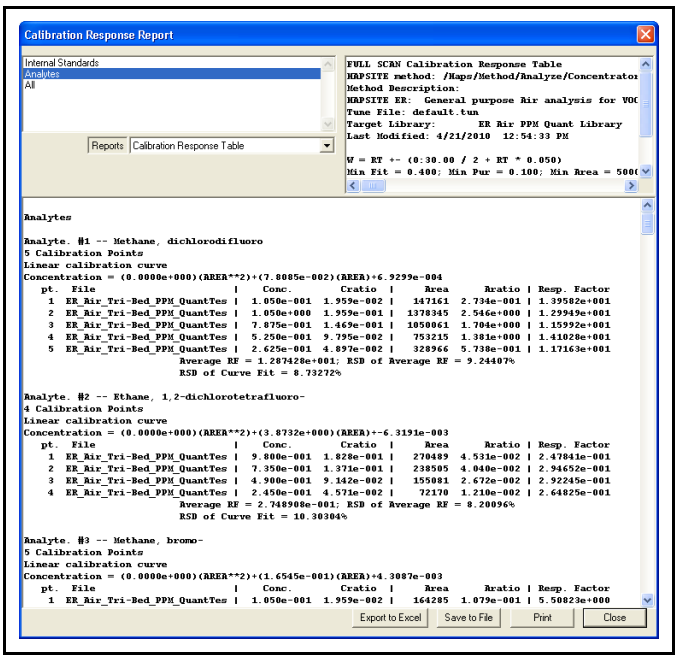
The default window that will be displayed is the **Internal Standard Calibration Response Table**. See Figure 10-76. This table will display the file names, the area of the peak and the response factor (the ratio between the signal produced by the analyte and the quantity of the analyte which produces a signal).

Figure 10-76 Internal Standard Calibration Response Table



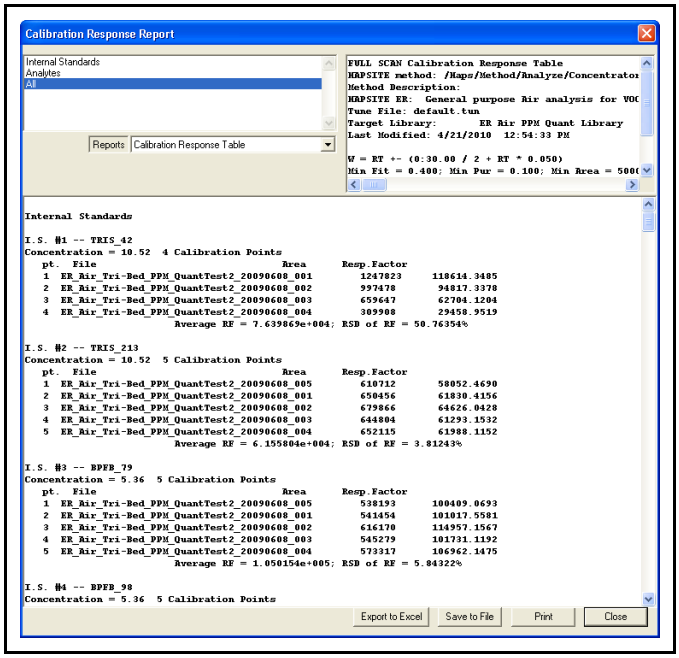
By selecting analyte from the drop-down menu, the **Analyte Standard Calibration Response Table** will be displayed. The **Analyte Standard Calibration Response Table** contains the same information as the **Internal Standard Calibration Table**, but pertains to the calibrated analytes. See Figure 10-77.

Figure 10-77 Analyte Standard Calibration Response Table



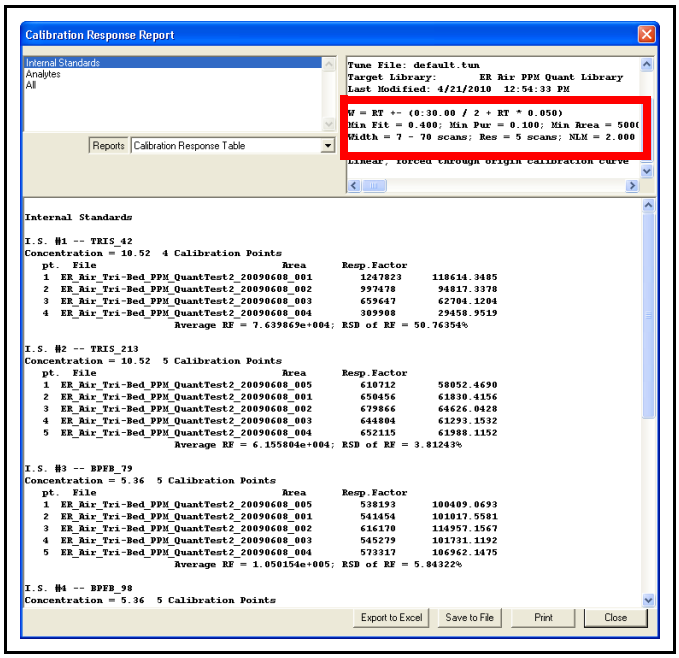
Selecting **All** will display the information contained in the **Internal Standard Calibration Report** and the **Analyte Standard Calibration Report**. (See Figure 10-78.)

Figure 10-78 All



The **Cal/Quant Report** can be viewed by selecting **Calibration Report** from the drop-down menu. See Figure 10-79. The **Cal/Quant Report** will display the same information as a **Quantitative Report**. Refer to section 8.4, Reports, on page 8-5 for more details. In the top right corner, the peak search parameters are also displayed. Refer to section 10.10.3, Peak Search, on page 10-44. (See Figure 10-79.)

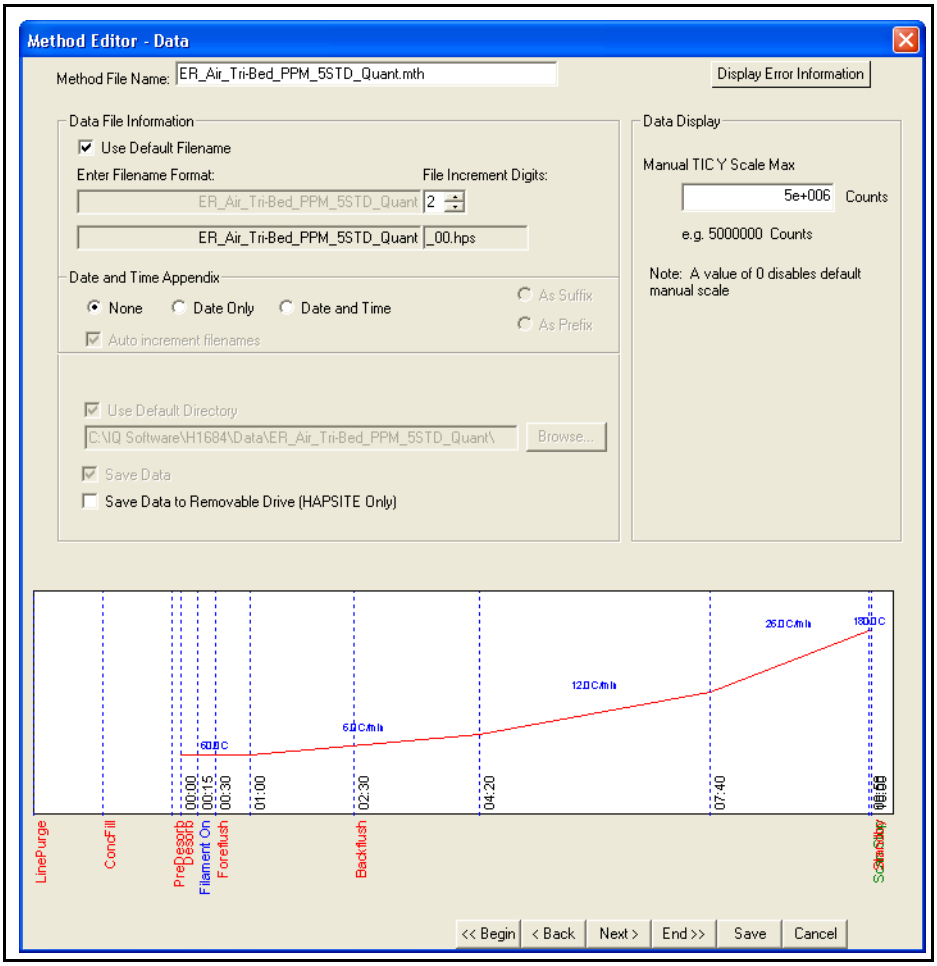
Figure 10-79 Cal/Quant Report



10.11 Data Page

The **Data Page** customizes the names and the storage location of the data files for the method. See Figure 10-80.

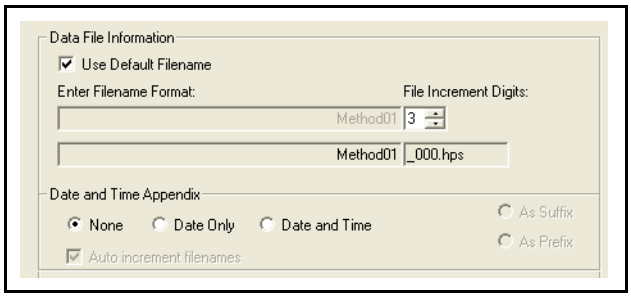
Figure 10-80 Method Editor Data Page



10.11.1 Data File Information

Use default filename . . . . . When checked, the method will use a default format for the data filename. The default filename is a combination of the method filename, the date and the sample run number. See Figure 10-81.

Figure 10-81 Use Default Filename



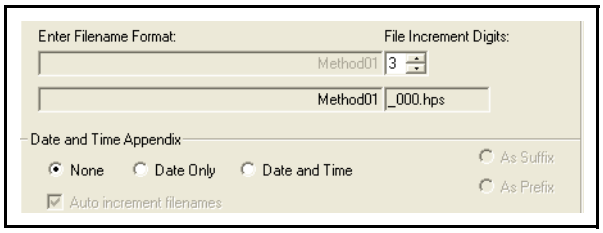
File increment digits . . . . . Sets the number of digits appended to the data file name. By default, **File Increment Digits** is set to three digits.

10.11.2 Date and Time Appendix

If desired, the data and time can be added to the data file name using the following options.

None . . . . . A date and time will not be added to the file name. See Figure 10-82.

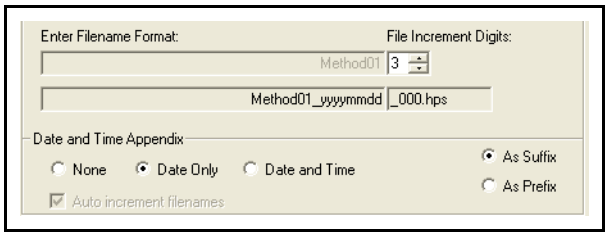
Figure 10-82 Date and Time Appendix- None Selected



Date Only . . . . . The date will add be added to the filename. See Figure 10-83.

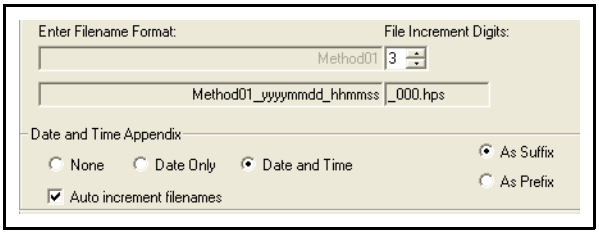
- yyyy is the year the data was collected
- mm is the month the data was collected
- dd is the day the data was collected

Figure 10-83 Date Only



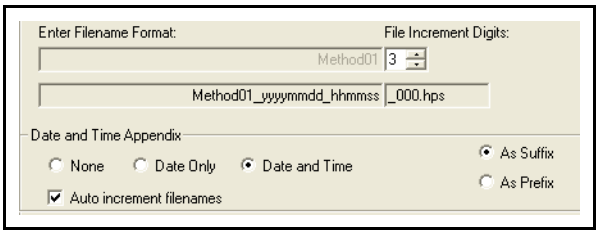
Date and Time . . . . . Both the date and time will be added to the data file name. See Figure 10-84. **hh** is the hour data collection was started. **mm** is the minute data collection was started. **ss** is the second data collection was started

Figure 10-84 Date and Time



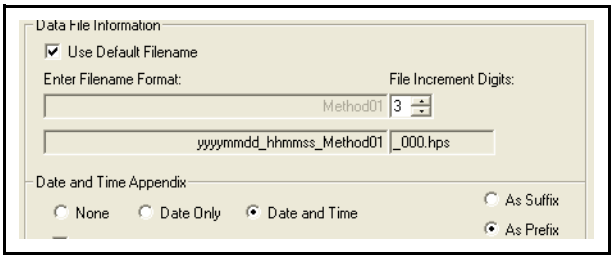
As Suffix . . . . . When **Date and Time** is selected, the date and time are added to the end of the filename. See Figure 10-85.

Figure 10-85 As Suffix



As Prefix . . . . . When **Date and Time** is selected, the date and time are added to the beginning of the filename. See Figure 10-86.

Figure 10-86 As Prefix

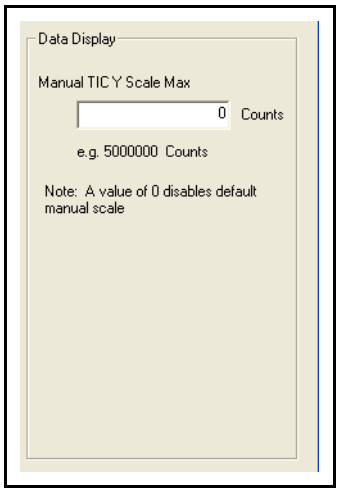


Save Data to Removable Drive . . . Data is saved to the USB on the HAPSITE ER as well as to the HAPSITE ER hard drive in the folder (directory) shown immediately above this check box.

10.11.3 Data Display

A **Manual Response Y** number can be entered, which will scale the Y-axis of the chromatogram to the desired counts. If there is not a number in this section, the TIC will automatically scale to the largest number. See Figure 10-87.

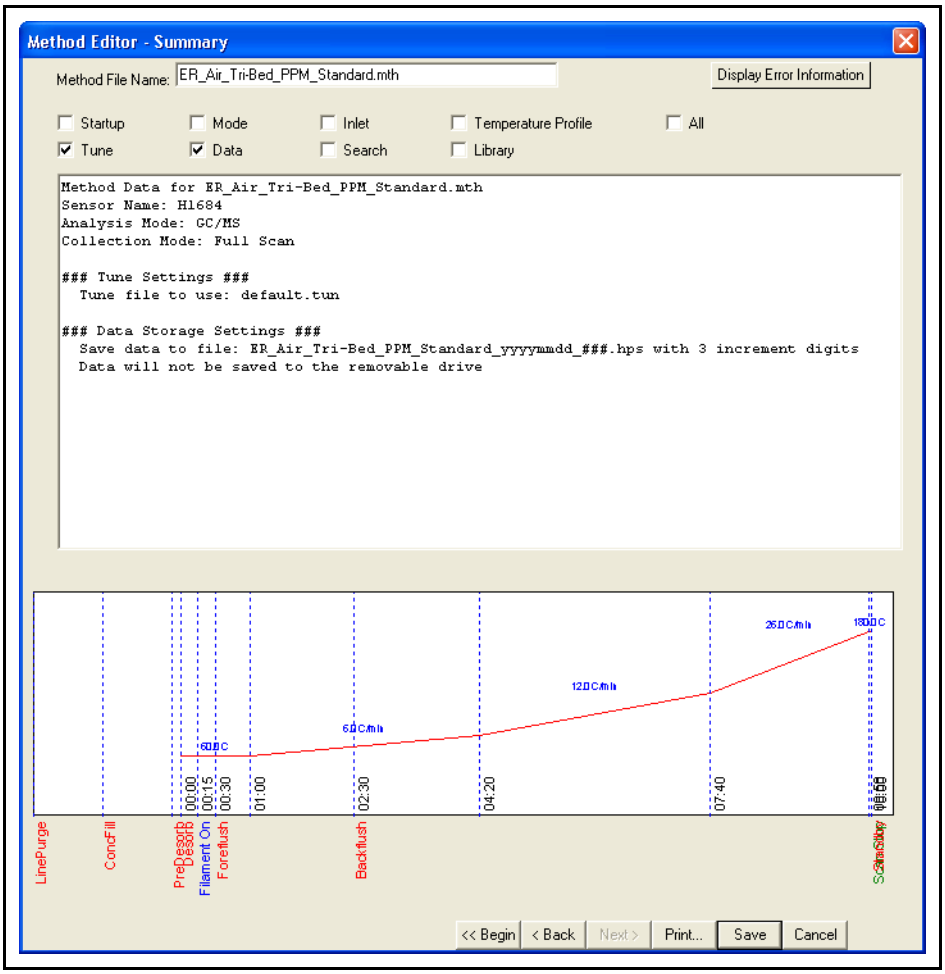
Figure 10-87 Data Display



10.12 Summary Page

The **Summary** page provides selections to display the selected components of the method in a text report. The method settings can be reviewed in this report before the method is saved. See Figure 10-88.

Figure 10-88 Method Editor Summary Page



10.13 Method Sequence

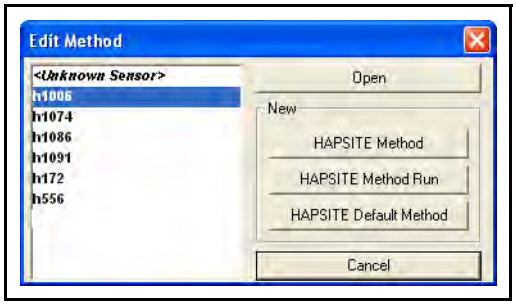
A series of methods can be configured to run back to back or at timed intervals. Follow the instructions below to sequence a method.

1 Double-click the **Method Editor** icon. See Figure 10-89.

Figure 10-89 Method Editor Icon

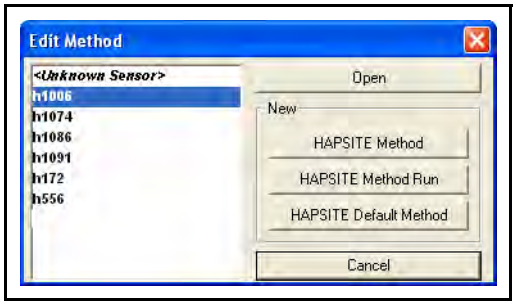
2 If more than one unit is connected to the laptop, click on the name of the desired HAPSITE ER. See Figure 10-90.

Figure 10-90 Selecting Desired HAPSITE ER



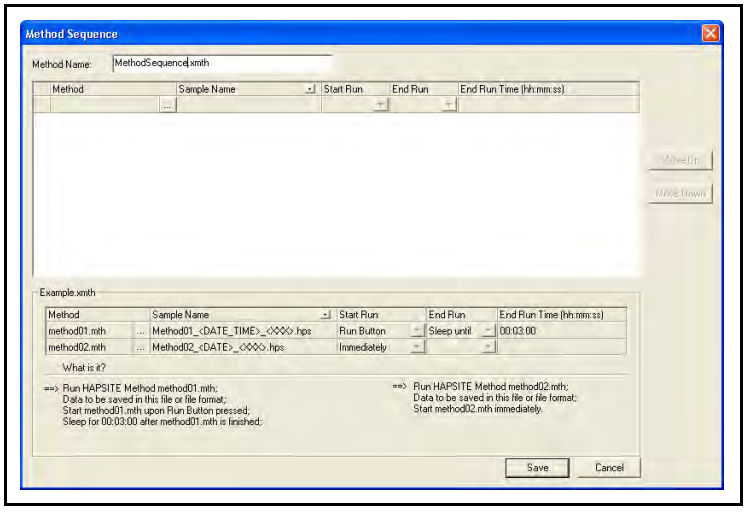
3 Click the **HAPSITE Method Sequence** option. See Figure 10-91.

Figure 10-91 HAPSITE Method Sequence



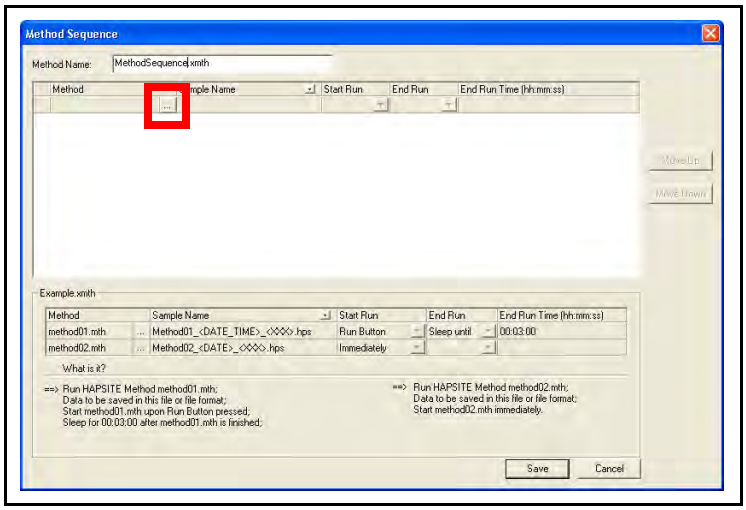
4 If desired, type in a new name for the method. Ensure that the file extension ends in **.xmth**. See Figure 10-92.

