



Operating Manual

HAPSITE® CDT

Chemical Identification System



INFICON

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1 | Warranty INFICON

1 Warranty

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3 | Safety Information INFICON

3 Safety Information

All work described in this document may only be carried out by persons who have suitable technical training and the necessary experience or who have been instructed by the end user of the product.

3.1 Safety Precautions When Using Instrument

Misuse of HAPSITE CDT can damage the instrument and may cause bodily harm. The safety messages in this document are provided to protect the user, as well as to optimize HAPSITE CDT performance. Before operating HAPSITE CDT, the user must read and understand all safety messages and take adequate precautions to mitigate hazards or equipment damage.

3.2 Definition of Safety and Informational Messages

When using this document, please pay attention to the safety and informational messages found throughout. For the purposes of this manual they are defined as follows:



⚠ DANGER

This type of message indicates a hazardous situation that will result in death or serious injury if proper precautions are not taken.



⚠ WARNING

This type of message indicates a hazardous situation that could result in death or serious injury if proper precautions are not taken.



MARNING

This type of message indicates that dangerous electrical voltages are present that could result in personal injury if proper precautions are not taken.



⚠ WARNING

This type of message indicates that high temperatures are present that could result in personal injury if proper precautions are not taken.

WARNING

This type of message warns against actions that could cause extensive equipment and/or environmental damage.

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A CAUTION

This type of message indicates a hazardous situation that could result in minor or moderate injury if proper precautions are not taken.

A CAUTION

This type of message cautions against actions that may cause an instrument malfunction, minor equipment damage, and/or the loss of data.

NOTICE

This type of message indicates information that is considered important but is not related to any type of hazard.



This type of message indicates information that is considered important but is not related to any type of hazard.

4 | Introduction INFICON

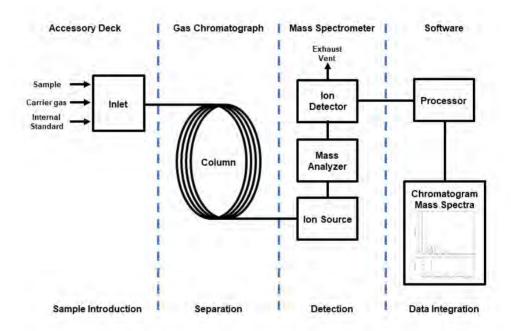
4 Introduction

4.1 Overview

HAPSITE CDT is a person-portable gas chromatograph/mass spectrometer (GC/MS), optimized for fast chromatography to decrease total run time and extended mass range to enable identification of a wide range of analytes.

4.2 Theory of Operation

GC/MS analysis is considered the gold standard in chemical identification and is used to separate and analyze complex mixtures. HAPSITE CDT consists of four main subsystems: sample introduction, separation, detection, and data integration.



4.2.1 Sample Introduction

A sample is introduced into the HAPSITE CDT GC/MS system through its sample inlet and accessory interface. HAPSITE CDT accepts gas samples preconcentrated on a sample cartridge and organic liquid samples injected through the split/splitless injection module. The accessory interface provides the pneumatic and electrical connections between HAPSITE CDT accessories and the GC/MS. Both the cartridge and injection module are heated during sample introduction, which allows for thermal desorption of the preconcentrated sample and vaporization of the injected liquid sample.

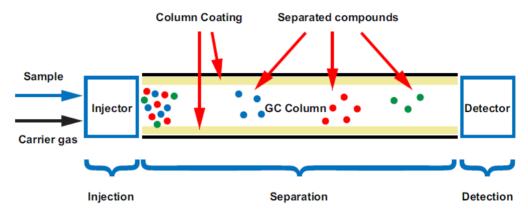
Carrier gas, also known as mobile phase, carries the sample of vaporized/gas phase analytes into the column for analysis.

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4.2.2 Sample Separation

Component separation of a sample injected onto a column is achieved through the component's relative vapor pressure and affinity for the column inner coating, also known as the stationary phase. The more time the analyte spends in the gas phase, the faster that compound travels through and exits the column, or elutes. Order of elution is primarily determined by the compound's volatility and polarity.

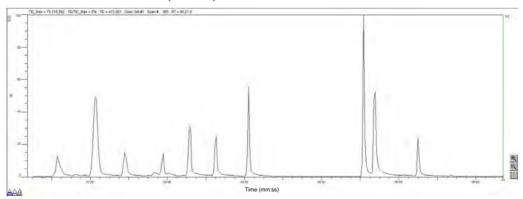
HAPSITE CDT uses nitrogen as the carrier gas to transport analytes through the column. The standard column is a fused silica capillary low-polarity cross-bond diphenyl dimethyl polysiloxane analytical column, 10 m length, 0.25 μ m film thickness, and 0.25 mm inner diameter.



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-programmed conditions remain the same between analyses, a specific compound will elute from the column at the same retention time on every analysis.

HAPSITE CDT uses internal standards to verify the performance of the GC and MS. The internal standard is composed of two volatile organic chemicals which are injected onto the sample cartridge prior to analysis. The internal standards' retention times and responses are used to ensure proper instrument performance and as a reference for quantitative analysis.

A graph of eluting compounds from the gas chromatograph is shown below. This graph is called a total ion chromatogram (TIC) and is plotted as a function of time (x axis) versus detector response (y axis).



4 | Introduction INFICON

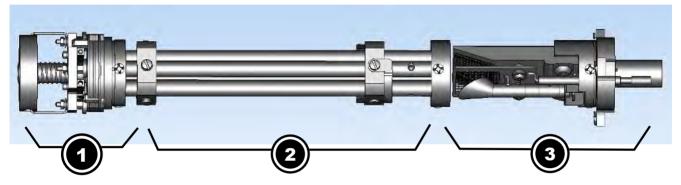
4.2.3 Sample Detection

The separated sample elutes from the GC column through the membrane inlet and enters the mass spectrometer.

The three main components of the mass spectrometer sensor are:

- 1. Ion source (ionizer)
- 2. Quadrupole mass filter
- 3. Detector/electron multiplier

These components are housed in a vacuum manifold that also includes: an inlet, two vacuum pumps, and a portion of the vacuum interconnect valve. The figure below is a representation of the three subsystems of the mass spectrometer.



After passing through the membrane inlet, analytes travel to the ion source. Within the ion source, analytes are subjected to a bombardment of electrons that 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 quadrupole mass filter by the different voltages on the ion volume and focusing plates.

The quadrupole mass filter is a mass analyzer. The mass analyzer is composed 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 degrees 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 quadrupole. 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 toward 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 transit the length of the quadrupole and impact the detector/electron multiplier.

When the ions exit from the quadrupole mass filter, they impact 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

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which generates more electrons. The result is a small burst of electrical current in response to each impacting ion. The signal from the electron multiplier is connected to the electronic amplifier and data integration system.

The ratio of RF to DC field strengths is varied (swept) to permit progressively heavier ions to transit the mass filter. The sweep, or scan, over the full range of masses (from 1 to 424 amu) allows for the production of a mass spectrum, a plot of the intensity of each mass fragment versus the size of the mass fragment. This mass spectrum is compared to a library of mass spectra, and if matches meeting search criteria are found, they are listed as probable identifications.

4.2.4 Data Integration

The HAPSITE CDT software system controls the GC/MS and processes the detector signal output for the sample being analyzed.