Figure 10-92 Typing in New Name



5 Click the button that is highlighted in the figure below. See Figure 10-93.

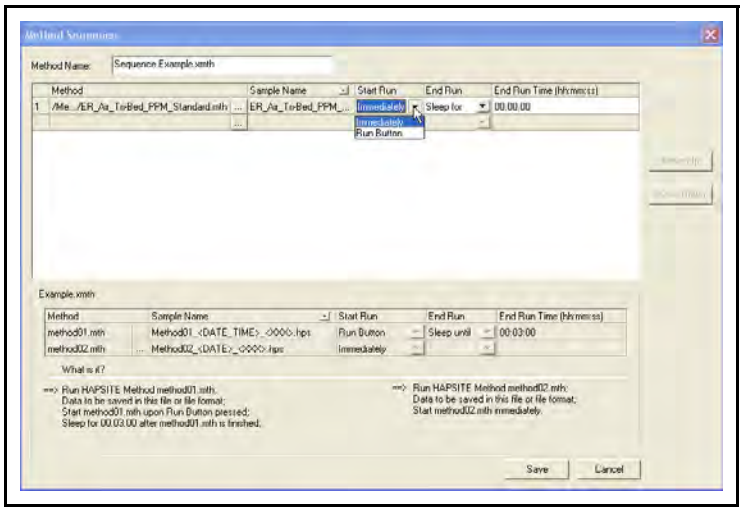
Figure 10-93 Click Highlighted Button



6 Double-click on the desired folder to access the desired method. For instructions on selecting folders, refer to section 8.3, Accessing the Data Review Feature, on page 8-2.

7 Select **Immediately** or **Run Button** from the drop-down menu to start the analysis. The **Immediately** option runs the next method as soon as the previous method has finished. The **Run Button** options requires the user to select **Run** to start the next method. See Figure 10-94.

Figure 10-94 Start Run



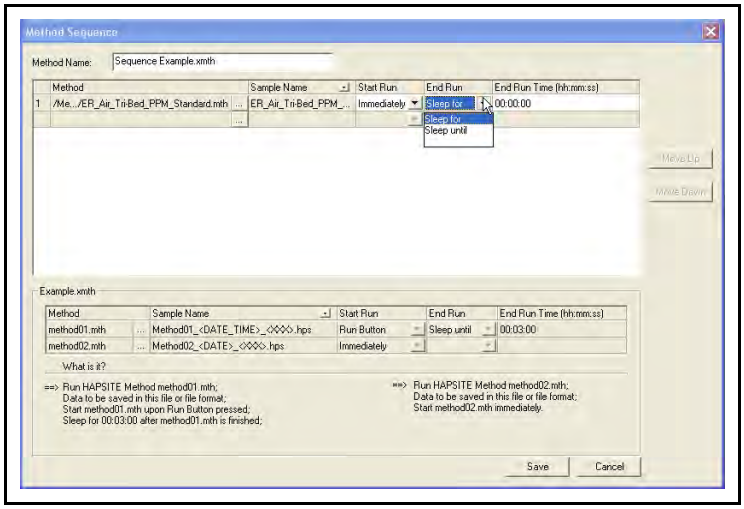
8 Select the timing between sample runs.

8a Select **Sleep for** if a lapse in time is desired. For example, if 1:30 is entered, the second method will run an hour and a half after the first method finishes. See Figure 10-95.

8b Select **Sleep until** to enter a specific time. For example, if 1:30 is entered, the second method will start at 1:30 a.m. See Figure 10-95.

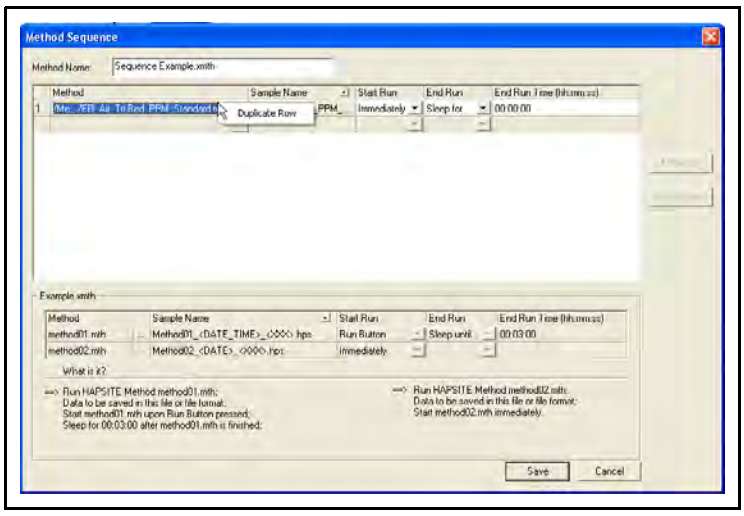
NOTE: Sleep until uses 24 hour notation.

Figure 10-95 End Run



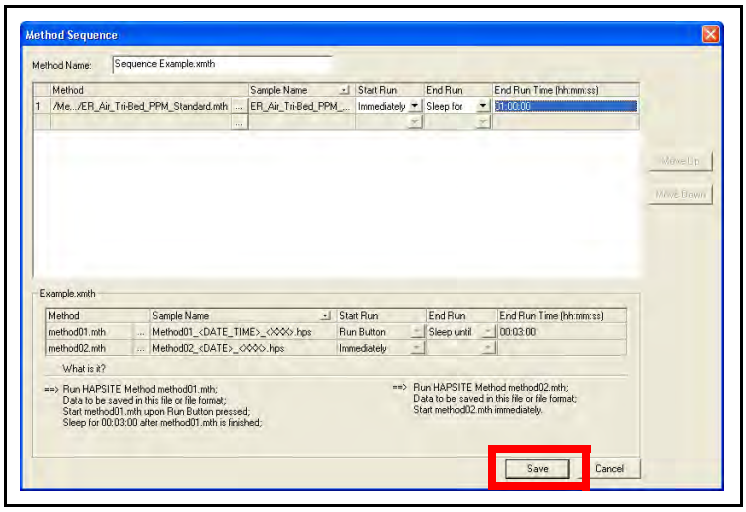
9 Add multiple runs by repeating Step 5 to Step 8b. Alternately, right-click and select **Duplicate Row**. See Figure 10-96.

Figure 10-96 Duplicate Row



10 Select **Save** to save the method. See Figure 10-97.

Figure 10-97 Saving Method



11 Select the desired location for saving the method. The method can be saved to the laptop or the HAPSITE by clicking the desired option at the top of the window.

Chapter 11
Calibration

11.1 Introduction to Quantitative Analysis

A **HAPSITE ER** method can be developed to collect and quantify sample data. Quantitative analysis involves creating a calibration library of target compounds, and associating target compound responses with concentration results. This library contains the analyte name, analyte area, the retention time and the response factor used to calculate the concentration of the analyte.

11.2 Calibrating a Method

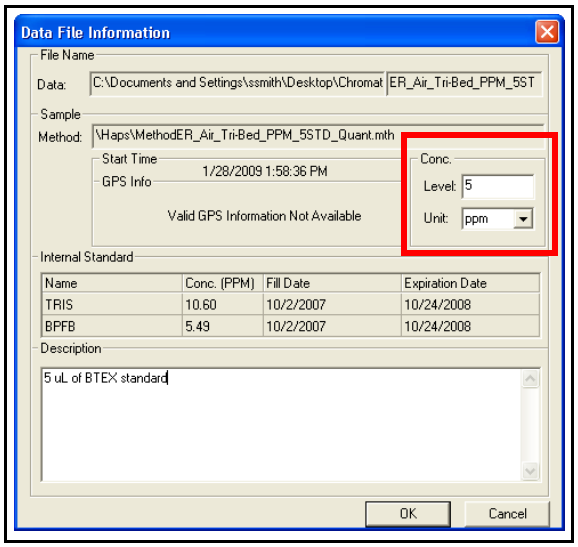
WARNING

Wear appropriate Personal Protective Equipment (PPE) as advised in the MSDS of the standard(s) being used.

1. Prepare the standards as necessary to achieve the desired concentrations.
2. Run each standard separately on HAPSITE ER using the desired method. Each standard will have its own separate run. The method used for HAPSITE ER can be a default method or custom method created with the **Method Editor**. See Chapter 11, Calibration.

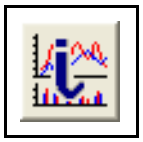
   NOTE: All other components of method development described in Chapter 10, Method Editor must be made prior to running the standards.
3. Enter the concentration of the standard and a description on the **Data File Information** window during each sample run. (See Figure 11-1.)

Figure 11-1 Data File Information page



3a Click the **Data File Information** window. (See Figure 11-2.)

Figure 11-2 Data File Information

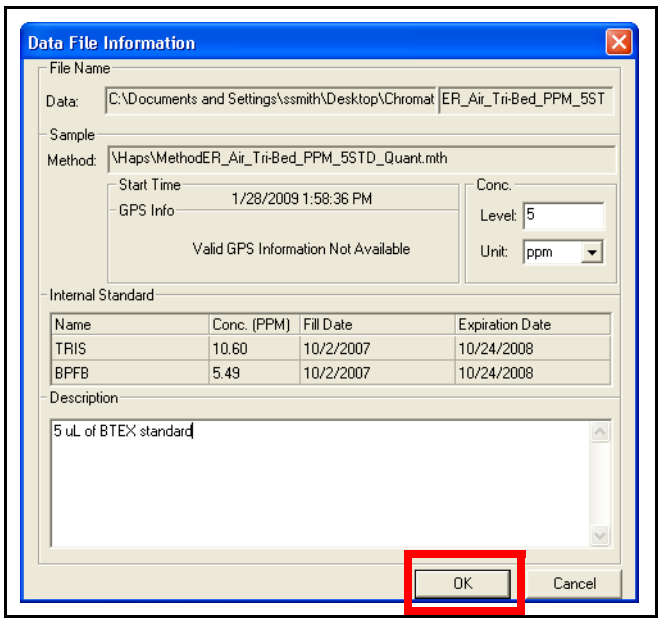


3b Enter in the concentration and the units into fields highlighted in Figure 11-1.

NOTE: If desired, a description can be entered into the **Description** field.

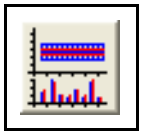
3c Click **OK**. (See Figure 11-3.)

Figure 11-3 OK



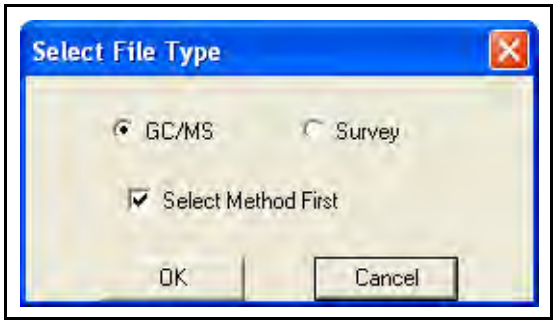
4 When every standards has finished running, double-click the **Calibrate** icon. (See Figure 11-4.)

Figure 11-4 Calibrate icon



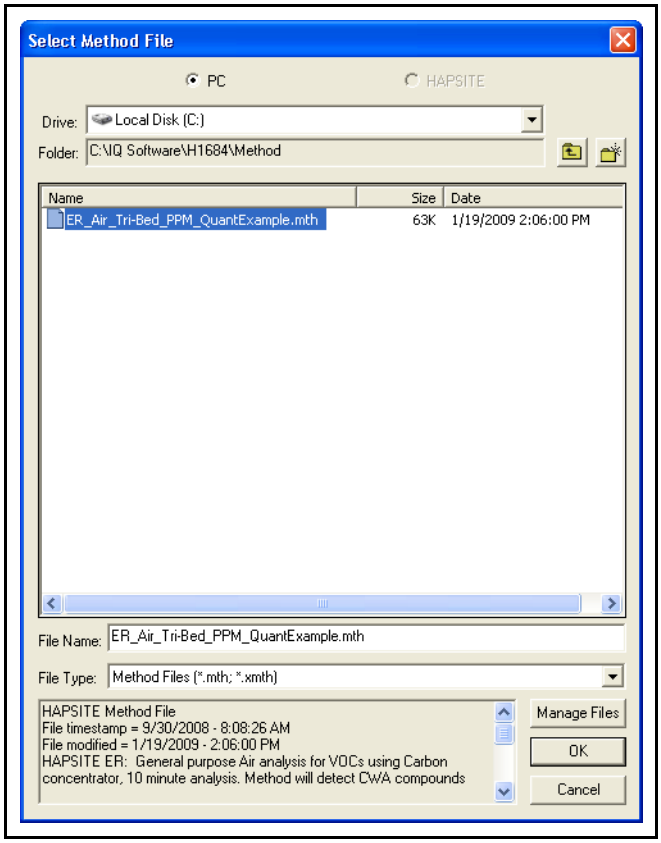
5 Selecting the **Calibrate** function will display a dialog box used to select either an **Analyze (GC/MS)** method or a **Survey** method. The **Select Method First** box should remain checked. Click **OK**. (See Figure 11-5.)

Figure 11-5 Selecting the Type of Quantitative Method



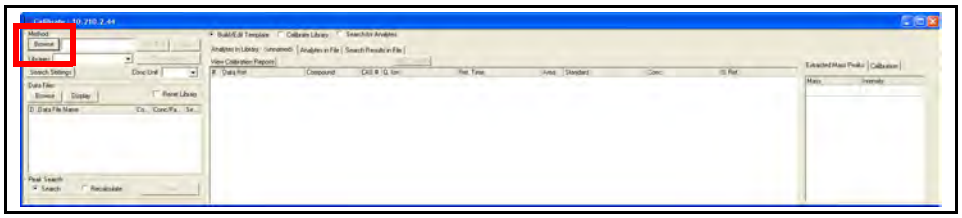
6 The **Method File** window will be displayed if the **Select Method First** box remained checked. (See Figure 11-6.)

Figure 11-6 Method File



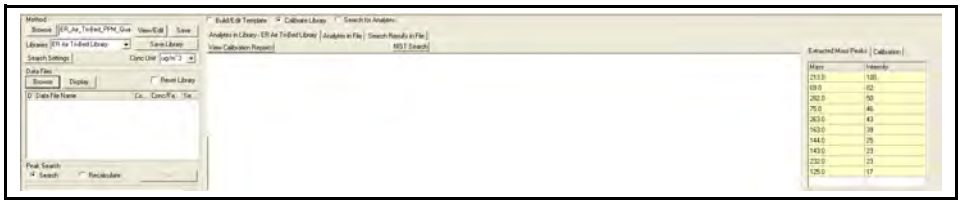
7 If the **Select Method First** box was unchecked, select the **Browse** button in order to select a method file. (See Figure 11-7.)

Figure 11-7 Browse button



8 Click the **Browse** button under **Data Files**. Select the desired data file for library template creation. (See Figure 11-8.)

Figure 11-8 Calibration Control Panel with Data File Selected



NOTE: It is recommended to use a high or mid range standard for calibration library development. Standards with low concentrations may have peaks too small to be detected with default **Search Settings**.

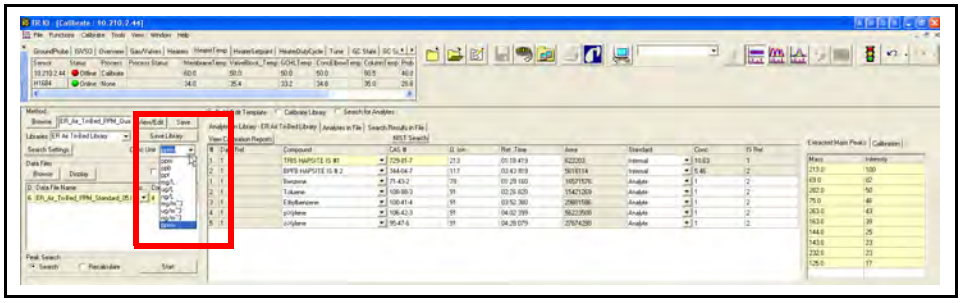
9 Select **Build/Edit Template**. (See Figure 11-9.)

Figure 11-9 Build/Edit Template

10 Select the units. (See Figure 11-10.)

NOTE: Step 10 will be automatically completed if the information was entered in the Data File Information window when the sample was run. Refer to Step 3.

Figure 11-10 Unit Selection



11 Set the **Concentration Reference** to **Global** or **Analyte**. (See Figure 11-11.)

NOTE: Select **Global** for standards that contain analytes that have the same concentration. This is most common with liquid standards diluted into a liquid.

NOTE: Select **Analyte** for standards that contain analytes with different concentrations. This is the most common with liquid standards that are diluted into a gas.

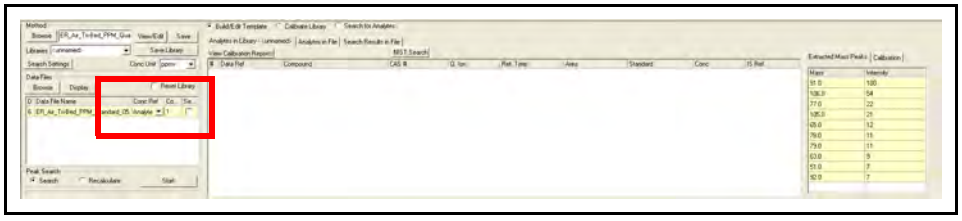
Figure 11-11 Global/Analyte

12 If **Global** is selected, enter in the concentration of the standard. Step 10 will be automatically completed if the information was entered in the **Data File Information** window when the sample was run. Refer to Step 3. (See Figure 11-12.)

Figure 11-12 Global

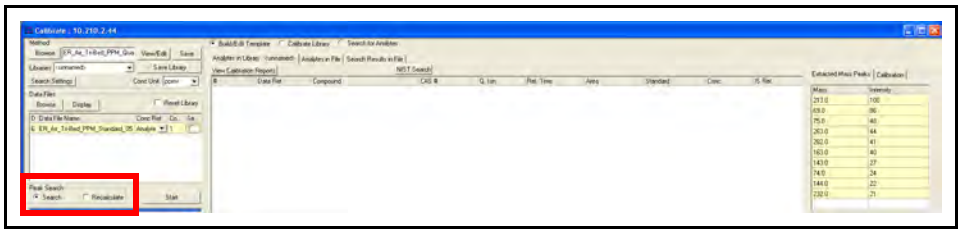
13 If **Analyte** is selected, enter the volume of standard used for the selected data file into the field highlighted below. For example, if an analyte was run at the concentrations of 5 ppb, 10 ppb and 20 ppb, the factor for the 5 ppb data file would be 1. For the 10 ppb, 2 would be the factor, and for the 20 ppb file, 4 would be the factor. The concentration of the standard would be entered into the concentration column in Step 28. (See Figure 11-13.)

Figure 11-13 Analyte



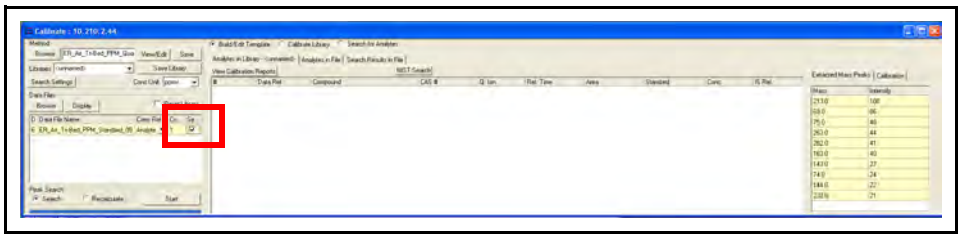
14 Set **Peak Search** to **Search**. (See Figure 11-14.)

Figure 11-14 Setting Peak Search



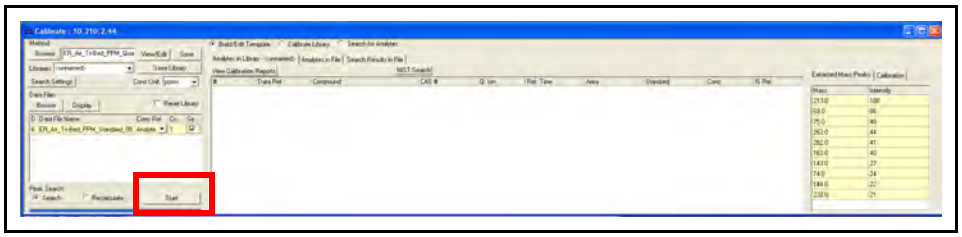
15 Check **Select**. (See Figure 11-15.)

Figure 11-15 Select



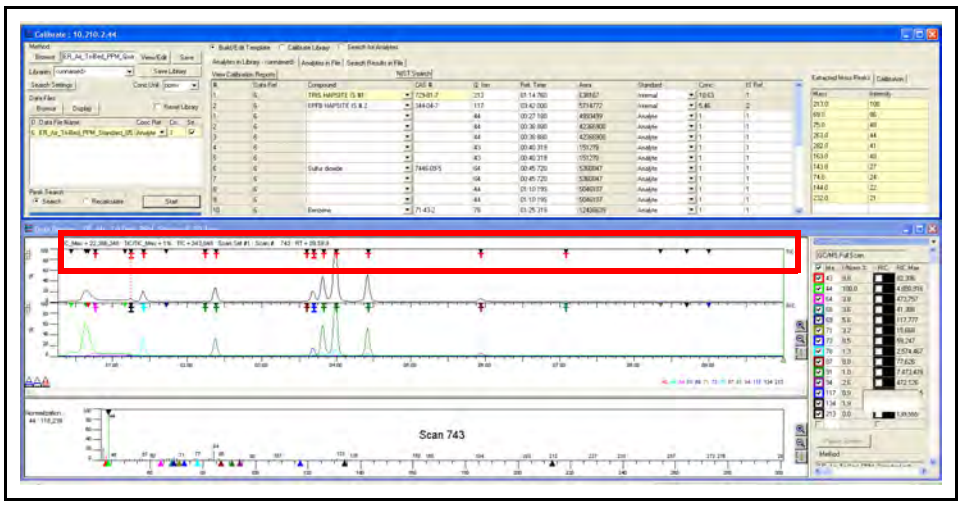
16 Click **Start**. (See Figure 11-16.)

Figure 11-16 Start



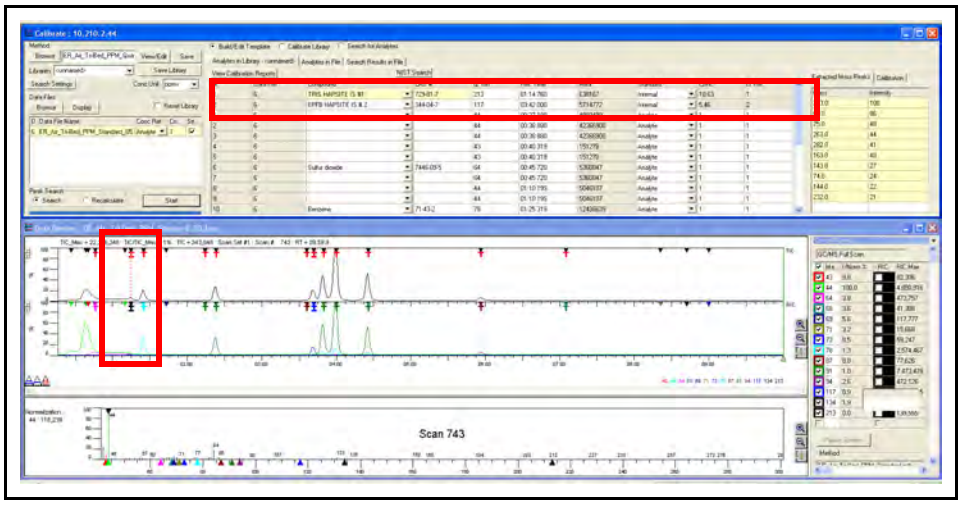
17 All compounds that have been identified by AMDIS will be labeled with a red T over the apex of the peak. (See Figure 11-17.)

Figure 11-17 Labeled Peaks



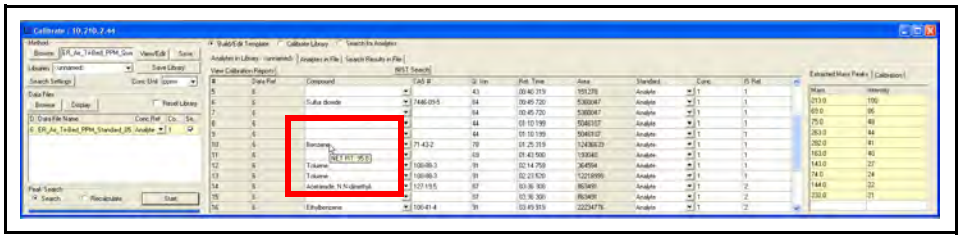
18 The highlighted compound in the library template will correspond to the peak with the red dotted line. (See Figure 11-18.)

Figure 11-18 Peak Correspondence



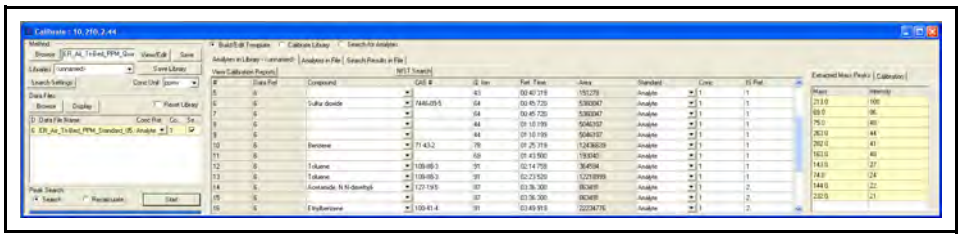
19 Verify that all analytes have a Net Fit greater than 70 by hovering the mouse over the analyte name. (See Figure 11-19.)

Figure 11-19 Net Fit



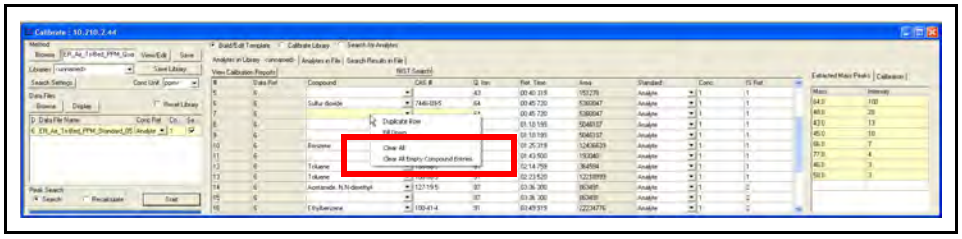
20 Verify that the retention times are correct. (See Figure 11-20.)

Figure 11-20 Retention Time Verification



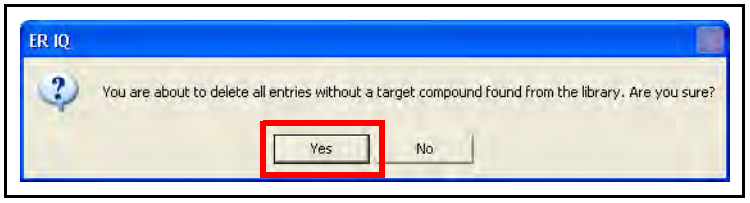
21 If unidentified compounds are present, which are indicated by a blank row, right click on a compound and select **Clear All Empty Compound Entries**. (See Figure 11-21.)

Figure 11-21 Clear All Empty Compounds



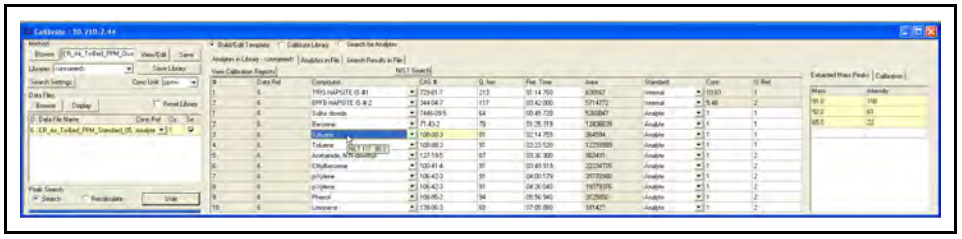
22 Click **Yes** to confirm the deletion of the unidentified compounds. (See Figure 11-22.)

Figure 11-22 Confirming Deletion



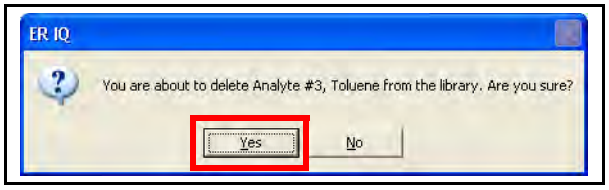
23 Delete any duplicate analytes, duplicate internal standards or undesired analytes from the template by highlighting the undesired compound and clicking **Delete** on the laptop keyboard. (See Figure 11-23.)

Figure 11-23 Deleting Duplicates



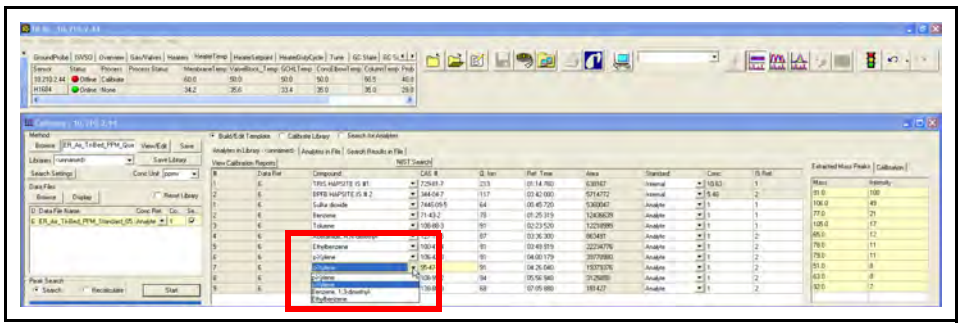
24 Click **Yes** to confirm the deletion of the undesired compounds. (See Figure 11-24.)

Figure 11-24 Confirming Analyte Deletion



25 If a compound was not correctly identified, type in the correct name. Alternately, the down arrow next to the compound name can be used to select a different name if AMDIS has identified more than one possible match. (See Figure 11-25.)

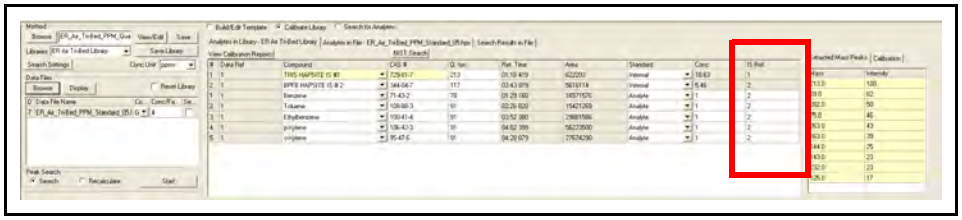
Figure 11-25 Correcting the Identification



26 Set the **IS Ref. (IS Reference)**. When using internal standards, best practice is to use a quant ion from the internal standard that is close in mass to the quant ion of the compound to be quantified. The software always selects the largest mass fragment in the spectrum as the quant ion. To change the quant ion, highlight the field and type in the new number. (See Figure 11-26.)

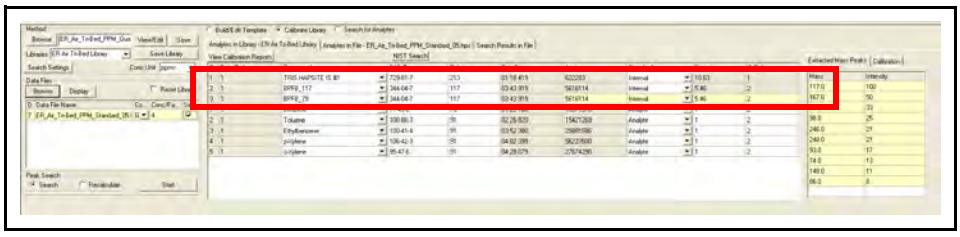
NOTE: The software will automatically recognize TRIS and BPFB. It will automatically enter the concentration from the IS canister into the method for calibration and quantization.

Figure 11-26 IS Reference



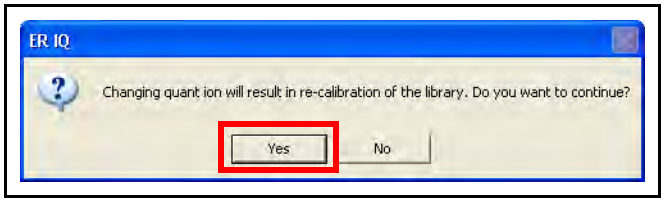
27 More than one quant ion can be used from a single internal standard peak. For example, highlight the second internal standard and right-click. Select **Duplicate Row**. Then, change the name of the internal standard peaks to **BPFB_79** and **BPFB_117**. The **Quant Ion** should be changed to **79** and **117**. (See Figure 11-27.)

Figure 11-27 Adding Quant Ions



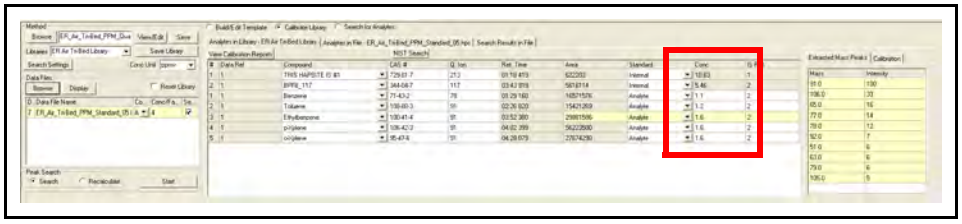
NOTE: When adding more than one quant ion, the following message will be displayed. Click **Yes** to allow for the recalibration to continue. (See Figure 11-28.)

Figure 11-28 Recalibration



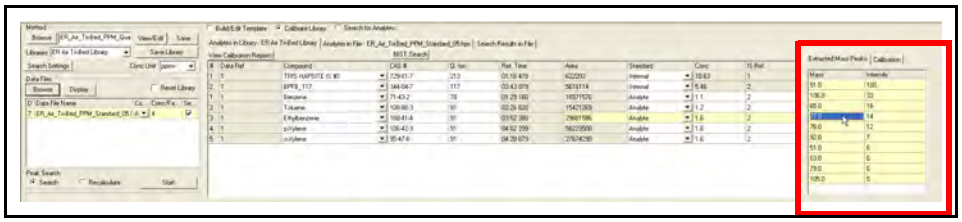
28 Enter the lowest concentration of each analyte into the **Conc** column if **Analyte** has been selected. If Global is selected, this step can be skipped. (See Figure 11-29.)

Figure 11-29 Entering the Analyte Concentration



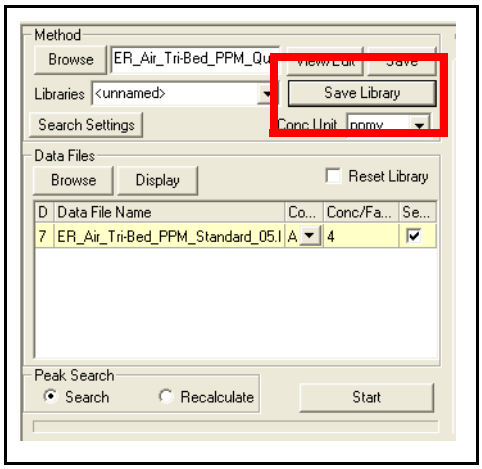
29 The **Extracted Mass Peaks** can also be edited to delete mass fragments. To delete unwanted mass fragments, highlight the field and press the delete key. Unwanted mass fragments would be those with intensities below 15%, unless the fragmentation pattern is not very distinct. (See Figure 11-30.)

Figure 11-30 Extracted Mass Peaks



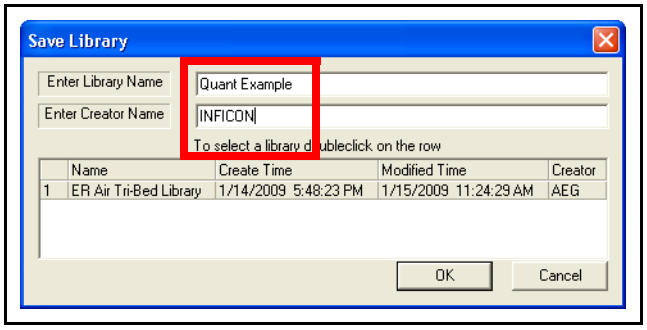
30 Save the template by clicking the **Save Library** button. (See Figure 11-31.)

Figure 11-31 Save Library



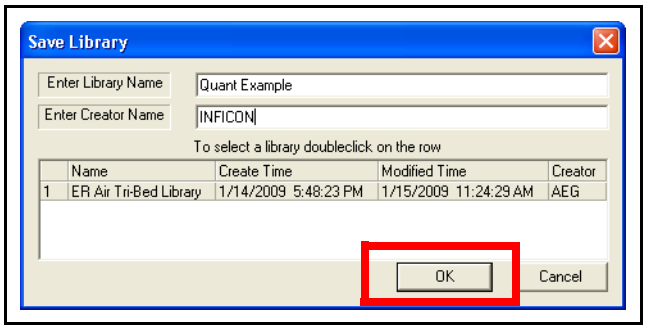
31 Enter a library name and a user name. (See Figure 11-32.)

Figure 11-32 Entering Library and User Name



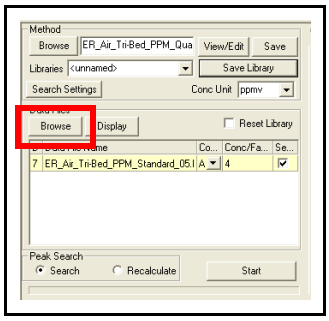
32 Click **OK**. (See Figure 11-33.)

Figure 11-33 Click OK



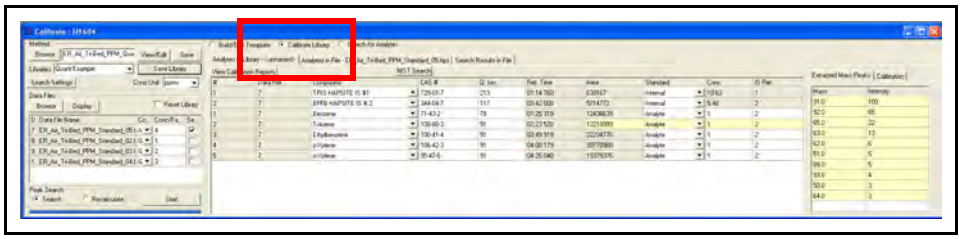
33 To calibrate the library, click **Browse** to select the desired data files. (See Figure 11-34.)

Figure 11-34 Browse to Select Data File



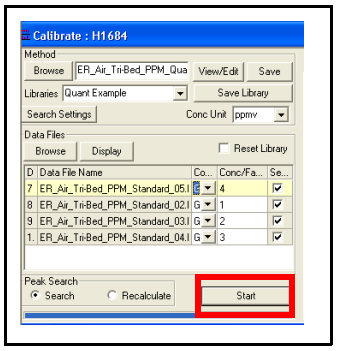
34 Select **Calibrate Library**. (See Figure 11-35.)

Figure 11-35 Calibrate Library



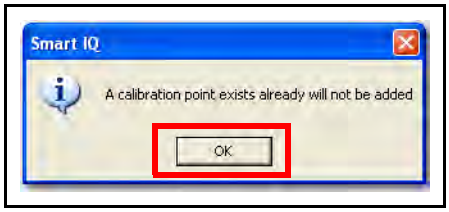
35 Check all of the data files and click the **Start** button under **Peak Search**. (See Figure 11-36.)

Figure 11-36 Start



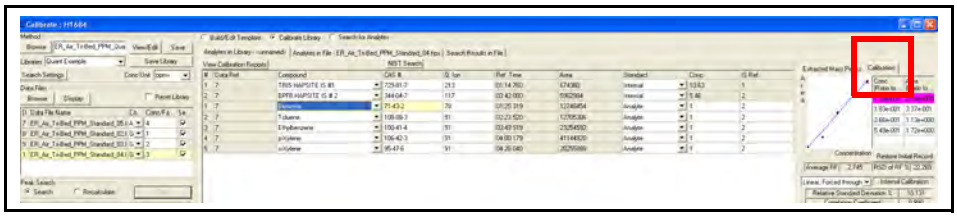
NOTE: Additional calibration points can be added to the curve by following Step 8 through Step 35. Click **OK** when the **A calibration point exists already will not be added** message is displayed. (See Figure 11-37.)

Figure 11-37 Confirming Additional Calibration Points



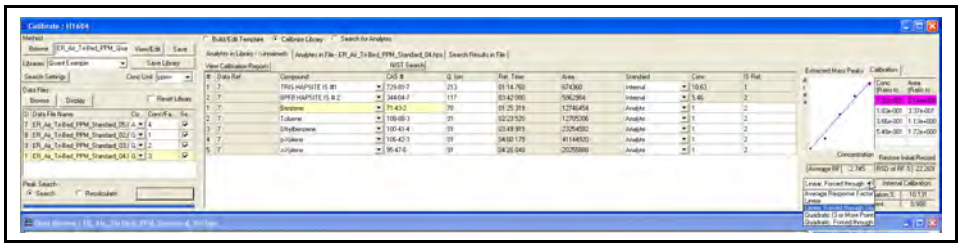
36 Review the curves for each analyte by clicking the **Calibrate** tab. (See Figure 11-38.)