- The instrument software reads methods, controls internal components to run a method, processes data, and performs compound identification. The front panel user interface allows for quick analysis and convenient instrument controls.
- The laptop software, CDT IQ, is a Windows®-based system for laptop use. CDT IQ is used to design and modify methods, view data, analyze results, and generate reports. The laptop is linked to HAPSITE CDT via an Ethernet or a wireless connection. This linkage permits data transfer and remote operation.

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4.3 Specifications

Operating Parameter	Specification
Weight	17.8 kg (39.3 lb.)
Dimensions (L \times W \times H)	50.6 cm × 51.4 cm × 19.3 cm
Installation (overvoltage)	Category II per IEC 60664
Power supply input	100-240 V (AC) ± 10%, 47-63 Hz
Power supply output	24 V (DC) at 250 W
Battery life	5 hours with cartridge analysis, 2 batteries at 25°C
Operating temperature	0-35°C (32-95°F)
Storage temperature	-40 to 55°C (-40 to 131°F)
Relative humidity	Up to 95%, noncondensing
Altitude	Up to 2000 m
Pollution degree	2 per EN61010-1
External communications	802.11b/g/n wireless or direct Ethernet

Instrument Parameter	Specification
Power requirement	24 V (DC) at 200 W
Internal storage	16 GB compact flash
External storage	USB
Display	8.0 in. 800 × 480 resolution with touch
GC column	Crossbond diphenyl dimethyl polysiloxane, 10 m, Rxi-5ms, 0.25 mm i.d., 0.25 µm df (standard)
Mass range	10-424 amu (1-424 using SIM)
Scan rate	Up to 250 amu/s at 10 points per amu
Ionization mode	70 eV electron impact
Mass analyzer	Quadrupole
Vacuum system	Non-evaporable getter (NEG) pump/ion pump and optional mechanical pumping accessory
Sample inlets	Air cartridge, split/splitless injector
Carrier gas	Nitrogen
Column temperature range	45-225°C (113-428°F), ramping up to 120°C/min
Maximum sample moisture content	95%, noncondensing
SIM channels	Up to 16 mass fragments
pH range of sample	2-11

5 Installation and Setup

5.1 Site Preparation

The following requirements should be taken into consideration prior to operating HAPSITE CDT.

5.1.1 Recommended Operating Conditions

HAPSITE CDT is a portable GC/MS designed for remote operation. It is recommended that operating temperatures be within $0-35^{\circ}$ C and with less than 95% relative humidity.

5.1.2 Space and Venting Requirements

During portable operation, HAPSITE CDT only requires the space of the exterior footprint of the instrument, which occupies a space of $50.6~\rm cm~x~51.4~\rm cm~x~19.3~\rm cm$. If HAPSITE CDT is being run off external power and is venting exhaust with tubing, allow an additional $15~\rm cm~(6~in.)$ of clearance on either side of the instrument. When operating HAPSITE CDT attached to the Service Module (SM), allow for clearance of the SM vents.

HAPSITE CDT is capable of external venting. This feature allows for less downtime between analyses and only requires clearance and airflow above and below the instrument, which can be obtained by using the handle as a support and positioning HAPSITE CDT at an angle.

5.1.3 Power Requirements

HAPSITE CDT uses a power supply input of 100-240 V (AC) \pm 10%, 47-63 Hz and a power supply output of 24 V (DC) at 250 W. The power requirement for HAPSITE CDT is 24 V (DC) at 200 W.

5.1.4 Computer Hardware Requirements

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

Component	Requirement
Processor	Intel® Core™ i3
RAM	8 GB or greater
Storage	10 GB
Display size	14 in.
Display resolution	1920 x 1080 pixels
Network	Ethernet or wireless
Operating system	Windows 10, 11

5 | Installation and Setup

5.1.5 Network Preparation

If HAPSITE CDT will be connected to a local area network (LAN) using a static IP address, the HAPSITE CDT host name and static IP address must be assigned by the LAN administrator.

It is not necessary for a LAN administrator to set up the HAPSITE CDT hostname and static IP address when Dynamic Host Configuration Protocol (DHCP) is used to assign the HAPSITE CDT IP address.

5.2 Ship Kit

Ship Kit Materials

Part Number	Description	Quantity
036-0015	Shoulder strap	1
074-290	Instruction sheet (shoulder strap)	1
059-0329	Quick disconnect stem	1
070-0972	Plunger contact	4
074-766-P1-A	HAPSITE CDT Quick Start Guide	1
600-1319-P2	Ethernet cable	1
937-3401-G1	CDT tool kit	1
937-3402-G1	Accessory deck maintenance	1
930-4652-P1	Permanent marker	1
930-612-P1	USB flash drive	1
937-469-G1	Universal power supply kit	1
937-3467-G1	Universal CDT battery charger kit	1

The ship kits for the laptops will vary; the items in the laptop ship kit are based upon the type of laptop ordered. Software will be pre-installed on the laptop, and the laptop kits will include the National Institute of Standards and Technology (NIST) Library Install CD.

5.3 Basic Assembly

HAPSITE CDT will be shipped from the factory with protection plugs installed on external components, including a yellow loop cartridge. There is no concentrator in the yellow loop cartridge; this cartridge is primarily used for system shipment. These protection plugs should be retained for the future, should the system need protection during shipment or external decontamination.

5.3.1 Protective Coverings Removal

1 Remove the protective shipping caps from the HAPSITE CDT exhaust and external carrier gas ports.



2 Remove the protective shipping caps from the HAPSITE CDT power, Ethernet, and communication ports.



3 Remove the protective loop cartridge. Slide the loop cartridge straight backward from the inlet until the cartridge releases from the inlet and guide pins.



5 | Installation and Setup

4 Install the sample cartridge. Align the cartridge using the guide pins on the accessory deck of HAPSITE CDT. Make sure the cartridge is flat against the accessory deck. Slide the cartridge toward the inlet until the cartridge clicks into place.



⚠ CAUTION

Leave the survey protection port cap installed. Removal of this cap will cause a leak to the GC during analysis.

5.3.2 Power Connection

HAPSITE CDT uses a power supply that accepts 100–240 V (AC) input and provides 24 V (DC) to the instrument.

A CAUTION

Connect the cables in the following order to avoid damage to the instrument.

- 1 HAPSITE CDT ships with a universal power supply kit. Connect the appropriate region specific power cord to the 24 V (DC) power supply.
- 2 Insert the Fischer® connector to the back right of the instrument, with the connector oriented to the three o'clock position so that the red dots align. A click will be audible when the power connector is properly connected.



Installation and Setup | 5

3 Connect the male end of the power cord to the 100-240 V (AC) power source.

⇒ With the power supply properly connected, HAPSITE CDT can be powered on by pressing the power button on the front panel.



A CAUTION

INFICON

Using an alternative power supply voids the warranty.

5.3.3 Gas Canister Installation

A CAUTION

Do not open the front panel door in a contaminated area.

HAPSITE CDT uses nitrogen as a carrier gas. Either a carrier gas canister or external carrier supply can be used to provide carrier gas. HAPSITE CDT uses two gas-phase internal standards to calibrate/tune the mass spectrometer and as a reference for quantitative analysis. The internal standards are:

- 1-Bromoheptadecafluorooctane (perfluorooctyl bromide, PFOB)
- Bromopentafluorobenzene (BPFB)

Both carrier gas and internal standard are needed for basic operation. Follow the instructions below for gas canister installation.

1 Open the front panel hinged door by rotating the guarter-turn fasteners.



5 | Installation and Setup INFICON

2 Insert a green-banded internal standard canister into the bottom round opening. This opening is marked with a green stripe.