Figure 11-38 Calibrate tab



37 Click each analyte to display the corresponding calibration curve. The curve should fit the data points. The drop-down menu provides four curve fit options: **Linear**, **Linear**, **Forced through the Origin**, **Quadratic** and **Quadratic, Forced through the Origin**. (See Figure 11-39.)

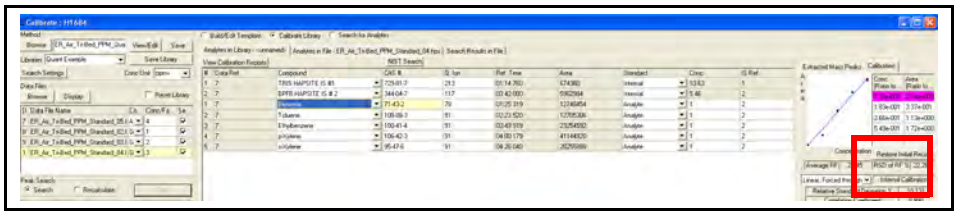
Figure 11-39 Curve Fit



NOTE: The RSD of the curve will vary depending upon the curve fit selected.

38 Verify that the RSD of RF% is acceptable. It is recommended that the RSD of RF% is 30% or lower. (See Figure 11-40.)

Figure 11-40 Verifying RSD of RF%

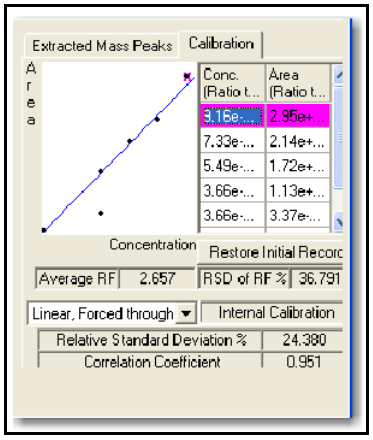


39 It is possible to delete points from the calibration curve. (See Figure 11-41.)

NOTE: Removal of points in the middle of a calibration curve is contrary to established analytical standards. Points can be removed from the highest and lowest level of the curve, but this will affect the calibration range.

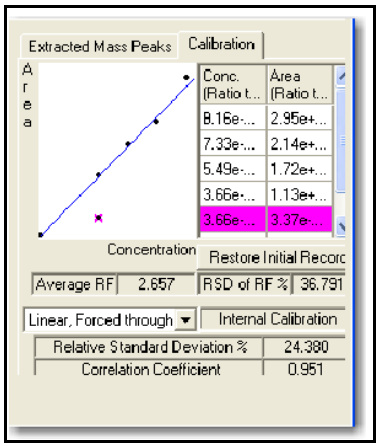
40 Click any number in the **Conc. (Ratio to IS)** column. The corresponding point will be overlaid with a pink X. (See Figure 11-41.)

Figure 11-41 Clicking in the Conc. (Ratio to IS) Column



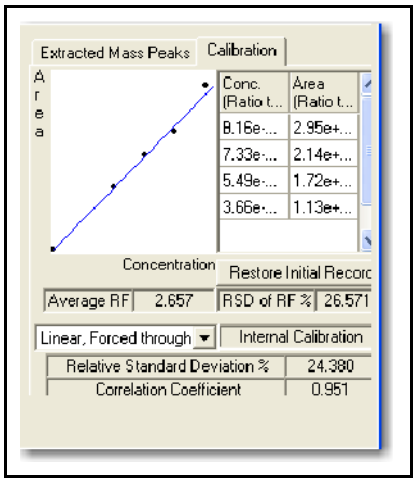
41 Use the up and down arrows to select the outlying point. (See Figure 11-42.)

Figure 11-42 Selecting the Outlying Point



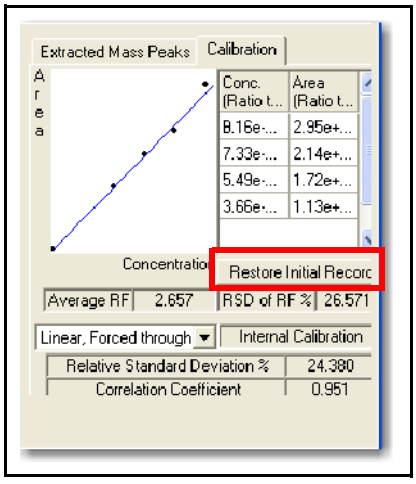
42 Click **Delete**. (See Figure 11-43.)

Figure 11-43 Deleting Point



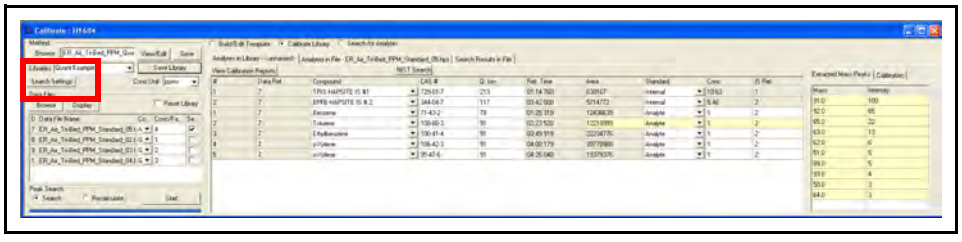
NOTE: If a point was inadvertently deleted, the original calibration points can be restored by clicking the **Restore Initial Record** button. (See Figure 11-44.)

Figure 11-44 Restoring Initial Record



43 If a point is missing because it does not meet the peak search criteria, the peak search parameters can be adjusted. Click **Search** settings to adjust all of the compounds at once. To adjust individual analytes, click **View/Edit**. Refer to () for more information. (See Figure 11-45.)

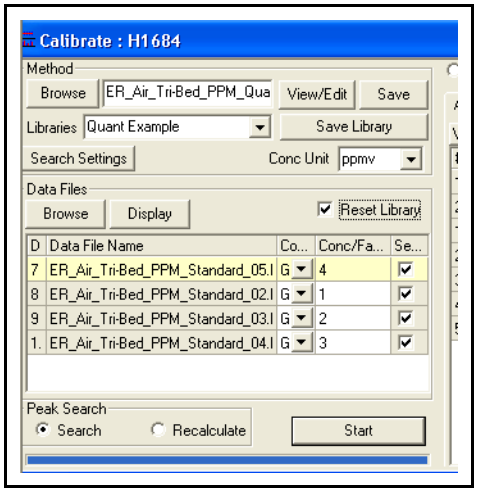
Figure 11-45 Adjusting Peak Search Settings



44 To recalibrate the library with the new parameters:

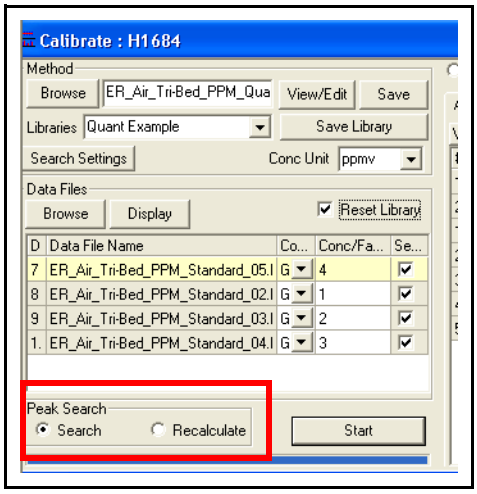
44a Check the **Reset Library** box. (See Figure 11-46.)

Figure 11-46 Reset Library



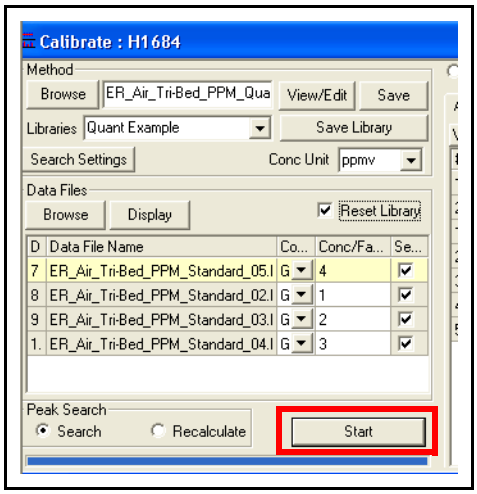
44b Verify that the **Peak Search** is set to **Search**. (See Figure 11-47.)

Figure 11-47 Search



44c Click **Start**. (See Figure 11-48.)

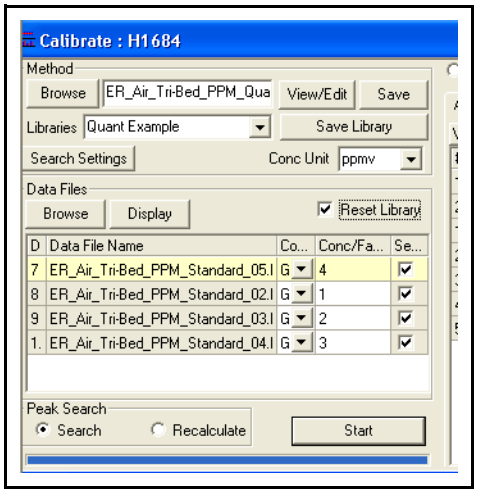
Figure 11-48 Start



44d Repeat Step 17 through Step 42.

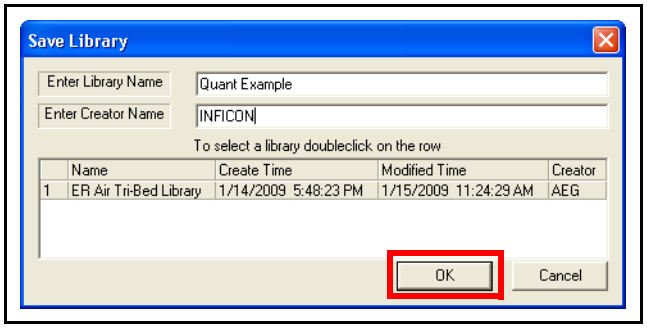
45 When the method is satisfactory, click **Save Library**. (See Figure 11-49.)

Figure 11-49 Saving Library



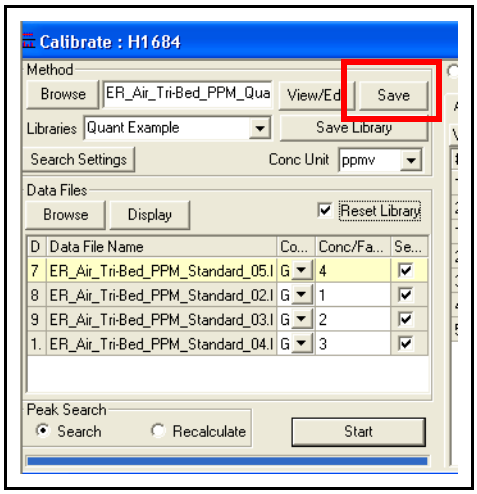
46 Click **OK**. (See Figure 11-50.)

Figure 11-50 Clicking OK



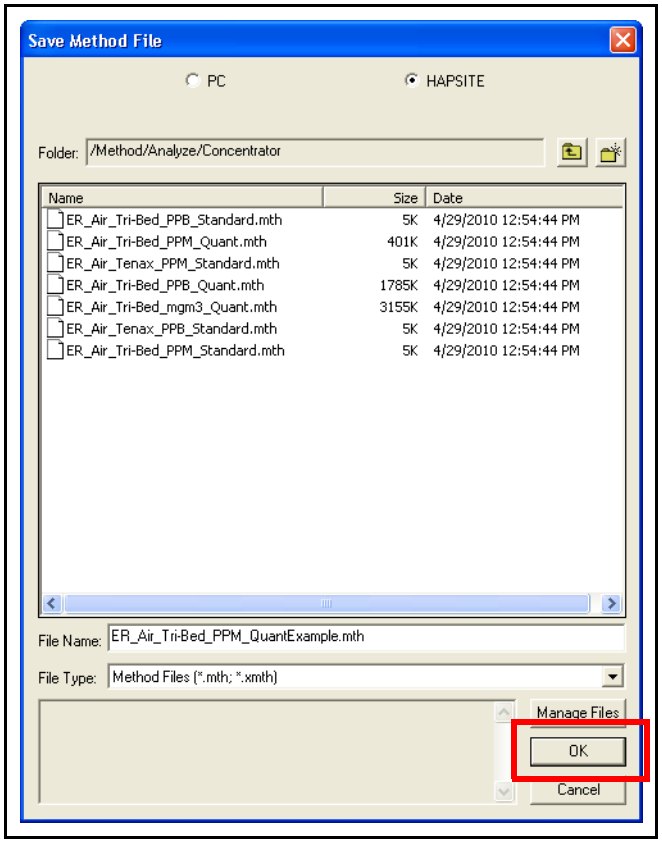
47 Save the library to the method by clicking **Save**. (See Figure 11-51.)

Figure 11-51 Saving Library to the Method



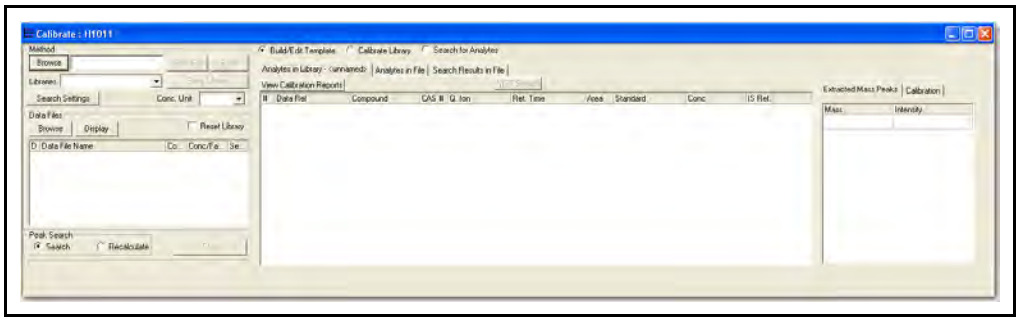
48 Click **OK**. (See Figure 11-52.)

Figure 11-52 Clicking OK



11.3 Definition of Terms in the Calibrate Window

Figure 11-53 Calibrate Window



11.3.1 Method

Browse . . . . . Allows the user to select a method for calibration.

View/Edit . . . . . Opens the **Method Editor** for the method that is currently being calibrated. See Chapter 10, Method Editor.

Save . . . . . Saves the current method.

Libraries . . . . . A drop-down menu that allows the user to select a previously saved library.

Save Library . . . . . Brings up the dialog box to save the library.

Search Settings . . . . . Displays the search parameter settings. See section 8.7.0.2, Peak Search Parameters, on page 8-33.

Conc. Unit . . . . . Used to select the concentration units.

11.3.2 Data Files

Browse . . . . . Used to select the data files for building and calibrating the library; when a data file is selected the data is listed as follows:

D . . . . . Shows the data file reference number.

Data File Name . . . . . Displays the data file name and storage pathway.

Conc Ref . . . . . Basis for calculating the concentration. Global (all analytes are at the same concentration) or Analyte (analytes are in file at specific concentrations).

Conc/Factor . . . . . Data file concentration of analytes if **Global** is selected, or concentration multiplier if **Analyte** is selected.

Selection . . . . . If checked, file will be processed upon clicking **Start**.

Display . . . . . Displays the chromatogram for the selected data file.

Reset Library . . . . . If checked, the calibration curve will be reset. All points currently contained in the library will be deleted.

11.3.3 Peak Search

Search . . . . . When **Build/Edit** is selected, **Search** performs a peak detection and integration on the selected files. When **Calibrate** is selected, **Search** calibrates the library and calculates the response factors.

Recalculate . . . . . Recalculates the peak areas and response factors without performing a peak search. This is most useful after manually editing the baseline points of the peak.

Start . . . . . Initiates the **Search** or **Recalculation**.

Build/Edit Template . . . . . **Build/Edit** must be selected if an analyte search, deletion of analytes or changing template parameters is desired.

Calibrate Library . . . . . Calibrate Library must be selected in order a calibration curve to be created with the desired data files.

Search for Analytes . . . . . Enables a search to be performed on the selected data file(s) without adding the detected analytes automatically to the library. This allows the data to be previewed before adding it to the library template.

NOTE: When adding compounds to an existing library or Template, use **Search for Analytes**. If using **Build/Edit Template**, the original template will be overwritten by the new search.

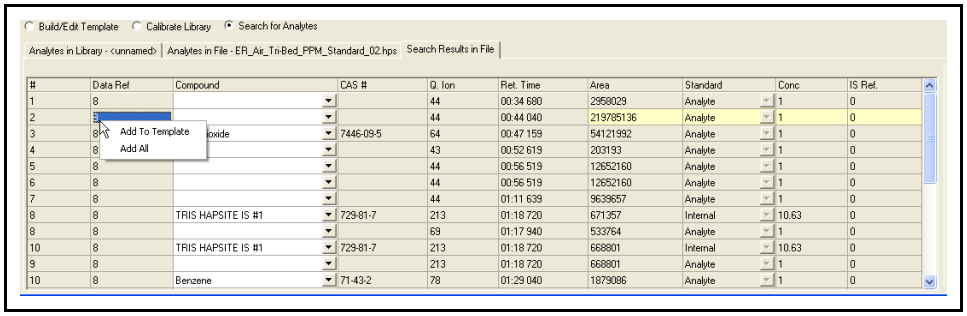
11.3.4 Analytes

Analytes in Library . . . . . Displays the analytes in the library.

Analytes in File . . . . . Displays the analytes in the currently displayed or selected file.

Search Results in File . . . . . If a search has been performed with **Search for Analytes** selected, a review of the analytes detected in the file is enabled. Individual analytes can then be added to the template by right clicking on the compound name and selecting **Add To Template**. To add all compounds detected in the file, select **Add All**. (See Figure 11-54.)

Figure 11-54 Search Results in File



11.3.5 Reports

View Calibration Reports refer to section 10.10.7, View Reports, on page 10-57**:**

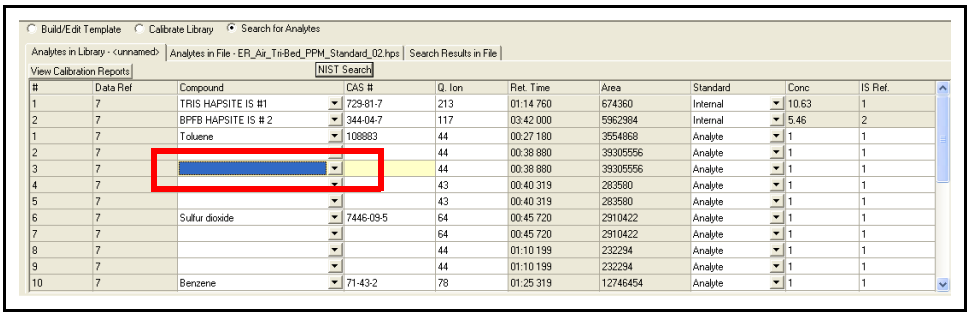
Calibration Response Table . . Report that displays the response factor and curve statistics based on the selected curve type.

Calibration Report . . . . . Report that displays the area fit and purity for the calibration standards.

NIST Search . . . . . The initial search when building a template/library is performed using the AMDIS library. If peaks are detected and loaded into the template without an identification, the **NIST Search** can be used to identify these compounds.