3 Press the PUSH lever while inserting the internal standard canister. Once inserted, press in the canister and PUSH lever together, then release the PUSH lever. Gently pull on the internal standard canister. It should remain fastened inside HAPSITE CDT.



A CAUTION

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

4 Insert a purple-banded carrier gas canister into the top round opening. This opening is marked with a purple stripe.



5 Press the PUSH lever while inserting the internal standard canister. Once inserted, press in the canister and PUSH lever together, then release the PUSH lever. Gently pull on the internal standard canister. It should remain fastened inside HAPSITE CDT.



↑ CAUTION

INFICON

The position of the gas canisters should not be interchanged. To prevent improper placement, the internal standard canister has a Teflon® ring that surrounds the inner stem on the top of the canister. Do not force the canisters into the wrong location, as this will contaminate and/or damage HAPSITE CDT.

MARNING

The HAPSITE ER internal standard canister is not compatible with HAPSITE CDT.

5.3.4 Gas Canister Removal

Removing the gas canisters is advised when HAPSITE CDT has been placed into extended standby. Also, the gas canister will need to be replaced when the canister is low. A low pressure warning will be displayed on the front panel when the canister needs replacement. Follow the instructions below to remove a gas canister.

5 | Installation and Setup INFICON

1 Press the PUSH lever located to the right of the canister. A slight twist of the canister may be required.



- ⇒ The canister will release.
- 2 Remove the canister.



MARNING

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

⚠ CAUTION

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

5.3.5 Ventilation

HAPSITE CDT has three vents built into the instrument's enclosure. To access the full benefits of this design, proceed with the following steps.

A CAUTION

Opening a vent while in a contaminated or harsh environment may cause contamination or damage to HAPSITE CDT. Make sure vents are rotated in a proper sealed position prior to entering a contaminated or harsh environment.

1 Use a 3 mm hex tool to loosen the socket head screws one-quarter turn on the vent covers. There are two vent covers on top and one on the bottom of the instrument.



2 Once the screws are loosened, lift and rotate each cover 180 degrees.



3 Use a 3 mm hex tool to tighten the socket head screws one-quarter turn.

5.3.5.1 Filter Replacement

1 Use a 3 mm hex tool to loosen the socket head screws one-quarter turn on the vent covers. There are two vent covers on top and one on the bottom of the instrument.



2 Once the screws are loosened, lift up and remove the vent cover and replace filter material.



3 Replace vent cover. Use a 3 mm hex tool to tighten the socket head screws one-quarter turn.



5 | Installation and Setup

5.3.6 Sample Cartridge Information and Installation

5.3.6.1 Tenax Cartridge

The Tenax® cartridge is used for analyzing samples with concentration levels in the low part per million to high part per trillion range. The Tenax cartridge will not effectively retain compounds with boiling points below -55°C, but may be more effective at retaining and releasing compounds with higher boiling points.

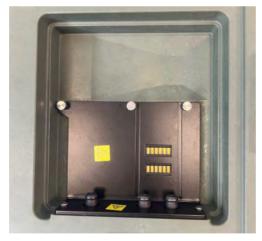


⚠ CAUTION

The Tenax cartridge will not effectively retain compounds with boiling points below -55°C.

5.3.6.2 Sample Cartridge Installation

1 To install the sample cartridge, position it with the tab oriented up and closest to the sample inlet. Make sure grooved channels on the sample cartridge are positioned above the accessory interface locking fasteners.



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2 Press the cartridge onto the accessory interface so that the locking fasteners are within the sample cartridge grooved channels.



3 While pressing the cartridge onto the accessory interface, slide the cartridge toward the sample inlet. Listen for an audible click. The cartridge should fit tightly.





A CAUTION

Accessory Interface Deck

HAPSITE CDT has a heated inlet. To avoid burns, use caution when installing.

A CAUTION

Inlet Pneumatic Connection

Take care to avoid contaminating the inlet with debris. Debris can cause slight leaks that may impact sample analysis. When not in use, be sure to install the protective sample loop or cartridge to maintain inlets free of debris. Contact INFICON support if debris is found in the sample inlet.

5 | Installation and Setup

5.3.7 Injection Port Information and Installation

1 Position the injection port with the flat side oriented closest to the sample inlet. Make sure that the grooved channels on the injection port are positioned above the accessory interface locking fasteners.



- **2** Press the injection port onto the accessory interface so that the locking fasteners are within the injection port grooved channels.
- 3 While pressing the injection port onto the accessory interface, slide the injection port toward the sample inlet. Ensure a good connection. The injection port should fit tightly.





A CAUTION

Accessory Interface Deck

HAPSITE CDT has a heated inlet. To avoid burns, use caution when installing.

A CAUTION

Inlet Pneumatic Connection

Take care to avoid contaminating the inlet with debris. Debris can cause slight leaks that may impact sample analysis. When not in use, be sure to install the protective sample loop or cartridge to maintain inlets free of debris. Contact INFICON support if debris is found in the sample inlet.

5.3.8 Battery Charging and Installation

- 1 To access the battery compartment, first adjust the handle forward toward the front panel so that there is a clear path for the battery compartment door.
- **2** Loosen the three fasteners on the battery compartment door. Swing the battery compartment door open.



3 To install a battery, position the battery so that its power connector and communication pads align with the power connector and pogo pins on the instrument.



4 Once aligned, push the battery down onto the power connector.

5 | Installation and Setup

5 Secure the batteries with the attached battery strap. Repeat with a second battery, if desired.





6 Close the battery compartment door and tighten the three fasteners.

MARNING

Only use INFICON-approved batteries. HAPSITE CDT Battery (937-3090-P1S), Ultralife UBBL13-01. Refer to UBM-5112 for battery safety information.

NOTICE

Batteries will charge only when external power is connected and instrument is in extended standby.

5.3.9 Wired Ethernet Connection

1. Connect an Ethernet cable to the Ethernet port on the right side of HAPSITE CDT near the rear of the system. The other end of this connection can be connected to a computer or Ethernet switching device.



INFICON Installation and Setup | 5

2. Hot zone use requires a sealed Ethernet cable. The Ethernet port should be covered with an Ethernet cap when not in use.



3. The system will be assigned a generic IP address at the factory. For instructions on Ethernet configuration, see Static Ethernet Configuration [\triangleright 40].

NOTICE

If HAPSITE CDT will be connected to a local area network, check with the network administrator prior to changing to static IP address to avoid conflicts.

5.3.10 Wireless Connection

The HAPSITE CDT wireless connection will be disabled as the default configuration. The system adopts a dynamic IP address and runs Dynamic Host Configuration Protocol (DHCP) by default when enabled. The user will need to assign a password for a secure wireless connection. HAPSITE CDT supports a direct wireless connection with the laptop computer, wireless connection through a network, or static wireless connection.

1 Enable the wireless signal by opening the front panel door and switching on the wireless switch.



2 For instructions on wireless configuration see Direct Wireless Configuration [▶ 41].

6 | Operation INFICON

6 Operation

6.1 Portable Operation

Portable operation refers to using HAPSITE CDT without the laptop computer. HAPSITE CDT portable operation via the front panel utilizes two possible user interfaces (UI): the Legacy UI and the CDT UI. Previous users trained on HAPSITE ER or earlier models will find similarities in the Legacy UI, while newer users will find an easy-to-use, streamlined CDT UI for sample cartridge analysis.

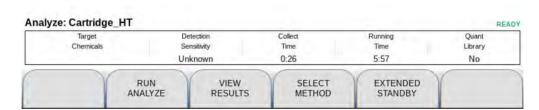
6.1.1 Standard User Interface

6.1.1.1 Home

The **Home** navigation tab is located on the left-hand side of the top menu bar.



Analyze is ready to run.

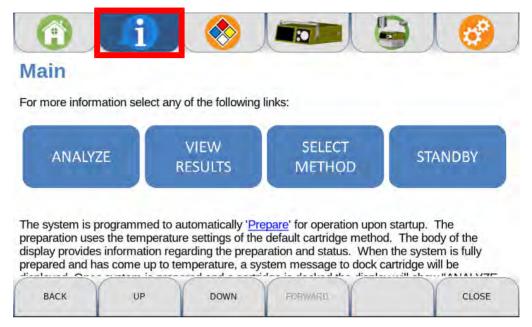


The **Home** screen displays the system status bar, status messages and progress, and the selected analyze method.

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6.1.1.2 Info/Help

The Info/Help navigation tab is located on the top menu bar, the second tab from the left.



The main Info/Help screen displays an Analyze link, a View Results link, a Select Method link, and a Standby link. Touching a link will provide instructions for performing the specified function.

6.1.1.3 Hazards Info

The **Hazards Info** navigation tab is located to the right of the **Info/Help** navigation tab on the top menu bar of the HAPSITE CDT screen. **Hazards Info** can be accessed by touching the **Hazards Info** navigation tab.



6 | Operation INFICON

The NIOSH Database screen is displayed. 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
- Toxicologic Review of Selected Chemicals

These publications provide information on exposure limits, synonyms, and detection limitations.

Scrolling to the bottom of the page accesses additional links.

- The Conversion Calculator converts concentration units.
- Hazard IDs 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. To access the database, scroll to the fourth option on the list and touch The NIOSH Pocket Guide to Chemical Hazards link.
- When the publication appears, touch INDEX with CHEMICAL NAMES and SYNONYMS.
- 3 Scroll down to display an alphabet. Touch the first letter of the desired compound.
- 4 A list of the chemicals that start with the selected letter is displayed.
- 5 Touch the desired chemical. The **Pocket Guide** for this specific chemical is displayed.
- **6** Scrolling down displays information about the exposure limit and additional information.
- 7 To access information regarding IDLHs, touch the first hyperlink on the Hazards Info screen.
- 8 Scroll down or touch **DOWN** until the **IDLH-Chemical listing and Documentation** link is displayed. Touch this 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.
- 10 Information regarding the compound's NIOSH REL, OSHA PEL, and toxicity data is displayed.

INFICON Operation | 6

6.1.1.4 System Status

The **System Status** navigation tab provides information on the status of the instrument and its consumables. Information regarding battery power, gas consumption, heaters, tune status, and GPS can be accessed through this screen.

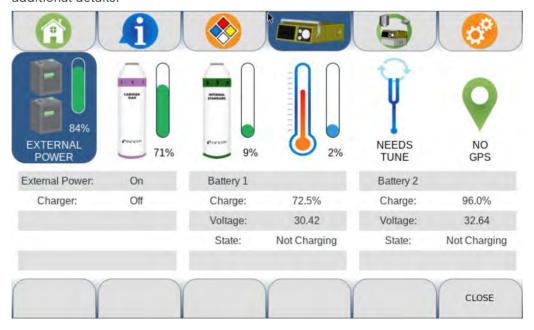


Analyze is ready to run.

Target	D	etection	Collect Time	Running	Quant Library
Chemicals	Se	ensitivity		Time	
	Ur	nknown	0:26	5:57	No
1					-
V	RUN	VIEW	SELECT	EXTENDED	
	ANALYZE	RESULTS	METHOD	STANDBY	

6.1.1.4.1 Batteries

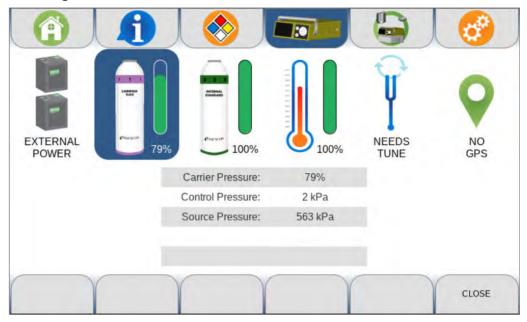
The total charge level of the installed batteries as a percent of full capacity is denoted as a vertical bar to the right of the battery icon. The charge level shown is based on the combined charge of two installed batteries. If one fully charged battery is installed, the charge level reads 50% initially. If two fully charged batteries are installed, the charge level reads 100% initially. Touch the **Batteries** icon to display additional details.



6 | Operation INFICON

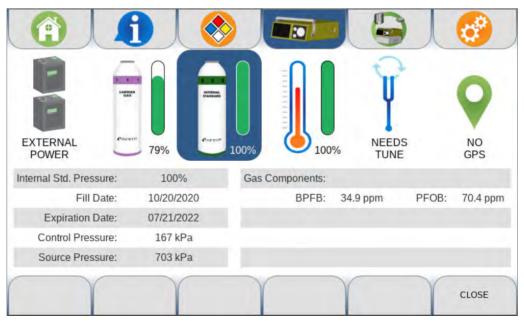
6.1.1.4.2 Carrier Gas

Touching the **Carrier Gas** icon will provide information about the pressure of the gas in the can. A vertical bar to right of the icon will provide a percentage of gas remaining in the canister.



6.1.1.4.3 Internal Standard

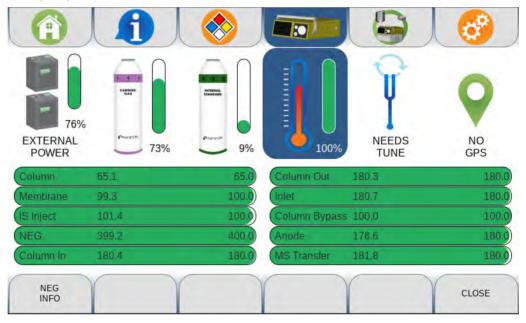
The Internal Standard icon uses a vertical bar to provide a percentage of gas remaining in the canister. Touching the icon displays the canister's fill date, the canister's expiration date, and the actual concentration of bromopentafluoro benzene (BPFB) and perfluorooctyl bromide (PFOB) in the HAPSITE CDT internal standard canister.



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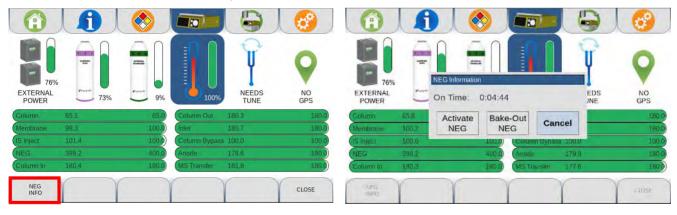
6.1.1.4.4 Heaters

The **Heaters** icon provides the current temperatures of HAPSITE CDT internal heaters. The bar located to the right of the **Heaters** icon represents the progress of the heaters. **NEG Info** provides additional information and actions regarding the NEG pump.