1 Click on an empty row without an identification. (See Figure 11-55.)

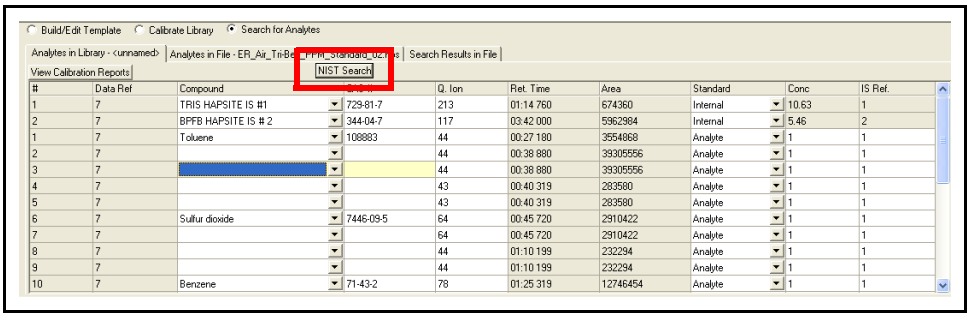
Figure 11-55 Unidentified Compound



#	Data Ref	Compound	CAS #	Q. Ion	Ret. Time	Area	Standard	Conc	IS Ref.
1	7	TRIS HAPSITE IS #1	729-81-7	213	01:14 760	674360	Internal	10.63	1
2	7	BPFB HAPSITE IS # 2	344-04-7	117	03:42 000	5962984	Internal	5.46	2
1	7	Toluene	108883	44	00:27 180	3554868	Analyte	1	1
2	7			44	00:38 880	39305556	Analyte	1	1
3	7			44	00:38 880	39305556	Analyte	1	1
4	7			43	00:40 319	283580	Analyte	1	1
5	7			43	00:40 319	283580	Analyte	1	1
6	7	Sulfur dioxide	7446-09-5	64	00:45 720	2910422	Analyte	1	1
7	7			64	00:45 720	2910422	Analyte	1	1
8	7			44	01:10 199	232294	Analyte	1	1
9	7			44	01:10 199	232294	Analyte	1	1
10	7	Benzene	71-43-2	78	01:25 319	12746454	Analyte	1	1

2 Click the **NIST Search** button. (See Figure 11-56.)

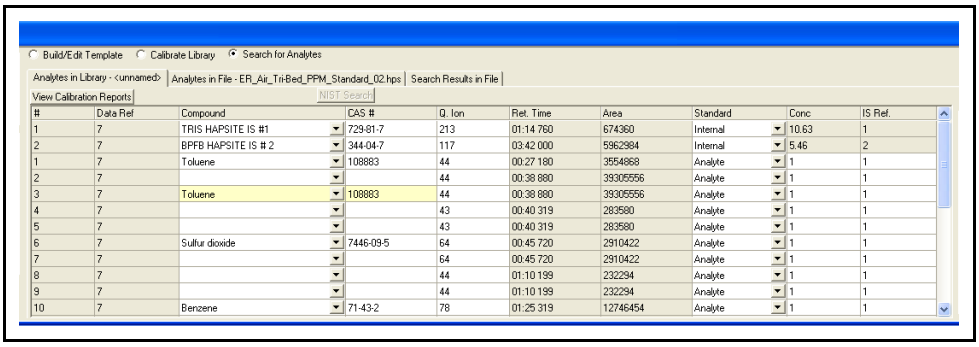
Figure 11-56 NIST Search



#	Data Ref	Compound	CAS #	Q. Ion	Ret. Time	Area	Standard	Conc	IS Ref.
1	7	TRIS HAPSITE IS #1	729-81-7	213	01:14 760	674360	Internal	10.63	1
2	7	BPFB HAPSITE IS # 2	344-04-7	117	03:42 000	5962984	Internal	5.46	2
1	7	Toluene	108883	44	00:27 180	3554868	Analyte	1	1
2	7			44	00:38 880	39305556	Analyte	1	1
3	7			44	00:38 880	39305556	Analyte	1	1
4	7			43	00:40 319	283580	Analyte	1	1
5	7			43	00:40 319	283580	Analyte	1	1
6	7	Sulfur dioxide	7446-09-5	64	00:45 720	2910422	Analyte	1	1
7	7			64	00:45 720	2910422	Analyte	1	1
8	7			44	01:10 199	232294	Analyte	1	1
9	7			44	01:10 199	232294	Analyte	1	1
10	7	Benzene	71-43-2	78	01:25 319	12746454	Analyte	1	1

3 The identification from the NIST library will be displayed. (See Figure 11-57.)

Figure 11-57 NIST Identification.



#	Data Ref	Compound	CAS #	Q. Ion	Ret. Time	Area	Standard	Conc	IS Ref.
1	7	TRIS HAPSITE IS #1	729-81-7	213	01:14 760	674360	Internal	10.63	1
2	7	BPFB HAPSITE IS # 2	344-04-7	117	03:42 000	5962984	Internal	5.46	2
1	7	Toluene	108883	44	00:27 180	3554868	Analyte	1	1
2	7			44	00:38 880	39305556	Analyte	1	1
3	7	Toluene	108883	44	00:38 880	39305556	Analyte	1	1
4	7			43	00:40 319	283580	Analyte	1	1
5	7			43	00:40 319	283580	Analyte	1	1
6	7	Sulfur dioxide	7446-09-5	64	00:45 720	2910422	Analyte	1	1
7	7			64	00:45 720	2910422	Analyte	1	1
8	7			44	01:10 199	232294	Analyte	1	1
9	7			44	01:10 199	232294	Analyte	1	1
10	7	Benzene	71-43-2	78	01:25 319	12746454	Analyte	1	1

. . . . . Shows the analyte number in the library.

Data Ref. . . . . Displays the reference to the Data File in which the analyte was found.

Compound . . . . . Shows the compound name that is either found in AMDIS, found in NIST or assigned by the user for the analyte.

CAS #. . . . . Shows the Chemical Abstracts Service number for the analyte from the AMDIS or NIST library.

Q Ion . . . . . Shows the **Quantitation Ion** for the analyte.

Ret. Time . . . . . Show the **Retention Time** for the analyte.

Area . . . . . Displays the integrated area of the quant ion.

Standard . . . . . Designates the compound as an analyte or an internal standard.

Conc . . . . . Shows the concentration of the analyte or internal standard in the displayed file.

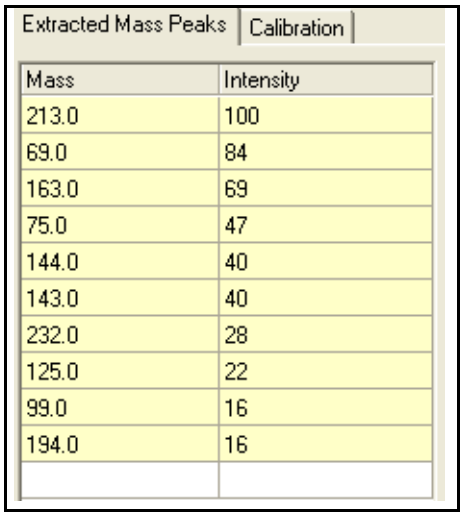
NOTE: This field is not used if the concentration flag is set to **Global**.

IS Ref. . . . . . Displays the internal standard reference number for analyte quantization.

11.3.6 Extracted Mass Peaks

Displays the mass peaks and relative percentages for the selected analyte. (See Figure 11-58.)

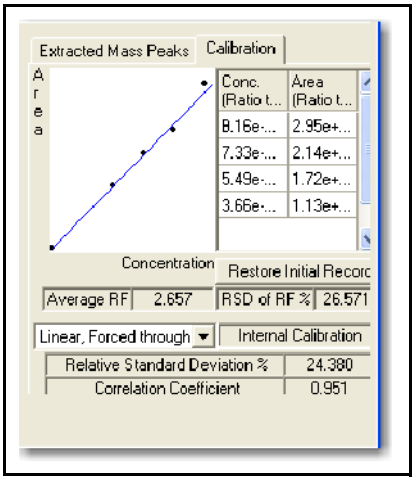
Figure 11-58 Extracted Mass Peaks



11.3.7 Calibration

Displays the calibration curve and curve statistics for the selected analyte. (See Figure 11-59.)

Figure 11-59 Calibration tab



11.4 Build/Edit Template Menu

When **Build/Edit** template is selected, right-clicking on the template will display the following options:

Duplicate Row . . . . . Creates a duplicate entry for the highlighted row.

Fill down . . . . . Replaces the contents of all rows below the highlighted row with the name of the selected compound.

Clear All . . . . . Erases all entries in the template.

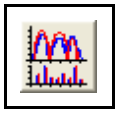
Clear All Empty Compound Entries . . . . . Deletes all entries that do not have a compound name associated with them.

11.5 ID Unknowns

The **ID Unknowns** functions allows the user to determine if all of the peaks in the chromatogram have been identified.

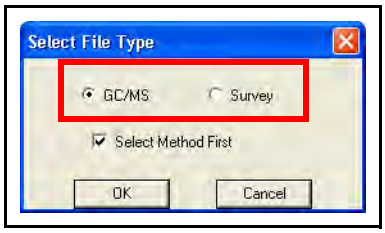
1 Double-click on the **ID Unknowns** function. (See Figure 11-60.)

Figure 11-60 ID Unknowns Icon



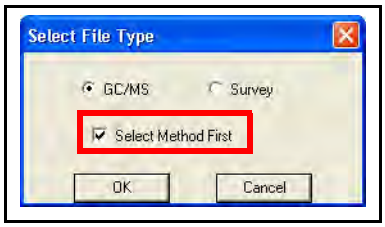
2 Select the type of file. (See Figure 11-61.)

Figure 11-61 Select File Type



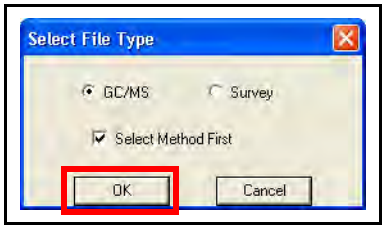
3 Verify that the **Select Method First** box is checked. (See Figure 11-62.)

Figure 11-62 Select Method First



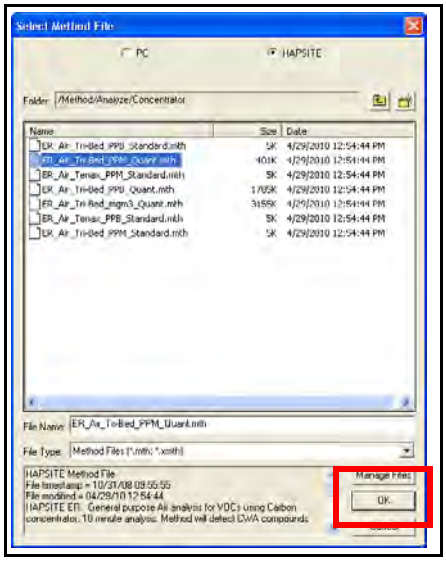
4 Click **OK**. (See Figure 11-63.)

Figure 11-63 Click OK



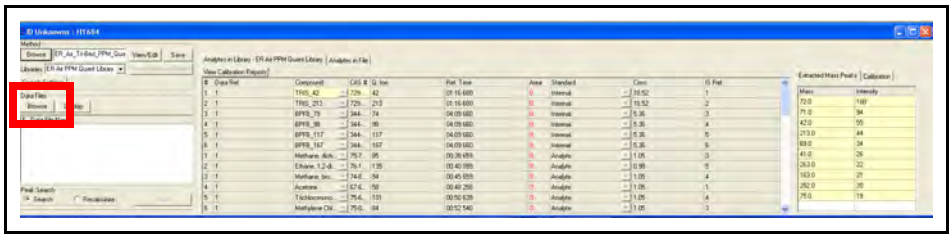
5 Select the desired method file. The data file that will be analyzed by **ID Unknowns** should have been generated from this file. Click **OK**. (See Figure 11-64.)

Figure 11-64 ID Unknowns



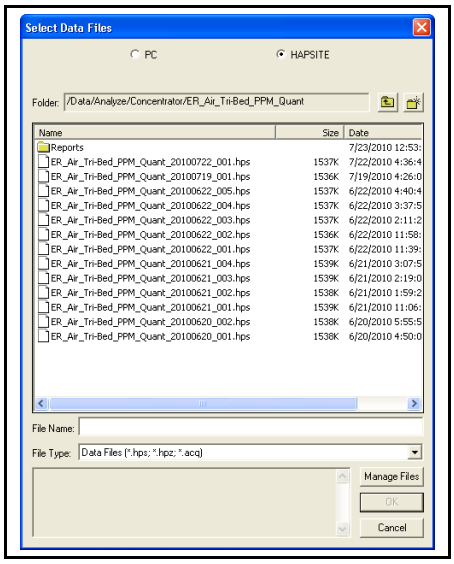
6 Click **Browse** in the **Data Files** section for the desired data file. (See Figure 11-65.)

Figure 11-65 Browse



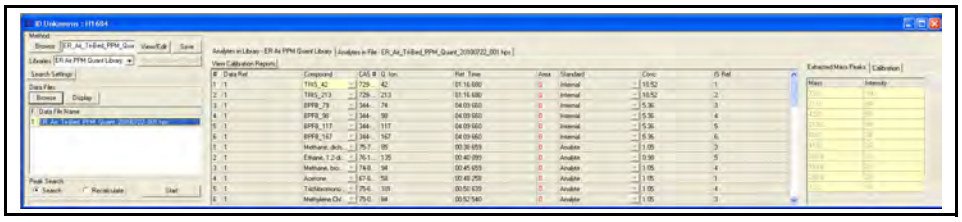
7 Select the desired data file. (See Figure 11-66.)

Figure 11-66 Selecting Data File



8 Click **Start** to open the **Quant Report** and the chromatogram. (See Figure 11-67.)

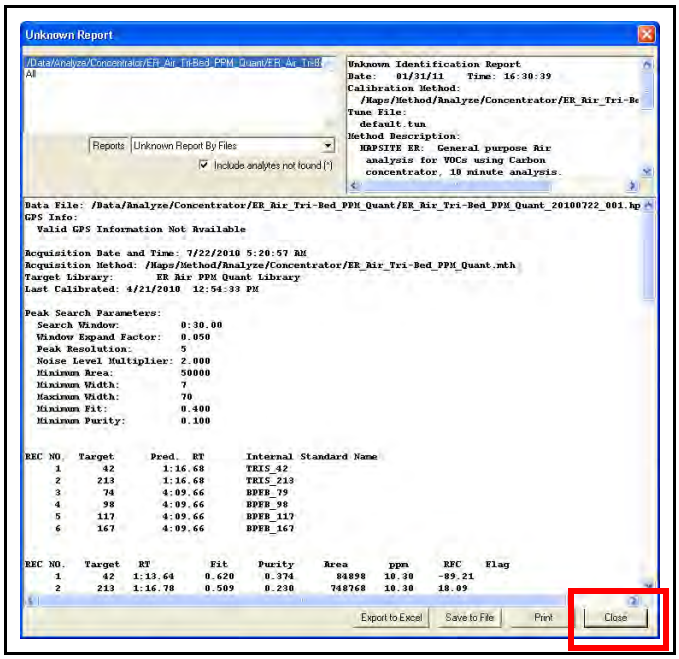
Figure 11-67 Start



9 For information on reading the **Quant Report**, refer to View Reports, see section 10.10.7 on page 10-57.

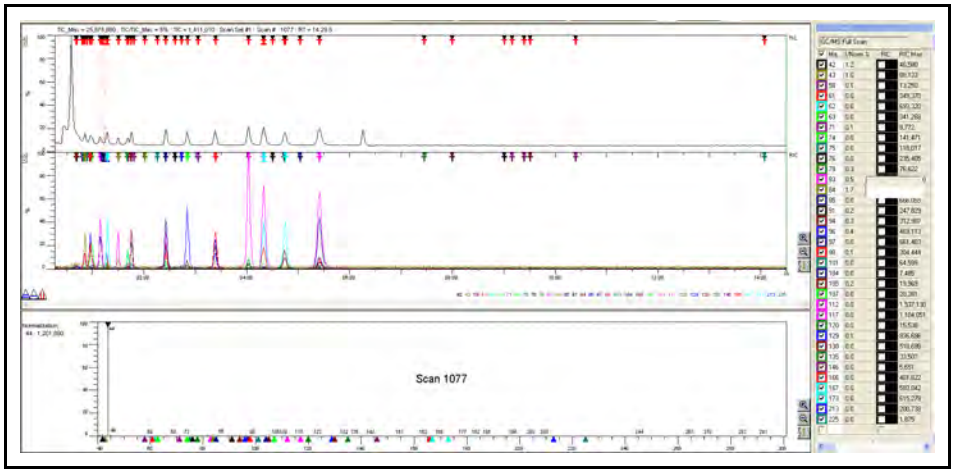
10 Click **Close** to exit the **Quant Report**. (See Figure 11-68.)

Figure 11-68 Closing Quant Report



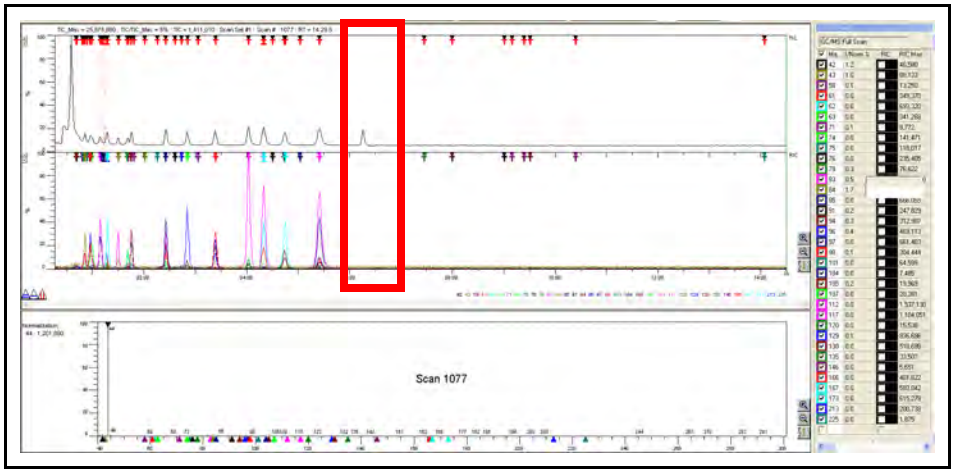
11 If the compound is part of the calibration library, **ID Unknowns** will label the peak with a “T”. (See Figure 11-69.)

Figure 11-69 Labelling Identifications



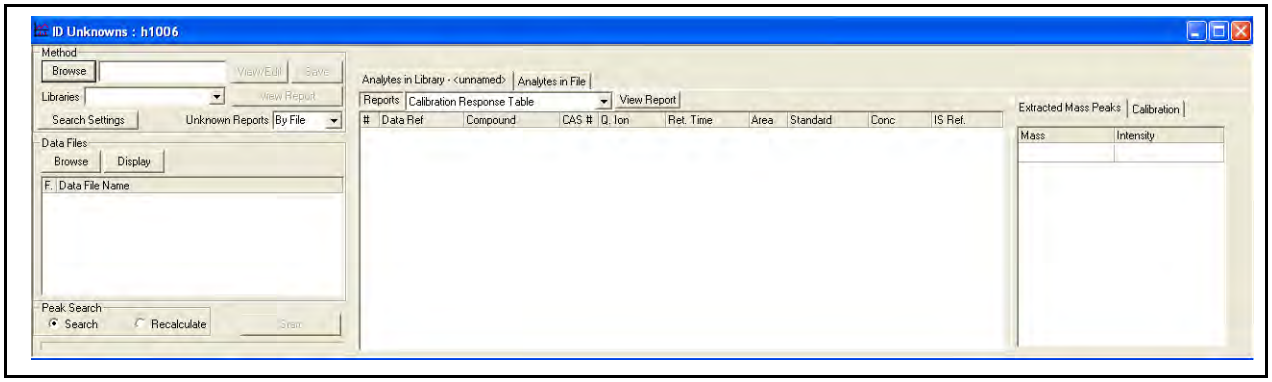
12 If the compound is not part of the calibration library, it is necessary to use AMDIS (refer to Analyzing Data Using AMDIS, see section 8.5 on page 8-16) or NIST (NIST Library Searches, see section 8.6 on page 8-24) to make an identification. (See Figure 11-70.)

Figure 11-70 Unidentified Compounds



11.6 Definition of Terms in the ID Unknowns Window

Figure 11-71 ID Unknowns Window



11.6.1 Method

Browse . . . . . Allows the user to select a method for calibration.

View/Edit . . . . . Opens the **Method Editor** for the method that is currently being calibrated. See Chapter 10, Method Editor.

Save . . . . . Saves the current method.

Libraries . . . . . A drop-down menu that allows the user to select a previously saved library.

Save Library . . . . . Brings up the dialog box to save the library.

Search Settings . . . . . Displays the search parameter settings. See section 8.7.0.2, Peak Search Parameters, on page 8-33.

Unknown Reports

By File . . . . . Displays report by file.

By Analyte . . . . . Displays report by analyte.

11.6.2 Data Files

Browse . . . . . Used to select the data file for analysis.

Display . . . . . Will display a chromatogram with a **T** over the compounds found in the calibration report. See section 11.7.

File Entry . . . . . Lists the reference number for the file.

Data File Name . . . . . Displays the data file name and pathway.

11.6.3 Peak Search

Search . . . . . Performs a peak detection and integration on the selected files. It produces the quantitative report.

Recalculate . . . . . Recalculates the peak areas and response factors without performing a peak search. This is most useful after manually editing the baseline points of a peak.

Start . . . . . Initiates the search for peaks or recalculates the peak search.

11.6.4 Analytes

Analytes in Library . . . . . Displays the analytes in the library.

Analytes in File . . . . . Displays the analytes in the currently displayed or selected file.

11.6.5 Reports

Calibration Response Table . . . . . Report that displays the response factor and curve statistics based on the selected curve type.

Calibration Report . . . . . Report that displays the area fit and purity for the calibration standards.

View Report . . . . . Displays the selected calibration report.

. . . . . Shows the analyte number in the library.

D . . . . . Data Reference: lists the reference to the Data File in which the analyte was found.

Compound . . . . . Shows the compound name found in AMDIS, NIST library or assigned by the user for the analyte.