6.1.1.4.4.1 NEG Info

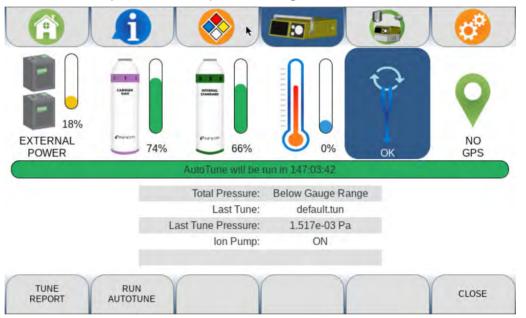
The **NEG Info** tab provides information regarding the hours of NEG use. From this dialog box, there are buttons to activate the NEG and for NEG bake-out. For more information, see Maintenance [> 219].



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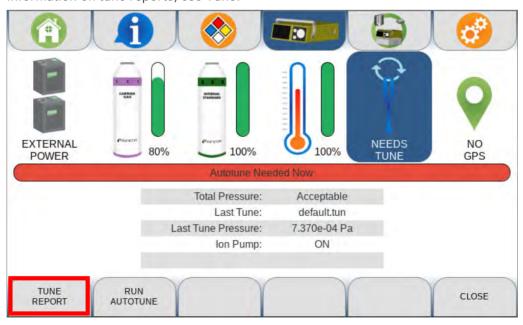
6.1.1.4.5 Tune

The **Tune** icon provides information about the state of the instrument's mass spectrometer (MS) tune. For more information regarding tune, see Tune [\triangleright 139]. The tune screen shows when an autotune is programed to run, the status of the ion pump, and the MS pressure during the last saved tune file. The current total MS pressure is also displayed. MS pressure can provide an indication of system health. The system will not tune or analyze samples if the MS pressure is too high ($>1 \times 10^{-2}$ Pa). Between 6×10^{-3} Pa and 1×10^{-2} Pa, a dialog box will indicate the system is above recommended pressure readings. It is recommended to contact INFICON service personnel if MS pressure is high or above recommended values.



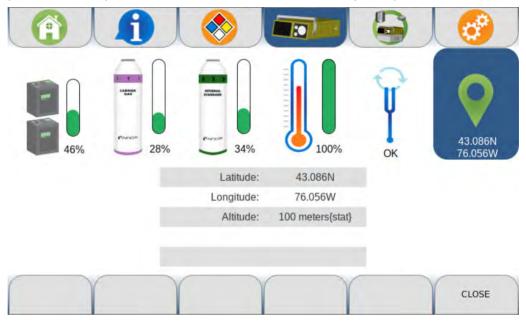
6.1.1.4.5.1 Tune Report

After the **Tune** icon has been touched, the **Tune Reports** tab will be shown at the bottom of the screen. This tab accesses data from the past tune report. For more information on tune reports, see Tune.



6.1.1.4.6 GPS

The **GPS** icon will give the latitude and longitude coordinates of the HAPSITE CDT position. It also provides the number of satellites found by the system.



6.1.1.5 Accessories/Devices

The Accessories/Devices navigation tab displays information regarding the current sampling configuration of the HAPSITE CDT.





The **Accessory** icon appears when a supported accessory is attached to HAPSITE CDT. Touching the icon displays additional information for the accessory.

Touching the **Service Module** icon displays additional information for the Service Module. Options for attaching and detaching the Service Module can be found on this screen. For more information on the Service Module, see the Service Module Operating Manual, available from the INFICON website.



6.1.1.5.1 Concentrator Cleanout

Concentrator cleanout, accessed by clicking the **Conc Cleanout** tab, allows for the cartridge to be cleaned out without the need to analyze a full system blank. Once concentrator cleanout is complete, a dialog box will be displayed showing the results of the cleanout.



6.1.1.6 Settings

The **Settings** navigation tab provides instrument information and allows the user to modify instrument settings. Within the Settings menu are icons for **System**, **Network**, **Switch UI**, **Language**, **Timezone**, and **Silent Mode**.



6.1.1.6.1 System

Clicking the **System** icon will open the System Settings, which provides additional system information. This information includes the system name, serial number, software version number, build date, maximum AMU range, and available system storage capacity. The user may set the preferred default user interface, update the software, and change the instrument name from the left side of the System Settings screen.



6.1.1.6.2 Network

Clicking the **Network** icon will open the Network Overview, which provides network configuration information. This information includes the host name, Ethernet and wireless IP addresses, prefixes, and gateways. Both Ethernet and wireless settings are user configurable.



6.1.1.6.2.1 Static Ethernet Configuration

- 1 Touch the **Settings** navigation tab.
- 2 Touch the Network icon.



3 Touch Ethernet Settings to configure the HAPSITE CDT Ethernet connection.



- 4 Select Static configuration type.
- 5 Select Auto Connect.
- 6 Edit IP Address to desired value; the factory default is 192.168.1.1.
- 7 Edit **Prefix** to match your local network.
- 8 Leave **Default Gateway** blank or use the gateway to match your local network.
- 9 Touch Save.
- 10 Touch Close.



6.1.1.6.2.2 Direct Wireless Configuration

- 1 Touch the **Settings** navigation tab.
- 2 Touch the Network icon.



3 Touch Wifi Settings to configure the HAPSITE CDT wireless connection.



4 Touch Host Mode configuration type.



5 Select Enable.



6 Enter password and then click **OK**.





The wireless password must be at least 8 characters long.

- 7 Touch Save.
- 8 Touch Close.

6.1.1.6.3 Switch User Interface (UI)

- 1 Touch **Settings** navigation tab.
- 2 Touch Switch UI icon.



3 Click Yes to switch to the Simplified UI.



6.1.1.6.4 Language

- 1 Touch **Settings** navigation tab.
- 2 Touch Language icon.





There are no additional languages installed at this time.

6.1.1.6.5 Time Zone

To change the date, time, or time zone:

- 1 Touch **Settings** navigation tab.
- 2 Touch Timezone icon.



3 Touch Change Time, Change Date, or Change TimeZone and adjust as necessary.



6.1.1.6.6 Silent Mode

To select Silent Mode:

- 1 Touch **Settings** navigation tab.
- 2 Touch Silent Mode icon.



6.1.1.7 Select Method

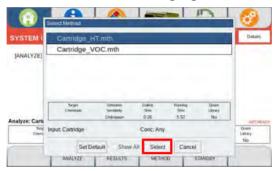
If the selected method is not the desired method, the method can be changed.

To select a new method, touch the Home navigation tab and then touch the Select Method tab on the bottom menu. If a method is preparing and the Preparing Analyze screen is displayed, touch Stop Prepare, then touch Select Method.





2 Scroll up or down and touch the desired method to highlight it. When the desired method is highlighted, touch **Select**.



3 The Preparing Analyze status is displayed.



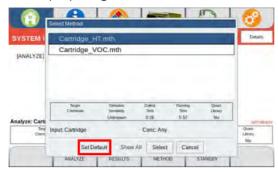
4 HAPSITE CDT begins preparing the new method.

6.1.1.7.1 Default Method

The default method for HAPSITE CDT can be changed. By changing the default method, HAPSITE CDT will automatically select that method when the associated accessory is installed.

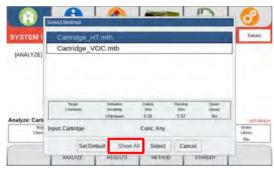
- 1 Touch Select Method.
- 2 Touch the desired method.

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



6.1.1.7.2 Show All

HAPSITE CDT will only show methods that are compatible with the currently installed accessory. By checking the **Show All** box, all loaded HAPSITE CDT methods will appear in the text box, regardless of configuration. Noncompatible methods will be shown in light gray. The noncompatible methods are for reference only and cannot be selected to run.



6.1.1.8 Prepare Analyze

Touching **Prepare Analyze** initiates the system to prepare the selected method. This drives heaters to the initial starting temperatures and sets carrier gas flows to initial pressures.



To prepare HAPSITE CDT for analysis, ensure the desired accessory is installed on the accessory interface and the correct method is selected.

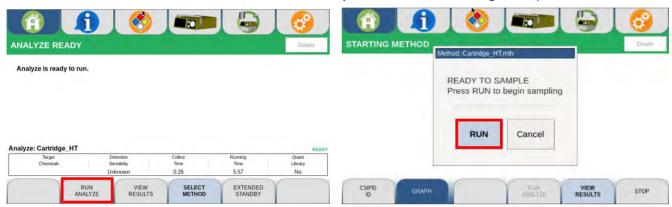
6.1.1.9 Procedure for Cartridge Analysis

NOTICE

A system blank analysis is recommended before analyzing a sample.

Before a cartridge method can be run, the system must be fully prepared. If the cartridge is installed when the system is not properly prepared, it can affect the analysis and peak shape.

- ✓ Verify that the appropriate method is selected and preparing.
 - 1 When HAPSITE CDT has finished preparing, an "Analyze Ready" message is displayed with a prompt to dock the cartridge to begin analysis.
 - 2 Dock the cartridge and ensure a firm connection. Once the cartridge is docked, touch **Run Analyze** and select **Run** to begin analysis.



3 After clicking **Run**, a window will appear where the user can capture the sample volume. Enter the sample volume and click **OK**.

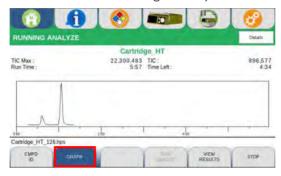


- **4** By touching **CMPD ID** during the analysis, a list of found compounds is displayed. This page displays the following information for each compound:
 - ⇒ CAS number
 - ⇒ Fit
 - ⇒ Retention time (RT)
 - ⇒ TIC (total ion count) maximum
 - □ Current TIC
 - ⇒ Remaining run time



Touching a compound on the list will display synonyms and exposure limit information if it is contained in the NIOSH database.

- **5** To view the chromatogram while the method is running, touch **Graph**. This screen displays:
 - ⇒ Total ion chromatogram (TIC) with compound identification
 - ⇒ TIC max
 - ⇒ Current TIC
 - ⇒ Time remaining in analysis





Touching the blue compound identification above the chromatogram will display synonym and exposure limit information.

6 A "Method Finished" message is displayed when the method has ended.





Another cartridge analysis can be started immediately after one has finished. Depending upon the temperature profile, the column may need to cool down before another analysis can begin.

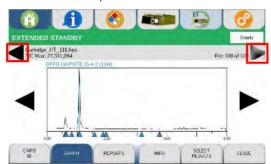
6.1.1.10 View Results/View Reports

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 home screen, touch the **Home** navigation tab.
- 2 Touch View Results.



3 The most recent file for the selected method is displayed on the screen. Use the upper black arrows to the left and right of the data file name to access other data files from the same method. If using the push buttons, use the front panel arrow keys. The left arrow key accesses earlier files. The right arrow key accesses later ones.



4 To view files from another method, touch Select Results.



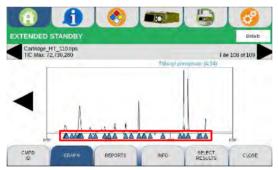
5 Scroll through the method files until the desired method is highlighted, touch **Select**.



6 The lower black arrows to the left and right of the chromatogram 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.



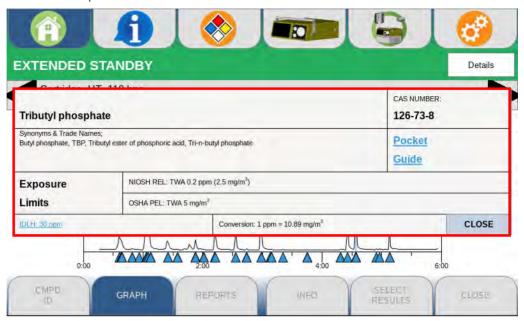
7 Touch the small blue triangles on the graph to display the compound identification and retention time for the compound directly above it.



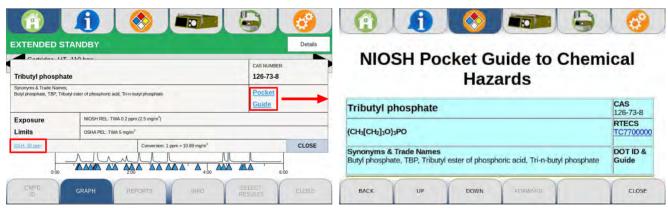


Most functions can be accessed using the push buttons. However, the blue triangles and blue arrows can only be accessed on the touch screen.

8 Touching a specific compound in the list displays that compound's Synonym and Exposure Limit.



9 A link to the NIOSH Pocket Guide to Chemical Hazards (NPG) is displayed in blue. The link is labeled **Pocket Guide**. In the bottom-left corner, there is a link to Immediately Dangerous to Life and Health Concentrations (IDLH). The link is blue and labeled **IDLH**. For further instructions about using NIOSH and other databases, refer to Hazards Info [** 31].



- 10 Touch Close to return to the data screen.
- 11 Touching CMPD ID (compound identification) while in View Results shows a list of the compounds identified during that specific analysis. The CAS number, the Net Fit, and the retention time for each identified compound are also shown.





HAPSITE CDT can detect and identify more compounds than those contained in the onboard library databases.

If the screen displays "N/A" and does not have links available, the compound is not included in these databases. Use laptop and full NIST library if this happens.

12 To view the run's Summary, Qualitative, and Quantitative Reports, touch Reports. Reports can be accessed from the Graph page or the CMPD ID from View Results.



13 The Summary Report can be found by touching **SUMM**. For each compound found, information regarding the Net Fit and the retention time is displayed.



14 The Qualitative Report can be found by touching QUAL. For each compound found, information regarding the Net Fit, the retention time, the CAS number, the area, and the number of hits is displayed.



The Quantitative Report can be found by touching **QUANT**. For each compound found, information regarding the target ion, the retention time, the Net Fit, the purity, the area, and the concentration is displayed.



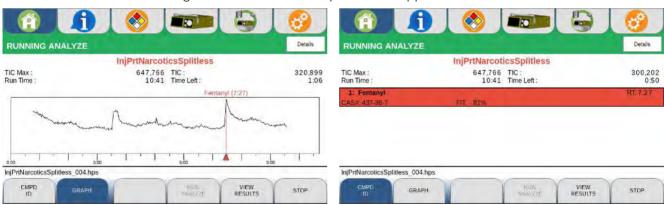


If the method is not quantitative, the message "No quant reports found" is displayed in the Quantitative Reports screen.

To determine if the method is quantitative, see the box in the bottom-right corner of the main screen.

6.1.1.11 Front Display Visual Alarms

Front display visual alarms for target analytes are user configurable through the alarm levels list. (To set alarm levels, see Set Alarm Levels [> 80].) If an analyte on the alarm levels list is identified in graph view, the method name will appear red instead of green, the small triangles denoting the identified compound will appear red instead of blue, and the identified compound name will appear red instead of blue. If an analyte on the alarm levels list is identified in CMPD ID view, the background color of the analyte line will appear red.