CAS # . . . . . Shows the Chemical Abstracts Services number for the analyte from the AMDIS or NIST library.

Q Ion . . . . . Shows the quantization ion for the analyte.

Ret. Time . . . . . Shows the retention time for the analyte.

Area . . . . . Displays the integrated area of the quant ion.

Standard . . . . . Designates the compound as an analyte or an internal standard.

Conc: . . . . . Shows the concentration of the analyte or internal standard in the displayed file.

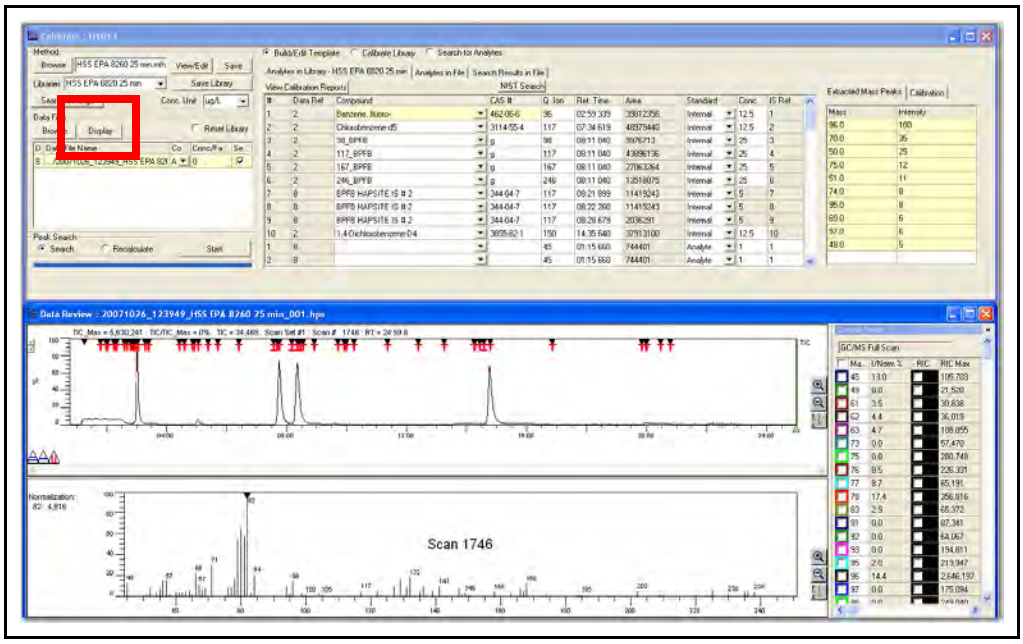
NOTE: The field is not used if the concentration flag is set to **Global**.

IS Ref . . . . . Displays the internal standard reference number for analyte quantization.

11.7 Display Function

The **Display** button in the **Data Files** section of both **Calibrate** and **ID Unknowns** shows the chromatogram and spectrum of the selected data file. This feature is beneficial when reviewing and revising identifications, selecting spectral peaks, adding to a library and manually integrating peak areas. (See Figure 11-72.)

Figure 11-72 Calibration Display File



Chapter 12
Maintenance

12.1 Introduction

This chapter outlines basic maintenance and troubleshooting procedures. It also provides an overview of common errors.

12.2 HAPSITE Symptom - Cause - Remedy Chart

Table 12-1 Diagnosing Problems - HAPSITE

Symptom	Cause	Remedy
Cannot power on HAPSITE	Battery is not charged.	Verify that battery is charged. Replace power source if necessary.
	Cable is not delivering power to the unit.	Verify that the cords are plugged into the unit. Do not power 2 HAPSITE ERs using a Y splitter as this will not deliver sufficient power.
HAPSITE periodically shuts off while in Extended Standby	Power is intermittent/fluctuating too much for AC/DC supply to regulate.	Add a dedicated uninterrupted power supply (UPS) upstream of the AC/DC converter.
N2 canister low error	Canister is nearly empty.	Replace with a new carrier gas canister.
Internal standard canister low error or internal standard expired error	Canister is nearly empty or expired.	Replace with a new, unexpired internal standard gas canister.
Sample carryover	System has become contaminated.	Run blanks until carryover is no longer present.
AutoTune failure	IS canister is expired or empty.	Replace with a new, unexpired internal standard gas canister and repeat AutoTune.
	There is a leak in the fluidic pathway.	Remove and replace all fluidic connections, ensure each is secured at both ends of the concentrator.
	Mass spectrometer parameters are out of range.	Repeat autotune. If failure persists after 3 tries, perform a manual tune. Refer to Chapter 9, Tune.

Table 12-1 Diagnosing Problems - HAPSITE (continued)

Symptom	Cause	Remedy
Concentrator clean out continuously fails	Concentrator is chipped or broken.	Reinsert the concentrator. Verify that the ferrules are in good condition and correctly oriented. Refer to section 3.3.7 on page 3-21.
	Concentrator is improperly seated or installed backwards.	Refer to section 3.3.7 on page 3-21.
	Concentrator is contaminated.	Replace Concentrator with new.
HAPSITE will not properly communicate with the laptop	HAPSITE is not properly configured to the laptop.	Refer to section 5.3 on page 5-9.
Retention time for BPFB is not within the 3:45±0:05 second range	GC pressure flow needs adjustment.	Refer to section 7.6.4 on page 7-31
GC column error	Concentrator is improperly seated.	Reinsert the concentrator. Verify that the ferrules are in good condition and correctly oriented. Refer to section 3.3.7 on page 3-21 and section 3.3.8 on page 3-29.
	Nitrogen carrier gas canister is nearly empty.	Replace with a new nitrogen carrier gas canister.
	Concentrator is chipped or broken.	Replace with a concentrator that is in good condition.
Probe is not recognized by the HAPSITE ER, but appears to be plugged into the port	The probe is not fully inserted into the port.	Insert the probe into the port until it clicks into place.
	Bent or broken pins on LEMO plug.	Gently straighten bent pins and reinsert probe.
Probe is plugged in but registers incorrect temperature	RTD of probe line may be damaged.	Install a different Probe in the AM, verify correct function. Install problem Probe into different AM, verify defective behavior. Contact INFICON for Service support.

Table 12-1 Diagnosing Problems - HAPSITE (continued)

Symptom	Cause	Remedy
Elevated baseline	Background contamination, MS leak, or improper MS tune.	Run a noise check in manual tune to verify MS is not leaking. Manually tune unit according to instructions in Chapter 9. Repeat blank run to verify that baseline is less than 10% of BPFB. Contact INFICON for technical support.
	Electronic connection inside the Probe is damaged.	Try using a different Probe- if this works, contact INFICON for support as original item will need to be serviced.
Zero baseline	Tune parameters are outside specifications.	Perform Manual tune, see sec. 9, and adjust threshold to 300 and baseline to 100.
IS canister is not recognized	Memory chip on canister is damaged.	Replace internal standard canister.
	Contact pins are damaged.	Repair or replace pins on the inside of the front panel.
Low sensitivity, Ionizer failure	Ionizer is depleted.	Contact INFICON for support- this component can only be replaced by trained INFICON service personnel.

Table 12-1 Diagnosing Problems - HAPSITE (continued)

Symptom	Cause	Remedy
High pressure error	NEG/Ion pump depleted Mass Spec requires service. Please review section 2.4.3 for details on the vacuum system.	Attach unit to Service Module and pump down for 24 hours. (See section 12.5, Attaching HAPSITE to the Service Module, on page 12-6.) Perform autotune with unit attached to SM. If autotune fails after 3 tries, perform a manual tune. Refer to Chapter 9, Tune. Detach SM and re-start. If problem persists contact INFICON for technical support. Consider replacing NEG. **NOTE:** HAPSITE ER ionizer cannot be replaced in the field-must be replaced by trained INFICON service personnel.
Filament shut off or will not open		
Electron multiplier fault		
Ion pump failure		
MS emission error		

WARNING

Attaching or venting HAPSITE ER with a NEG that has not cooled will cause total NEG consumption and possibly result in severe damage to the HAPSITE Mass Spectrometer components. It may also result in physical injury since extreme heat generation from NEG consumption will create hot surfaces.

12.3 Saturation of the Probe and Probe Line

12.3.0.1 Symptoms

Symptoms of contamination in the probe and probe line include a high continuous base line with the same or similar identification in Survey Mode. It can also be seen as a persistent peak in Analyze (GC/MS) Mode.

12.3.0.2 Decontaminate Saturation

1. Remove the probe from HAPSITE ER.
2. Hold the probe and probe line in a “U” shape.
3. Holding the probe, pour methanol from a squeeze bottle into the probe nut.

WARNING

For safety precautions, wear appropriate PPE according to the manufacturer’s MSDS.

4. With each end of the probe in a separate hand, move each hand up and down to allow the methanol to flow through the probe.
5. Empty the methanol remaining in the probe line by tipping one end of the probe line downward until all of the methanol drains from the probe line. Repeat this procedure to allow the methanol to flush contaminants from the probe line.
6. Blow out the probe line with nitrogen to remove any residual methanol that may be left in the probe line. Allow the probe to fully dry.
7. Reattach probe line to HAPSITE ER.

WARNING

Continue to wear PPE while blowing out probe and be sure that both ends of the probe are facing away from the user when blowing out occurs.

12.4 NEG Troubleshooting

A high pressure warning indicates that the on-board NEG and ion pump cannot maintain appropriate vacuum, and that loading the unit on a Service Module to re-create the vacuum may be necessary. For instructions on how to load the instrument onto a service module, please see section 12.5, Attaching HAPSITE to

the Service Module, on page 12-6. The high pressure error may also indicate that the NEG pump is worn and needs replacing. (See Figure 12-1.) Please continue reading for information on how to troubleshoot NEG pumps.

Figure 12-1 MS Pressure Error

To view the MS pressure:

1 Touch **HAPSITE** icon.

2 Touch the **Tune** icon.

3 Locate the MS pressure. In order for HAPSITE to properly operate, the pressure must be below 6 e-03. If pressure is too high, ionizer will not activate.

If the NEG pump has 150 hours or less consider trying a bakeout to extend the life of the NEG pump. To check the NEG pump hours, refer to section 7.6.5 on page 7-32

NOTE: If the NEG pump has more than 250 hours, a bakeout can be tried, though the results are likely to be limited.

12.5 Attaching HAPSITE to the Service Module

CAUTION

Prior to attaching HAPSITE to the Service Module, unplug the black NEG cable inside the HAPSITE front panel. This will ensure that the NEG will not heat when using the Service Module to provide vacuum.

WARNING

Attaching or venting HAPSITE with a NEG that has not cooled will cause total NEG consumption and possibly result in severe damage to the HAPSITE Mass Spectrometer components. It may also result in physical injury since extreme heat generation from NEG consumption will create hot surfaces.

NOTE: If the HAPSITE is turned on with the NEG at 400 C, then the NEG must be cooled before preceding. Turn off the HAPSITE and allow it to cool for approximately 24 hours or until the NEG is at room temperature.

If the Service Module has been in storage, refer to HAPSITE Service Module operating manual, section 4.2.1, Setting Up the Service Module, on page 4-2 before continuing.

HAPSITE must be turned on before continuing (refer to HAPSITE Service Module operating manual, section 5.4, Starting Up HAPSITE on the Service Module, on page 5-9).

Physically attach HAPSITE to the Service Module (refer to HAPSITE Service Module operating manual, section 5.2, Placing HAPSITE on the Service Module, on page 5-2).

HAPSITE can be electronically attached to the Service Module using the IQ Software, or using the HAPSITE front panel. Refer to the appropriate HAPSITE model operating manual for more instruction on front panel usage.

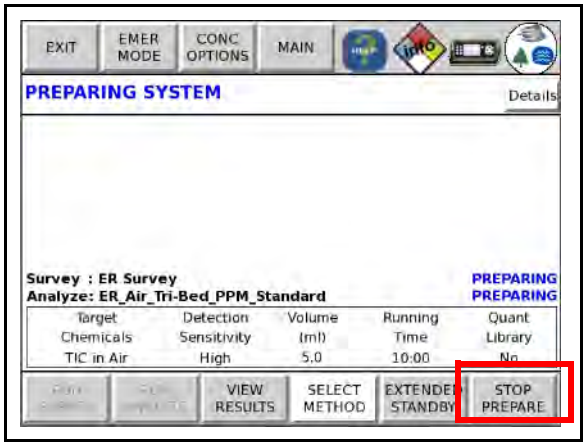
CAUTION

When operating the Service Module, the vents must be kept clear to allow free airflow. Air flows from right to left through the Service Module to allow cooling of the pumps. A blockage can prevent the air from cooling the pumps properly and may cause the over-temperature protection sensor to automatically shut down the pumps.

12.5.1 Attaching HAPSITE to the Service Module Using IQ Software

1 Make sure that HAPSITE does not heat, or is in the **NOT READY** state. As soon as the HAPSITE screen is displayed, tap **STOP PREPARE** or using ◄▲▼►, highlight **STOP PREPARE** and tap **OK SEL**. (See Figure 12-2.)

Figure 12-2 STOP PREPARE button



CAUTION

Prior to attaching HAPSITE to the Service Module, unplug the black NEG cable inside the HAPSITE front panel. This will ensure that the NEG will not heat when using the Service Module to provide vacuum.

2 Connect HAPSITE to the computer using wireless communication or the crossover cable.

3 Open IQ Software.

4 Click the desired HAPSITE sensor icon.

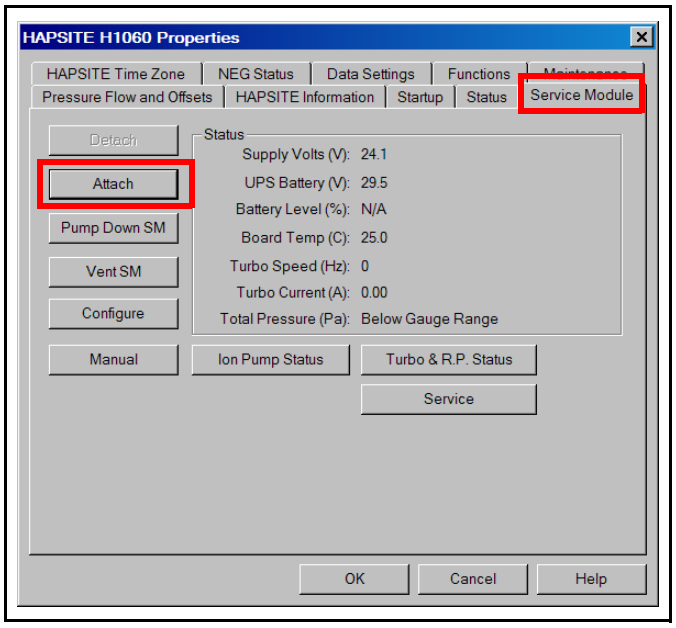
5 Double-click the **Service Module** icon. (See Figure 12-3.)

Figure 12-3 Service module icon

6 The **Service Module** tab on the **HAPSITE Properties** window displays.

7 Click **Attach**. (See Figure 12-4.)

Figure 12-4 HAPSITE properties window



8 **Are you sure you want to attach the service module?** confirmation message is displayed. Click **Yes**. (See Figure 12-5.)

Figure 12-5 Confirmation message

9 The Roughing Pump will start first, then the Turbo Pump will begin, as shown on the Turbo Speed (Hz) line in Figure 12-4 above. The speed is initially displayed as 0, then increases.

NOTE: After clicking **Attach**, the **HAPSITE Properties** window can be closed.

The procedure typically takes about five minutes to complete. While attaching, the **Attaching Service Module Please Wait** message is displayed. (See Figure 12-6.)

Figure 12-6 Attach In Process

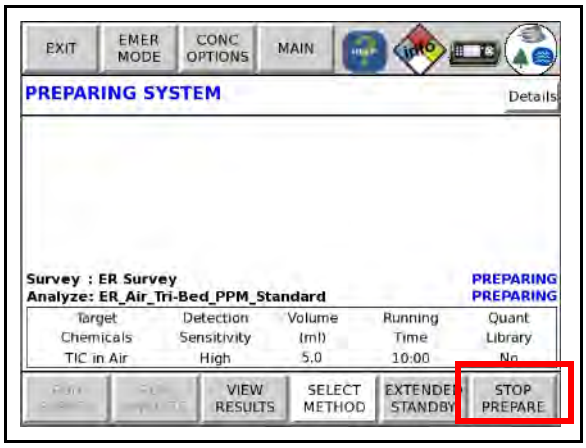
10 When the procedure is finished, the **HAPSITE is Attached** message is displayed. (See Figure 12-7.)

Figure 12-7 HAPSITE is Attached

12.5.2 Attaching HAPSITE to the Service Module Using the HAPSITE Front Panel Controls

1 To avoid running the start up method or AutoTune, tap **STOP PREPARE**. (See Figure 12-8.)

Figure 12-8 STOP PREPARE button



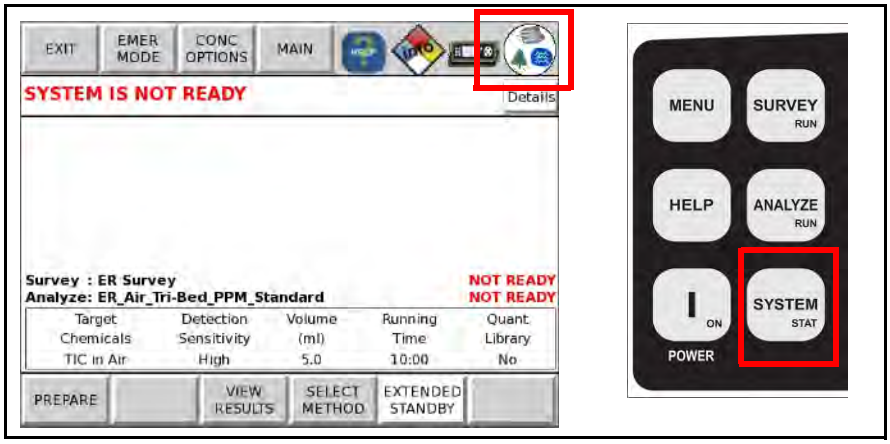
1a If using the push button keys, highlight **STOP PREPARE** with ◄▲▼►. Tap **OK SEL**. (See Figure 12-9.)

Figure 12-9 Arrow Keys

2 The **SYSTEM IS NOT READY** message will appear at the top of the screen.

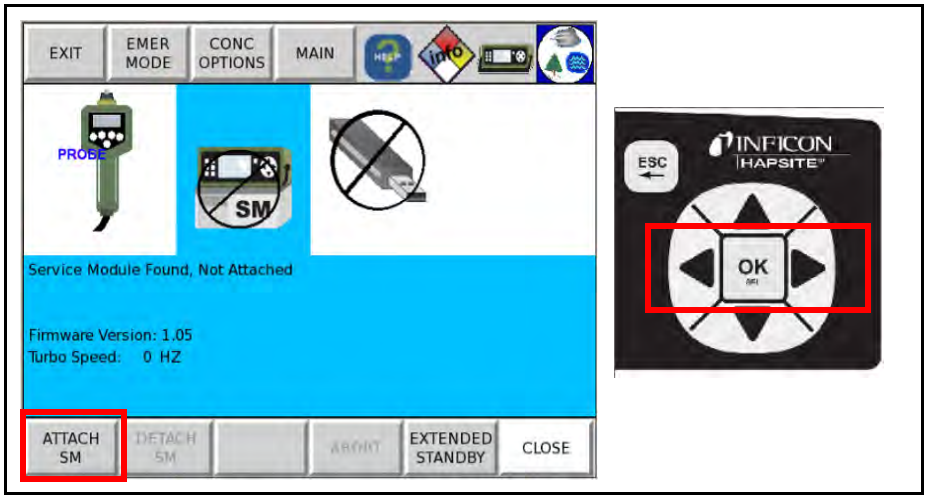
3 Tap the **Accessory** icon, or push the **SYSTEM/STAT** button until the accessory page appears. (See Figure 12-10.)