6.1.1.12 Extended Standby

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

Extended Standby maintains vacuum in the MS and allows the system to prepare faster.

6.1.1.12.1 Enter Extended Standby

Proceed as follows to place the system into Extended Standby.

1 Touch the **Home** navigation tab, and then touch **Extended Standby** on the bottom menu.



2 When the screen prompts "Do you want to go into Standby?", touch Yes.

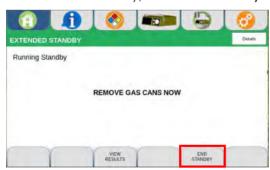


3 HAPSITE CDT goes into Extended Standby. Remove the gas canisters.



6.1.1.12.2 Exit Extended Standby

1 To end standby, touch End Standby.



2 When the system prompts "Do you want to end Standby?", touch Yes.

6.1.1.13 System Blank Analysis

A system blank cleans out the system prior to analysis. This is an important step in ensuring the instrument and its accessory are ready for sample analysis. System blanks also allow for basic troubleshooting and provide an indication of overall system health. It is recommended that system blanks are analyzed on a weekly basis or during daily system use.

NOTICE

When not in use, keep HAPSITE CDT in Extended Standby with the gas canisters removed. To enter Extended Standby, HAPSITE CDT must be connected to external power.

1 Ensure the cartridge is properly installed. If the cartridge is not installed, install the cartridge prior to analysis. Align the cartridge using the guide pins on the accessory deck of HAPSITE CDT. Make sure the cartridge is flat against the accessory deck. Slide the cartridge toward the inlet until the cartridge clicks into place.



2 To prepare the system to run, open the front panel door by rotating the quarter-turn fasteners.



3 Insert the green-banded internal standard canister into the bottom round opening and insert the purple-banded carrier gas canister into the top round opening. These openings are marked with the corresponding color label.



4 Press the PUSH lever while inserting the canister. Once inserted, press in the canister and PUSH lever together, then release the PUSH lever. Gently pull on the canister. It should remain fastened inside HAPSITE CDT.

A CAUTION

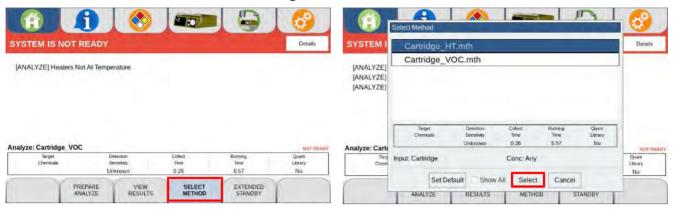
Closing the front panel door when the canisters are not properly installed may damage HAPSITE CDT and/or the canisters.



5 Touch End Standby.



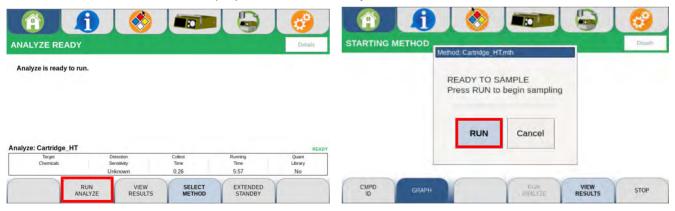
6 Ensure that the desired method is selected or select it from the list of methods in the method directory (sample method file: Cartridge_HT.mth). If Cartridge_HT.mth is not selected touch Stop Prepare, then Select Method. Choose Cartridge_HT.mth from the list. Touch Select.



7 Then touch **Prepare Analyze** and the following window will pop up, indicating that the analysis preparation has begun.



8 When HAPSITE CDT has finished preparing, an "Analyze Ready" message is displayed. Touch **Run Analyze** and then select **Run** to start the method.



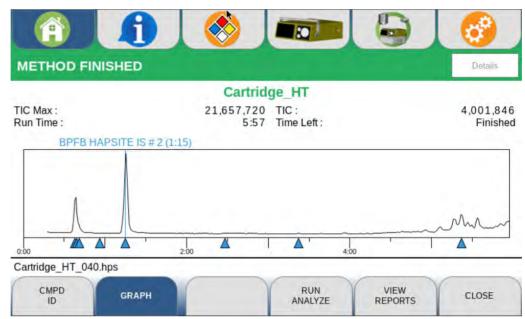
9 Touch Skip for blank analysis.



When the method is finished, look for a flat baseline with an intensity of less than 10% of BPFB HAPSITE #2 peak height.

Look for the two internal standard peaks:

- ⇒ Locate PFOB HAPSITE #1
- ⇒ Locate BPFB HAPSITE #2



11 After the blank analysis data has been verified, HAPSITE CDT can be put into Extended Standby. Touch **Close**.





Other small peaks may be present in the background. However, if the background peaks are greater than 10% of the BPFB peak, continue to run blanks until only the internal standard peaks remain. If peaks remain after several blank analyses and do not decrease in area, these compounds may be from a source of contamination or may be present in the room air. Try sampling in a ventilated area or from a clean air source; additionally, try a different cartridge.

12 Touch Extended Standby. When prompted "Do you want to go into Standby?", touch Yes.



13 Remove the gas canisters by pressing the PUSH lever while twisting the gas canister. Close the front panel door.

6.1.1.14 Quick Reference SOP: Cartridge Analysis

Required Materials:

- HAPSITE CDT (analytical module)
- · Internal standard gas canister
- · Carrier gas canister
- Charged battery or a power supply adapter
- Sample cartridge

Procedure:

1 Insert the internal standard and carrier gas canisters.



- 2 Insert a charged battery or connect the power supply. If installing a charged battery, follow the steps below and then continue on with step 4. If connecting to a power source, skip this step and continue on to step 3.
 - ⇒ Adjust the handle forward, toward the front panel so that there is a clear path for the battery compartment door.
 - \Rightarrow Loosen the three fasteners on the battery compartment door. Swing the battery compartment door open.



⇒ To install a battery, position the battery so that its power connector and communication pads align with the power connector and pogo pins on the instrument.



- ⇒ Once aligned, push the battery down onto the power connector.
- ⇒ Secure the batteries with the attached battery strap.



 \Rightarrow Close the battery compartment door and tighten the three fasteners.

3 Connect the appropriate region specific power cord to the 24 V (DC) power supply.

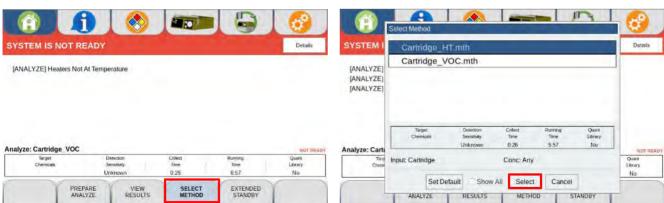
⇒ Connect the power cable to the back of the instrument, orient the connector so that the red dot is in the three o'clock position. A click will be audible when the power connector is properly connected.



- \Rightarrow Connect the male end of the power cord to the 100-240 V (AC) power source.
- 4 Press the **Power** button on the front panel. An indicator illuminates.



5 HAPSITE CDT boots up in approximately one minute. Ensure that the desired method is selected or select it from the lists of methods in the method directory (sample method file: Cartridge_HT.mth). If Cartridge_HT.mth is not selected touch Stop Prepare, then Select Method. Choose Cartridge_HT.mth from the list. Touch Select.