Figure 12-10 Accessory Button and SYSTEM/STAT



4 Tap the **ATTACH SM** button or using ◄▲▼► highlight the **ATTACH SM** button and tap **OK SEL**. (See Figure 12-11.)

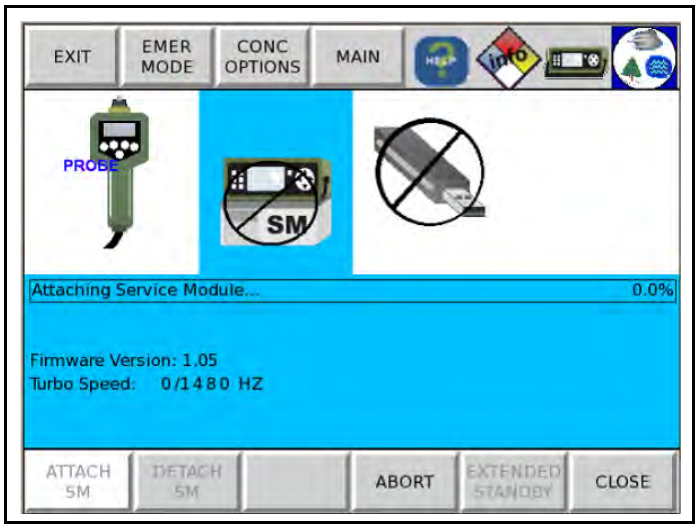
Figure 12-11 Service Model Attach Button



5 A status bar displaying the progress of the attach procedure will be displayed. (See Figure 12-12.)

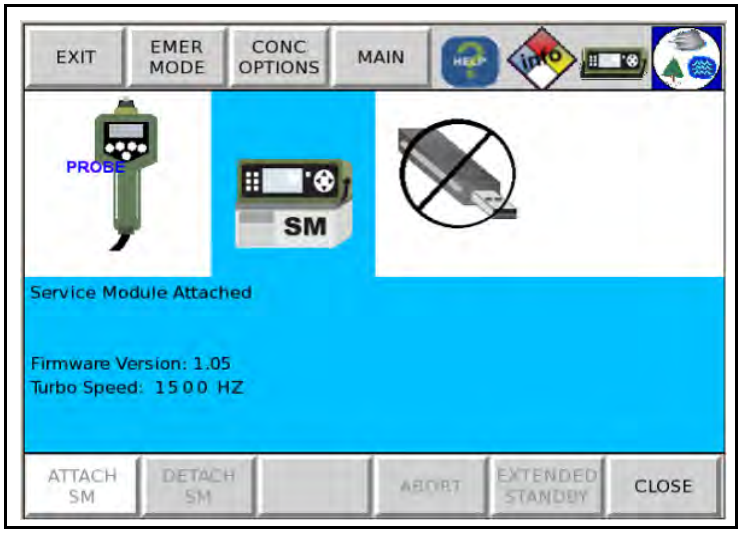
NOTE: The **ATTACH SM** button will be grayed out.

Figure 12-12 Attach progress



6 When the Attach has successfully completed, the **Service Module Attached** message will be displayed. (See Figure 12-13.)

Figure 12-13 Service Model Attached



NOTE: Both **ATTACH SM** and **DETACH SM** buttons will be grayed out immediately after a successful attach while the system prepares.

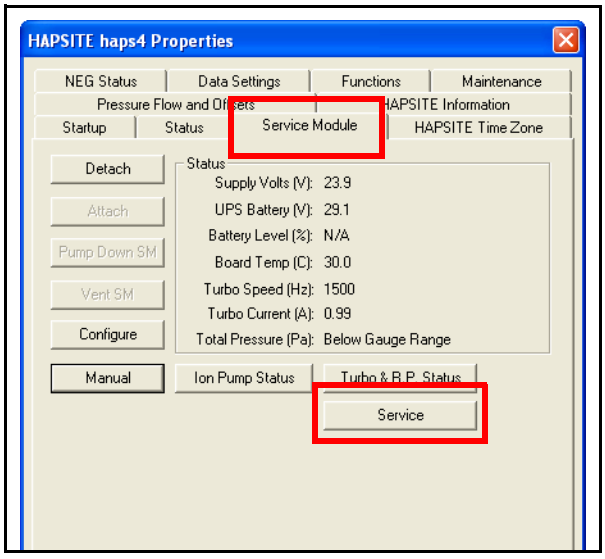
12.6 Bakeout Procedure

A bakeout can be performed with or without the use of the Service Module. A bakeout heats the NEG pump to 700°C for a specified length of time. (The default time setting is two hours). Contact INFICON technical support before performing this procedure.

1 Click on the **Service Module** tab of the **Properties** menu.

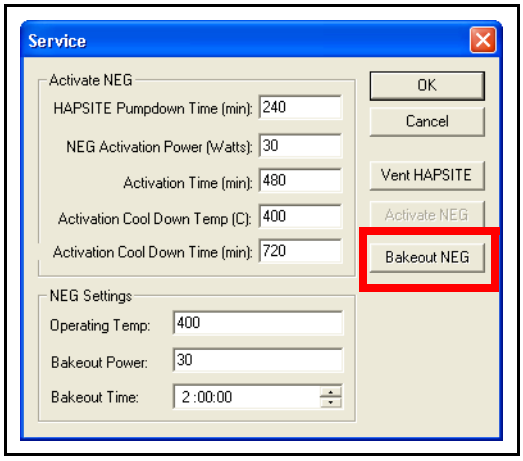
2 Click on the **Service** button. (See Figure 12-14.)

Figure 12-14 Service Button on the Service Module tab



3 Verify that the settings match the setting displayed below and click **Bakeout NEG**. (See Figure 12-15.)

Figure 12-15 Service window



4 If the bakeout is complete, run a blank method. If the bakeout was successful HAPSITE ER will be operational. If the bakeout was unsuccessful, a high pressure error will occur.

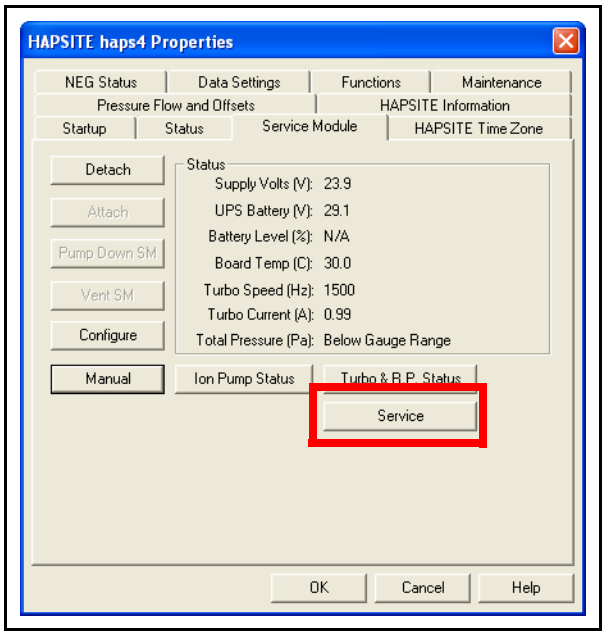
12.6.1 Reactivating the NEG Pump

Reactivating the NEG pump requires having the Service Module attached to HAPSITE for at least 22 hours. This procedure is the same procedure that is used to activate a new NEG pump.

1 Click on the **Service Module** tab of the **Properties** menu.

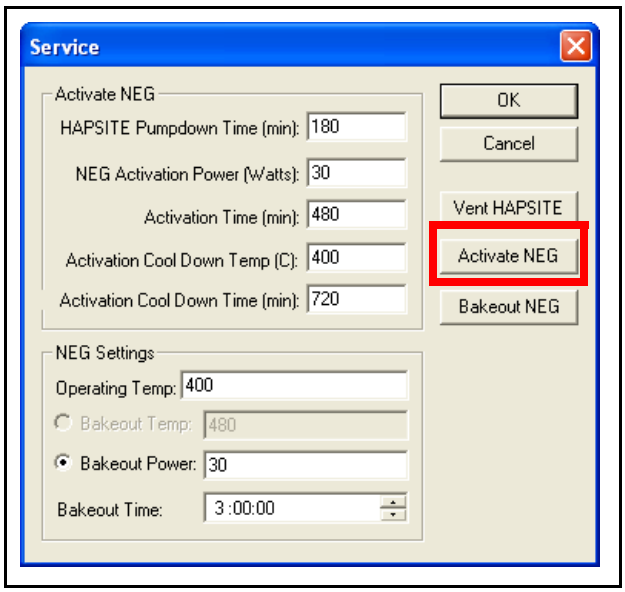
2 Click on the **Service** button. (See Figure 12-16.)

Figure 12-16 Service Button on the Service Module tab



3 Use the Activate NEG settings below as a guideline. However, change the HAPSITE Pumpdown Time to **180**. (See Figure 12-17.)

Figure 12-17 Service window



4 Click the **Activate NEG** button.

5 At the end of the reactivation, the program will detach the HAPSITE from the Service Module as part of the process.

Chapter 13
Part Numbers

13.1 HAPSITE Part Number

Table 13-1 HAPSITE Part Numbers

Part Number	Product Feature Options	HSER
930-2100-G10	HS Analytical Module w/Standard Column No NEG Pump, Green	1
930-2100-G11	HS Analytical Module w/Standard Column No NEG Pump, Green	2
930-2100-G20	HS Analytical Module w/Standard Column NEG Pump Installed, Blue	3
930-2100-G21	HS Analytical Module w/Standard Column NEG Pump Installed, Blue	4
930-850-G5	120V HAPSITE ER	1
930-850-G6	230V HAPSITE ER Continental Europe	2
930-850-G7	230V HAPSITE ER United Kingdom	3
930-850-G8	230V HAPSITE ER Australia/China	4
930-206-G6	Hand Control Unit, Green	1
930-206-G7	Hand Control Unit, Blue	2
930-0371-G1	NIST and HAPSITE software only, No Laptop	A
930-261-G6	Laptop with Windows XP	B
930-261-G7	Ruggedized Laptop with Windows XP	C
930-262-G6	Laptop with Windows XP (Europe)	D
930-262-G7	Ruggedized Laptop with Windows XP (Europe)	E
930-263-G6	Laptop with Windows XP (United Kingdom)	F
930-263-G7	Ruggedized Laptop with Windows XP (United Kingdom)	G
930-264-G6	Laptop with Windows XP (Australia/China)	H
930-264-G7	Ruggedized Laptop with Windows XP (Australia/China)	J

Table 13-1 HAPSITE Part Numbers

Part Number	Product Feature Options	HSER
930-202-G1	Service Module 100-240 V	1
930-202-G3	Service Module 24 VDC	2
930-035-G1	HAPSITE ER IQ Software, English (Installed in Laptop and AM)	A

13.2 HAPSITE ER Accessories

931-205-G1 . . . . . Headspace Sampling System

932-220-G2 . . . . . HAPSITE SituProbe Sampling System

934-290-G1 . . . . . HAPSITE SPME Sampling System

934-708-G1 . . . . . HAPSITE TDSS Sampling System

13.3 HAPSITE ER Spare Parts

059-329 . . . . . Quick Disconnect Stem for N2

068-002 . . . . . Battery Charger / Service Module Power Cord, U.S.

074-5009-G1 . . . . . HAPSITE ER User Guide CD

Cables

600-1319-G2 . . . . . Ethernet Communication Cable (Crossed) - Black Cable (12 ft.)

930-246-G1 . . . . . Hot Swap Cable (Battery Test Bracket)

Kits

930-021-G1 . . . . . Gasket Kit

930-0221-G1 . . . . . Concentrator Tube Nut and Ferrule Kit, 10 each

930-022-G1 . . . . . Tool Kit with Torque Wrench Kit

930-0231-G1 . . . . . Probe Nut and Ferrule Kit, 5 each

930-2020-G2 . . . . . Decon Cap Plug Kit

930-705-G1 . . . . . Sample Loop Tube Kit

930-206-G6 . . . . . Hand Control Unit (Probe)

930-249-G2 . . . . . Concentrator Cover

930-250-G1 . . . . . Sample Loop Cover

Concentrator Tubes

930-251-G1 . . . . . w/Heater, Tenax

930-716-G1 . . . . . w/Heater, Tri-Bed Concentrator Tube Kit

930-4051-P1. . . . . Cold Weather Insulating Bag

930-4061-G1 . . . . . Battery

Line Insulation

070-1545 . . . . . Probe Insulation

NIST

930-4071-G1 . . . . . NIST Version Upgrade

930-4081-G1 . . . . . NIST (with AMDIS)

930-4292-G1 . . . . . VX Conversion Tubes, 10 each

930-4293-G1 . . . . . TDSS Conversion Tubes, 10 each

930-4551-G1 . . . . . Backpack, HAPSPACK

Shipping Cases

930-464-P1. . . . . HAPSITE

930-4131-P1. . . . . HAPSITE Accessory Case

930-469-P1. . . . . 110 V(ac) - 24V(dc) HAPSITE Power Supply

930-470-G1 . . . . . Battery Charger

13.4 HAPSITE Consumables

NEG Pumps

930-242-G1 . . . . . Installed and Activated at Factory

930-425-P1. . . . . Spare Pump

Carrier Gas Canisters

930-432-P6. . . . . 6 each

930-432-P12. . . . . 12 each

930-432-P24. . . . . 24 each

Extended Life Carrier Gas Canisters

930-730-G1 . . . . . Extended Life Carrier Gas Deployment Kit (110 liter)

930-4611-P1 . . . . . Extended Life Carrier Gas (110 liter cylinder)

Internal Standard Canisters

930-433-P6. . . . . Canister, Internal Standard Gas, 6 each

930-433-P12. . . . . Canister, Internal Standard Gas, 12 each

930-433-P24. . . . . Canister, Internal Standard Gas, 24 each

Combo Pack Canisters

930-477-P1. . . . . Gas Combo Pack (4 Carrier Gas and 2 Internal Standard)

071-747 . . . . . Performance Standard Concentrator / Air (5 analytes) in Methanol 1.2 mL

071-760 . . . . . HAPSITE Chemical Standards Kit, 12 part (for training/practice)

13.5 Headspace Spare Parts

070-1204 . . . . . Sample Vials, Case of 100

931-702-G10 . . . . . Vial Needle Guide,10 each

Syringes

070-1205 . . . . . 25 mL Gastight (not supplied with needle), each

070-1206 . . . . . 10 µL Gastight w/Removable Needle, each

070-1223 . . . . . 10 µL w/Fixed Needle, 6 each

070-1224 . . . . . 50 mL Luer Lock, each (not supplied with needle)

070-1207 . . . . . Replacement 10 µL Needle for Syringe (070-1206), each

931-402-P1 . . . . . Sample Needle, Headspace

071-748 . . . . . Performance/IS Standard Headspace (4 analytes) in Methanol 1.2 mL

930-4151-P1 . . . . . VX Conversion Pads (Headspace), 10 sets

931-406-P1 . . . . . Shipping Case, Headspace

Line Insulation

931-401-P3. . . . . 4 ft Line

931-409-P2. . . . . 6 ft Line

931-405-P1. . . . . Thin Line

931-408-P1. . . . . Heavy Line

600-1131-P30. . . . . Y Power Cable

13.6 Service Module Spare Parts

068-0002 . . . . . Battery Charger / Service Module Power Cord, U.S.

930-0211-G1. . . . . Torque Wrench Kit

930-465-P1. . . . . Shipping Case, Service Module

600-1001-P15. . . . . RS232 Cable (15 ft.)

13.7 HAPSITE SituProbe Spare Parts

940-700-G1 . . . . . SituProbe Vessel and Plugs

933-700-G1 . . . . . Collection Tube Replacement Kit

931-401-P3. . . . . 4 ft Transfer Line

931-409-P2. . . . . 6 ft Transfer Line

Line Insulation

931-405-P1. . . . . Thin

931-408-P1. . . . . Heavy

600-1131-P30 . . . . . Y Power Cable

932-220-G1 . . . . . HAPSITE SituProbe Accessory (6'), Replacement

Chapter 14
Glossary

14.1 Glossary

Air peak . . . . . A response by the mass spectrometer to the components of air. This set of compounds typically elutes 1 to 1.5 minutes from the start of analysis.

Alignment . . . . . A part of the tuning process which assures that the mass peaks fall at their calibrated position on the mass scale.

AM . . . . . Analytical Module, also called the HAPSITE and HAPSITE ER.

AMDIS . . . . . Automated Mass Spectral Deconvolution and Identification System Software

AMU . . . . . (Atomic Mass Unit) an unit that is used for indicating mass on an atomic scale

Analyte . . . . . That portion of a sample which comprises compounds to be analyzed.

AutoTune . . . . . A process that occurs when the instrument is initially started up; it automatically performs mass alignment, resolution adjustment and adjustment of relative intensity of the peaks. AutoTune will take place once the heated zones have reached the proper temperature.

Baseline . . . . . A measure of the intensity of the background noise of the mass spectrometer. This is determined using the Noise Check feature in the Tune program.

Carrier Gas . . . . . The pure inorganic gas used to aid the flow of sample gas through the chromatograph for analysis. VOC-free nitrogen is the carrier gas for the HAPSITE ER.

Column . . . . . The column is a long glass capillary which is lined with a material (called the “stationary phase”) with which the analytes interact based on their physical characteristics, slowing their flow. The degree of this interaction progressively separates the different compounds from one another during elution.

DAC . . . . . Digital to Analog Converter. An element of the electronic circuitry which converts the microprocessor’s digital instructions to the analog requirements for control of the instrument.

DOC . . . . . Declaration of Contamination document. All chemicals that have been run through the HAPSITE must be listed on the form prior to service and repairs.

Elution time . . . . . The elapsed time from injection of a specific compound onto the column until the compound exits the column (same as retention time).

ET . . . . . Elapsed time of sample run. Used in Survey method instead of retention time.

Filament . . . . . A hot wire in the ionizer from which electrons are emitted.

Filament Delay . . . . . This specifies the amount of time between the start of analysis and the time which the HAPSITE turns on the filament. Filament delay allows components of the air peak or solvents to pass through the mass spectrometer before the filament is turned on.

GC . . . . . Gas Chromatograph.

GUI . . . . . Graphical User Interface.

Inlet State . . . . . This refers to the valve states in the HAPSITE The states of the valves control sampling, analysis, clean-out of the HAPSITE ER.

Internal Standard . . . . . A mix of known compounds with known concentrations. They are mixed with the sample analytes to validate the response of the HAPSITE ER.

Ion Energy. . . . . These settings in the tune program directly affect the intensity of mass peaks. Ion energies are commonly used to set the relative mass intensities of the tuning ions.

Ion Volume . . . . . The specific space in the ionizer where ionization of the sample takes place.

Ion . . . . . An atom or molecule which carries an electric charge due to depletion or addition of one or more electrons.

Ionizer . . . . . The assembly of parts in the mass spectrometer into which the sample flows and which projects a beam of mixed ions into the mass filter.

I.S. Reference . . . . . This section of the **Calibrate** screen identifies the target ion of the internal standard which will be used for quantification of the chosen compound.

kPa. . . . . Kilo Pascal. Unit of pressure measurement which is equivalent to approximately 0.145 PSI.

LCD . . . . . Liquid Crystal Display. This refers to the display screen on the front panel of the HAPSITE ER.

Library. . . . . A user compiled list of compounds, which includes both analytes and internal standards (if chosen). The library keeps information such as the name, target ion, concentration, retention time, relative mass intensities, and compound specific search parameters (if selected).

Mass Calibration . . . . . A function of the HAPSITE ER which uses internal standard gas to check the alignment of masses, and also to check the relative intensities of the tune masses.

Mass Fragment. . . . . A molecule (or ion) resulting from the break-up of a parent molecule.

Mass Defect . . . . . The effect on a mass spectrum of the difference between the atomic weight of a compound or fragment and a whole number.

Mass spectrum . . . . . A display of the amount of each mass fragment present at the specific time, plotted as amplitude vs. molecular weight.

MDP . . . . . Molecular dispersion pump.

Membrane Isolation Valve . . . . . The valve which supports the Mass Spectrometer's inlet membrane and (when closed) interrupts the flow of analyte from the membrane into the Mass Spectrometer.

Method. . . . . A set of instructions for a function of the HAPSITE.

Molecular Weight . . . . . The amu representation of the total number of protons and neutrons in a specified molecule.

MS . . . . . Mass Spectrometer

ms . . . . . milliseconds

MSDS . . . . . Material Safety Data Sheet

Multiplier Voltage . . . . . The voltage applied to the multiplier in the mass spectrometer, which directly effects the amplitude of signal and background noise.

NEG . . . . . Non-evaporative getter as a vacuum source

NIST Library . . . . . NIST stands for National Institute of Standards and Technology Mass Spectral Library. This is a library of spectra of compounds which can be searched to tentatively identify unknown compounds.

Noise Check . . . . . An option in the Tune program which checks the system for background noise. The results of the noise check are used to discriminate against baseline noise during analysis.

Pascal (pa) . . . . . Unit of pressure, equal to 1 dyne per cm^2. Equivalent to 7.5×10^{-3} Torr and 1.45×10^{-4} PSI.

PEEK . . . . . A contamination resistant material used for a number of fittings in the HAPSITE ER.

Phase . . . . . The coating on the inside of the gas chromatograph column by which organic vapors are retained.

PPB . . . . . Parts per billion concentration level.

PPE . . . . . Personal Protective Equipment.

PPM . . . . . Parts per million concentration level.

PPT . . . . . Parts per trillion concentration level.

Remote Power . . . . . Power supplied to the HAPSITE and HSS either from the Service Module (for the HAPSITE) or external AC - 24 V(dc) converter.

Resolution . . . . . These settings in the tune program affect the way the mass spectrometer resolves peaks. Increasing the resolution narrows the peaks in that mass range, while lowering the resolution will broaden the peaks.

Retention Time . . . . . The elapsed time from injection of a specific compound onto the column until the compound exits the column (same as retention time).

Reverse Search . . . . . A function of the NIST search (tentative unknown identification) library which allows compounds which are specified in the user library to be identified as part of the search.

RH . . . . . Relative humidity.

RIC . . . . . (Reconstructed Ion Chromatogram) A presentation of the chromatographic record which extracts from the TIC and displays the intensity of the ion or ions specified.

Round Trip Time . . . . . The amount of time required to complete a scan of all the masses specified in a SIM method. This includes the number of masses, integration time, number of extra measurements, lead in time, and peak width.

RMA . . . . . Return material authorization document. Returning material can not be sent back without this document.

% RSD . . . . . Percent Relative Standard Deviation. This is a measure of the linearity (using mathematical regression analysis) of the concentration levels in the calibration curve for each compound.

Sample Loop . . . . . The portion of the gas chromatograph through which the inlet flow is directed and from which the injection is made.

Scan Method . . . . . This method specifies the masses to be scanned by the MS, length of the run, filament delay, and scan and integration times.

Scan Time . . . . . In **Full Scan** analysis, this refers to the cumulative time required to make a scan of all the masses in the range specified. The calculation of scan time includes the integration time and the points/amu.

SIM . . . . . **Selected Ion Monitoring**. Mass analysis of one or several ion peaks without scanning the entire spectrum.

Target Ion . . . . . The specific ion mass which will be used for quantification or primary identification of a compound in the library.

Temperature Programmable . . . . . Software controlled temperature programming that allows the user to reach temperatures from 55°C to 225°C in a controlled ramp.

Threshold . . . . . A measure of the amplitude of the background noise of the mass spectrometer. This is determined using the **Noise Check** feature in the tune program.

TIC . . . . . (Total Ion Chromatogram) A graph of time verses signal intensity.

TMP . . . . . Turbo Molecular Pump

Torr. . . . . Unit of sub-atmospheric pressure. Equivalent to 133.3 pa.

Vacuum Interconnect Valve. . . . . The two-part valve which seals the HAPSITE manifold, when closed, and opens it to the vacuum pumps in the Service Module, when open. The Vacuum Interconnect Valve is powered by a motor within the Service Module, under direction of the HAPSITE.

VSO Valve . . . . . Voltage Sensitive Orifice valve. This valve uses voltage applied to the valve to control the size of its orifice. This in turn controls the flow rate of gas through the HAPSITE ER.

Chapter A
HAPSITE Target Compounds

A.1 Compounds in Order of Elution

Name	Formula		k	Quantion AMU	I.S. AMU	CAS #
Chloromethane	CH3Cl	a	0.08	50	50	74-87-3
Vinyl Chloride	CH2=CHCl	a	0.11	62	50	75-01-4
Bromomethane	CH3Br	b	0.17	96	9	74-83-9
Chloroethane	CH3CH2Cl	b	0.19	64	69	75-00-3
Acetone	CH3COCH3		0.27	43,58	50	67-64-1
1,1-Dichloroethylene	CCl2=CH2	c	0.37	98	99	75-35-4
Methylene Chloride	CH2Cl2	c	0.39	86	99	75-09-2
Carbon Disulfide	CS2		0.46	76	69	75-15-0
trans-1,2-Dichloroethylene	CClH=CHCl		0.51	96	69	540-59-0
1,1-Dichloroethane	CHCl2CH3	d	0.57	65	69	75-34-3
Vinyl Acetate	CH3COOC(H)CH2	d	0.57	43,86	50	108-05-4
2-Butanone	CH3COCH2CH3		0.63	43,58	69	78-93-3
cis-1,2-Dichloroethylene	CClH=CClH		0.73	96	99	540-59-0
Chloroform	CHCl3		0.78	83	69	67-66-3
1,3,5Tris(trifluoromethyl)benzene	C6H3(CF3)3	e	0.96	Note 1		729-81-7
1,2-Dichloroethane	CClH2CClH2	e	0.98	64	69	107-06-2
1,1,1-Trichloroethane	CCl3CH3		1.07	97	99	71-55-6
Benzene	C6H6		1.22	78	69	71-43-2
Carbon Tetrachloride	CCl4		1.26	117	125	56-23-5
1,2-Dichloropropane	CH2ClCHClCH3		1.51	63	69	78-87-5
Bromodichloromethane	BrCl2CH	f	1.59	83	69	75-27-4
Trichloroethene	ClCH=CCl2	f	1.61	130	99	79-01-6
cis-1,3-Dichloropropene	CClH=CCClH2(H)	g	2.08	75	69	542-75-6
4-Methyl-2-Pentanone	CH3COCH2CH(CH3)CH3	g	2.11	43,58	69	108-10-1
trans-1,3-Dichloropropene	CClH=C(H)CClH2		2.44	75	69	542-75-6
1,1,2-Trichloroethane	CHCl2CH2Cl		2.56	97	99	79-00-5
Toluene	C6H5CH3		2.8	91	79	108-88-3
2-Hexanone	CH3CO(CH2)3CH3	h	3.08	43,58	79	591-78-6
Dibromochloromethane	Br2ClCH	h	3.16	127	117	124-48-1
Tetrachloroethylene	Cl2C=CCl2		4.02	129	167	127-18-4
Chlorobenzene	C6H5Cl		5.07	122	117	108-90-7
Bromopentafluorobenzene	C6BrF5		5.59	Note 2		344-4-7
Ethyl Benzene	CH3CH2C6H5		5.91	91	79	100-41-4
Bromoform	CHBr3	i	6.24	173	167	75-25-2
m-Xylene	C6H4(CH3)2	i	6.35	106	117	1330-20-7
p-Xylene	C6H4(CH3)2	i	6.35	106	117	1330-20-7
Styrene	C6H5CH=CH2		7.25	104	117	100-42-5
o-Xylene	C6H4(CH3)2	j	7.52	91	79	1330-20-7
1,1,2,2-Tetrachloroethane	CHCl2CHCl2	j	7.52	83	79	79-34-5

Internal Standards

Note 1: 69, 75, 99, 125

Note 2: 79, 117, 167

NOTE: k is the partition coefficient of a volatile.

Appendix B
Calibrating Gas Mixtures

B.1 Acquisition, Preparation, and Handling

CAUTION

Failure to calibrate the instrument may give you inaccurate identifications when sampling.

WARNING

When using chemicals, wear the appropriate PPE according to the MSDS.

HAPSITE (or any GC/MS instrument) must be calibrated at one or more concentration levels of the organic compound(s) of interest for quantitative analysis. In the case of the HAPSITE, the compounds of interest must be supplied to the instrument as a gaseous mixture of known volume/volume composition (mole/mole % or ppmv levels in air or nitrogen) and at atmospheric pressure.

There are a number of important factors to consider in acquiring, preparing, and handling gaseous standard calibration mixtures. These can be organized in three groups:

1. How to establish the desired concentrations of the required compounds. See section B.1.1 on page B-1.
2. Correct delivery of the mix to the inlet of the HAPSITE. See section B.1.2 on page B-3.
3. Gas cylinder safety, contamination checks and corrective steps in the equipment. See section B.1.3 on page B-5.

B.1.1 How to Establish the Desired Concentrations

There are two basic ways to obtain several concentrations of a given mix of compounds. The compounds can be bought, premixed to specification, in cylinders containing the several concentrations desired. A master cylinder of the compounds can also be purchased at the highest concentration needed, and diluted to the lower required concentrations. Each of these options is discussed in the following sections.

B.1.1.1 Using Cylinders Charged with Each Concentration

A gas supplier (such as Scott Specialty Gases[1]) can provide a choice of cylinder sizes with the compounds of interest mixed in a suitable matrix at the requisite concentrations. The matrix (or balance gas) for the mixture should be specified as "VOC-free Nitrogen" or "VOC-free Air", to minimize the level of background VOC's in the calibration mix.

The concentrations for calibration of the various compounds of interest will probably be defined in the method being followed. The method may specify, for example, 0.1 ppm, 1 ppm, and 10 ppm of each compound. Calibrate the HAPSITE to bracket the concentrations at which the compounds of interest will occur in the samples.

The mixtures received will be tagged with the precise value of the concentration of each compound as delivered. The concentration supplied will generally be within ±10% tolerance; this is termed the *blend accuracy.*

The precise values should be used in the course of building the calibration libraries and are accurate to +2 -20%, depending on the target concentration levels and the certification methods used. This is termed the *analytical accuracy.* The certified concentrations in each cylinder mixture will generally be stable at room temperature conditions for about six months.

The selected gas supplier should be able to advise about the reactivity of the compounds needed, and the materials of cylinder construction to provide the best long term stability of the concentration. The supplier will recommend the use of stainless steel regulators with stainless diaphragms. To minimize stagnant volumes where VOCs can accumulate, the regulator body should be designed with minimum internal dead-volume. Use 1 in. diameter gauges, or eliminate the gauges altogether. The regulators and the tubing following should be rated for high purity, mildly corrosive (or corrosive) service if any halogenated VOC's are to be delivered.

NOTE: A regulator/transfer line system must be well purged with pure nitrogen or air to remove any residual VOCs prior to use with a cylinder containing a lower concentration mix.

Transfer fittings should be composed of the stainless steel Swagelok[2] type, and transfer lines should be clean, stainless steel or nickel 1/8 inch tubing. Teflon tubing should be avoided due to its permeability. Ideally, regulators and transfer lines should be heat-traced to maintain above ambient temperatures (35-55 °C) and to reduce adsorption of the higher boiling VOC's.

1.Scott Specialty Gases: (215) 766-8861
2.Swagelock (Crawford Fitting Company): (216) 248-4600

B.1.1.2 Diluting the Gas On-site

Guidelines to verify acceptable performance of suitable dynamic gas mixing/dilution systems are suggested in the Federal Register (vol. 59, No. 148, Aug. 3, 1994 Proposed Rules, 40 CFR Part 51 Method 205).

Systems conforming to the Method 205 suggestions are available commercially from Environics[3] (Series 2014 Computerized VOC Gas Dilution System) and Alltech[4] (GB-2 Gas Blender).

The materials in the flow stream must be inert to the VOC compounds of interest, and heat-traced to prevent condensation and accumulation of any VOC's in the flow channels. A well performing gas mixing system minimizes future outlay in certified cylinder gas standard mixes. In this system, only the cylinders at the highest calibration concentration levels are required. Lower concentrations (by as much as a factor of 1000) can be prepared by serial dilution (with VOC-free Nitrogen or air) of these cylinder mixes to the desired calibration levels with the gas mixing system. This is probably the most economic route for labs which must frequently do multi concentration re-calibrations for known VOC mixtures.

B.1.2 Correct Delivery of the Mix to the Inlet of the HAPSITE

The HAPSITE is designed to draw samples at atmospheric pressure. Internal standard gas is mixed with the sample in a ratio which is dependent on the flow rate of the sample gas and the suction of the pump.

WARNING

Connecting the inlet of the probe to a sample at a pressure above or below atmospheric will cause the mixing ratio of the internal standards to be incorrect, so the resultant calibration will be invalid.

There are two basic approaches to assuring that the calibration mix is at atmospheric pressure: a free flow of gas or capture of the gas mixture in an inert sample bag.

B.1.2.1 Free Flow of Gas

The free flow of gas from the regulator of a pressure cylinder is reduced to atmospheric pressure when the impedance to flow is small. This can be achieved by placing a sampling tee at the point where the line becomes large in diameter. The connection of the HAPSITE sample probe inlet should be at right angles to the direction of gas flow with 1/8 in. stainless steel Swagelok fittings.

3.Environics: (203) 429-5040
4.Alltech: (800) 255-8324

WARNING

The excess vent flow (overflow) from this sampling tee (in the gas flow direction) should exit through stainless steel fittings of at least 1/4 in. size and a short vent line to a fume hood or other exhaust system.

The smaller “leg” of the sampling tee is coupled to the HAPSITE ER. The total flow to the sampling tee should be approximately 1 liter/min. to allow sufficient excess over the HAPSITE sampling flow rate which is approximately 100 cc/min. and to prevent external air from being drawn back into the vent “leg” of the sampling tee which would alter the concentrations delivered from the cylinder or mixer.

B.1.2.2 Inert Sample Bag

Ultra clean Tedlar sample bags, dedicated to a given VOC compound mix/concentration level, will be the most economic option for regular calibration (more than once a week) and eliminates the waste of certified gas mix out of the sampling tee vent. The dedicated Tedlar bag can be filled directly from the associated gas cylinder or gas mixing system effluent.

WARNING

Regulate the gas delivery to avoid overfilling the bag. The bags are not designed to be pressurized.

Alternatively, a bag can be filled by delivery of a set volume of the diluent gas (via a mass flow meter), then adding a set volume of the certified cylinder VOC gas mix, followed by mixing to homogeneity in the bag to obtain the proper dilution. A 12-liter Tedlar bag will allow about 60 HAPSITE samplings of the contents between refills.

The use of properly filled Tedlar bags inherently assures that the gaseous contents are at atmospheric pressure for sampling. The bag should not be filled to the point where the bag appears like a firm “air pillow”, as the bag would then be at above atmospheric pressure, and could not be sampled accurately by the HAPSITE. In addition, this would lead to eventual leakage along the bag seams, destroying the integrity.

Clean Tedlar bags to be filled with a certified gas mix should be filled once with the gas mix and allowed to stand several minutes for preconditioning, then evacuated with a transfer line and a diaphragm vacuum pump and refilled again with the mix.

Fittings on the Tedlar bags are typically 3/16 in. diameter; the inlet systems for the HAPSITE are 1/8 in. diameter. Connection of the probe to the Tedlar bag can be made with a stainless steel Swagelok type adapter, 3/16 in. to 1/8 in. The recommended parts for this adapter include:

3/16 in. to 1/8 in. Reducer . . . . . (Swagelok part# SS-300-R-2)

3/16 in. Teflon Ferrule Set . . . . . (Swagelok part# T-300-Set)

1/8 in. Nut . . . . . (Swagelok part# S-S-202-1)

1/8 in. Ferrule Set . . . . . (Swagelok part# SS-200-Set)

The 3/16 in. O.D. tube on the Tedlar bag valve will slip into and out of the 3/16 in. nut on the adapter, which can be easily finger tightened to seal, leak-free, on the Teflon ferrule set. Care should be taken to not completely unscrew the 3/16 in. nut from the adapter each time a Tedlar bag is removed. This will prevent the dropping of nuts and ferrules. The 1/8 in. end of the adapter is a swaged connection to the 1/8 in. male Swagelok fitting on the end of the HAPSITE ER probe, so wrenches will be required to make a leak free connection.

The Tedlar bag valve should be open only during the HAPSITE sample taking cycle to save gas usage.

B.1.3 Gas Cylinder Safety, Contamination Checks, and Corrective Steps

WARNING

Safety of operations should always take precedence in the working environment. Gas cylinders should be properly affixed to lab benches with clamps, or chained to the wall for safety. A safety certified gas cylinder cart should be available in the vicinity of where the cylinders are normally used, for moving them and replacing empty cylinders. Gas cylinders should never be transported with the regulator attached!

Tedlar bags may be cleaned for reuse, or replaced with new bags. To clean a Tedlar bag for use with different VOC's or concentrations, partially fill with VOC-free N_2 or VOC-free air, heat it to 40-50°C by wrapping the bag with an electric blanket for several minutes, then evacuate the bag contents through the open valve with a clean transfer line to a diaphragm vacuum pump. This operation should be repeated 10 times for a normal cleaning. Then the bag may be stored filled with VOC free N_2 or VOC-free air until needed.

A supply of clean Tedlar bags can be useful for quick standards preparation by direct liquid injection of VOC's not regularly analyzed into an N_2 or air matrix in the bags. This allows a more convenient and rapid alternative to gaseous cylinder mixes in such uses as new applications development or verification of unknown VOCs by component spiking. Accurate gas standard preparation by direct liquid injection is only recommended at levels greater than 5 ppmv, because the minimum liquid volume deliverable by syringe at an acceptable accuracy and precision is about 0.5 μL. This corresponds to approximately 10 ppmv in a 12 liter Tedlar bag, or approximately 3 ppmv in a 40 liter Tedlar bag. Larger Tedlar bags are available, but convenience in regular handling and the possibility of target compound adsorption on the larger interior surface area may be matters of concern.

Appendix C
Shipping the HAPSITE and Consumables

C.1 Introduction

The HAPSITE instrument and its Service Module are designed to ship to remote locations. The instruments can be reshipped in the cardboard boxes (with the same cut-foam inserts) in which they were received. However, these boxes will not suffice for frequent shipping. A heavy-duty fitted shipping case for HAPSITE is available from INFICON (part number 930-464-P1). The case for the Service Module is part number (930-465-P1). The protection provided by these cases will allow the instruments to survive handling by most airline, air freight and trucking handlers.

While there is room for the necessary cables in each case, additional boxing must be used for certain accessories and consumables, as detailed below.

CAUTION

The batteries should be removed from the HAPSITE and the Service Module before shipping, as their weight, under the shock-loads of shipment, will damage the respective instrument. They will require their own packaging for shipment. The computer, if required at the remote site, should be hand-carried.

NEG Pumps can easily be shipped in the box in which they are received. A NEG Pump installed in HAPSITE will not be damaged by shipment.

WARNING

When shipping canisters follow DOT regulations for packaging, labeling and methods in which hazardous materials can be shipped.

C.2 Shipping the Canisters

The canisters of carrier gas and internal standards gas are pressurized to 700 kPa (100 psig) or more. The canisters are approved by the Department of Transportation (DOT), but they are considered hazardous cargo because they are pressurized. They are permitted to be transported on passenger aircraft, but not in the passenger compartment, nor checked as luggage. The labeling of the cartons and the paperwork required can be tedious. The easiest approach is to contact

INFICON and order the required gases to be shipped directly to the site. If previously purchased gases are to be shipped, the original cartons can be used. If new cartons must be used, refer to the old shipping packages for the required labeling.

WARNING

Do not ship canisters installed in the HAPSITE; they are still hazardous and can damage the unit during transport.

The regulations governing shipments of hazardous goods are found in the DOT portion of the Code of Federal Regulations: Part 171, 172 and 173 of 49 C.F.R. The gas canisters, pressurized, are classified as hazardous materials under Section 172.101. When shipped from INFICON, they meet all the packaging requirements set forth in Section 173.

Federal Express, UPS, and the passenger airlines are forbidden to accept such cargo unless it is accompanied with the required "Shipper's Declaration for Dangerous Goods" in four copies. Both FedEx and UPS have their own version and will provide instructions. The generic version, for use with airlines, is shown after page C-3, and for instructions on filling out the form, see below.

In filling out the form, it is important to be precise. In the "Transport Details" box, firmly *cross out* the term "Cargo Aircraft Only". To the right of the box, *cross out* the term "Radioactive".

The "Proper Shipping Name" and "UN or ID NO." are either:

- Nitrogen, Compressed, UN 1066, or
- Compressed Gases, n. o. s., UN 1956 respectively (Bromo-pentafluorobenzene, Nitrogen)

The "Class or Division" is *2.2*. "Packing Group" and "Subsidiary Risk" are left blank. "Quantity and Type of Packing" for a single six-pack would read: *6 DOT 2M Canisters in Fiberboard Box X 0.04 Kg*.

For two six-packs in a single larger box (which must carry the green diamond and other placarding), this would read *12 DOT 2M Canisters in 2 Fiberboard Boxes X 0.08 Kg (Overpack Used)*. The Kg number refers to the total mass of the gas, not the gross weight.

In the "Packing Inst." column write *200*. The "Authorization" column is left blank. The signature section is very important; fill it out completely.

The "Shipper's Declaration for Dangerous Goods" is a "Style F83R" from Label master in Chicago; their phone number is 800 621-5808. They are carbon-less, four-part forms and may be available from local stationary suppliers. The form, and all its copies, must have red markings along the borders; black and white copies will not be accepted.

Although the airline will carry the box of canisters in the same cargo hold as the baggage, they will not accept hazardous materials at the check-in counter. Take the box of canisters with the form filled out to the desk of your airline at the ***air freight terminal*** at your airport. They will be able to assist you with transporting the gas.

C.3 Empty Canisters

It is important to remember that it is the *pressure* of the gas in the canisters which is considered hazardous. The gases themselves are mostly nitrogen. (The amount of the organic internal standards compounds is 50 ppm and 100 ppm.)

To discard the canisters, simply discharge them outdoors by inserting any small point into the valve. Once they are empty, they can be disposed of as aluminum scrap.

WARNING

When discharging the canisters, point them away from people and stand upwind of the discharge. Whenever possible discharge canisters into a hood.

If the empty canisters cannot be recycled or disposed, they may be shipped back to their point of origin for disposal:

Be certain that they are empty (less than 30 psi) then package them in a *plain* cardboard box, *without* any green diamond label. Mark the box as "**Empty Canisters for Destruction"**. Ship them, prepaid, to

Scott Specialty Gases
2330 Hamilton Boulevard
South Plainfield NJ 07080

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www.inficon.com reachus@inficon.com