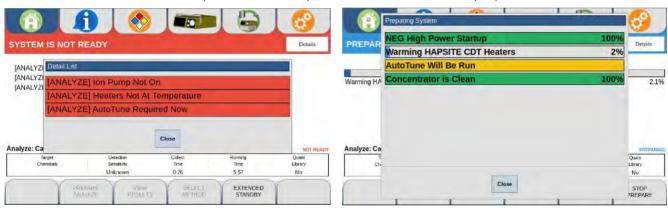


6 During the preparation period, the front panel displays the "Preparing Analyze" message. This message occurs when a system is not at the method's temperature setpoint.

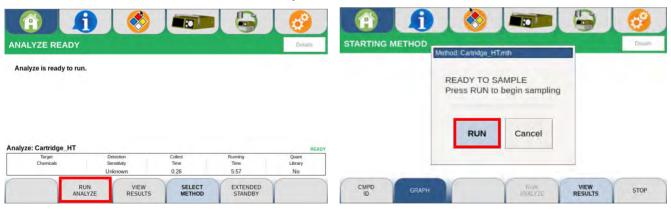
7 To view the preparation details' progress, touch **Details**.



8 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.



- 9 When HAPSITE CDT is ready to run samples, a green "Analyze Ready" message is displayed.
- 10 If "Analyze Ready" is displayed, then dock the prepared sample cartridge. Touch Run Analyze, then select Run.



6.1.1.15 Quick Reference SOP: Injection Port Analysis

Required Materials:

- HAPSITE CDT (analytical module)
- Internal standard gas canister
- Carrier gas canister
- Power supply
- · Injection port
- 10 μL glass syringe

Procedure:

1 Insert the internal standard and carrier gas canisters.



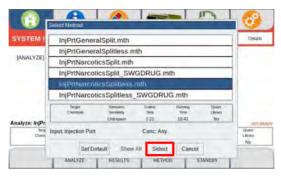
- 2 Insert a charged battery or connect the power supply. For further instruction see Quick Reference SOP: Cartridge Analysis [> 59].
- 3 Install injection port.



4 Press the **Power** button on the front panel. An indicator illuminates.



5 HAPSITE CDT boots up in approximately one minute. To prepare the instrument, select the appropriate method for your application, then touch Select.



6 Confirm that the correct method is selected and then press **Prepare Analyze**.





7 During the preparation period, the front panel displays the "Preparing Analyze" message.



8 To view the details of the preparation progress, touch **Details**.



9 The progress of the preparation is shown by a bar graph. If a heater is in the process of being prepared, it will be shown in blue. When a heater is ready, it will be shown in green. If a heater 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.



- 10 During these system preparation steps, ready the syringe with the prepared sample; refer to Quick Reference SOP: Sample Preparation for Surface Wipes of Unknown Powder Residue [> 210].
- 11 When HAPSITE CDT is ready to analyze samples, a green "Analyze Ready" message is displayed.





12 If "Analyze Ready" is displayed, lift the injection port cover, press Run Analyze on the screen. Analysis begins shortly; there is a three-second window to inject the sample. When prompted with Inject Now, insert the syringe through the septum nut and inject the sample.





A CAUTION

Injection of any substance other than the diluted or extracted sample in organic solvents may damage HAPSITE CDT.

6.2 Laptop Operation

6.2.1 CDT IQ Software

6.2.1.1 CDT IQ

CDT IQ is the laptop software that controls instrument operation, runs analyses, manages files, and creates reports. Data collected with HAPSITE CDT can be viewed on and interpreted using CDT 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 function of the CDT IQ software allows access to previously acquired data for review and analysis, or to view data that are being acquired in real time. CDT IQ operates with Microsoft Windows.

The software is loaded onto the laptop at the factory. If reinstallation is necessary, contact INFICON for support.

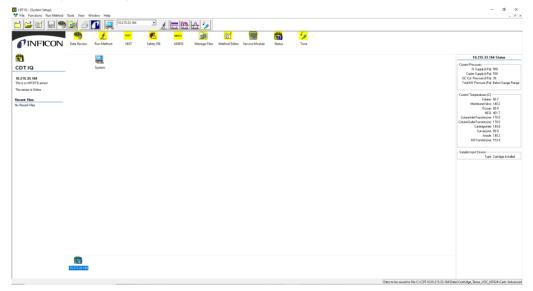
6.2.1.2 System Setup

Upon opening CDT 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 CDT components.

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



2 When opening CDT IQ, the main window of the software is the System Setup screen.



6.2.1.2.1 System Startup Menu

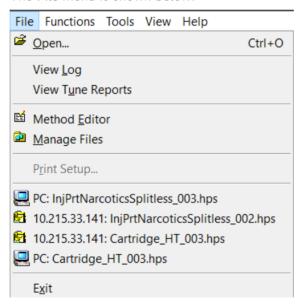
The default main menu toolbar includes File, Functions, Tools, View, and Help options. Additional menu options will appear when certain actions are taken:

- If a log has been opened, the menu will include Log View Options.
- If a method is prepared, the menu will include Run Method.
- If a calibrate screen is opened, the menu will include Calibrate.
- If a data file is opened, the menu will include Data Review.
- If a window is opened, the menu will include Window.



6.2.1.2.1.1 File Menu

The File menu is shown below.

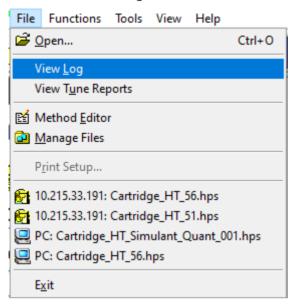


- Open will open a data file from either CDT IQ or the laptop.
- View Log allows for event .log files to be opened. Examples of files logged are warnings, errors, and run history.
- View Tune Reports allows for tune reports (.tun) to be opened. For more information on tune reports, see View Tune Report [▶ 151].
- Method Editor opens the Method Editor function. It performs the same function as the Method Editor icon. See Methods [▶ 153] for further instructions.
- Manage Files opens the Manage Files function. It performs the same function as the Manage Files icon. See Manage Files [> 79].
- 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 CDT IQ.

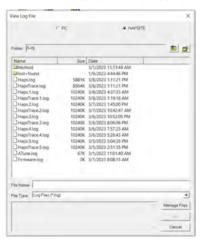
6.2.1.2.1.1.1 View Log

HAPSITE CDT will log errors, warnings, and events, if desired. See Maintenance [86] 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.



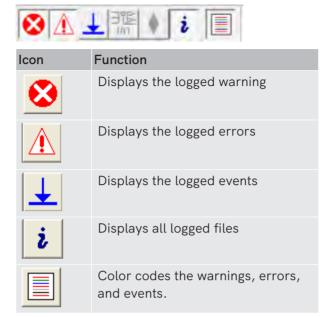
2 Double-click the desired log file.



3 The log file will be displayed.

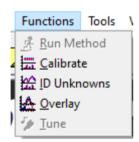
6.2.1.2.1.1.2 Log File Toolbar

The following icons will be displayed on the **Log File Toolbar**. These are the same options available in the Log View Options menu.



6.2.1.2.1.2 Functions Menu

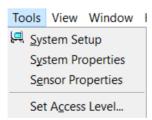
The Functions menu is shown below.



The **Run Method**, **Calibrate**, and **Overlay** options function identically to the icons of the same name.

6.2.1.2.1.3 Tools Menu

The **Tools** menu is shown below.



System Setup toggles the System Setup screen.

System Properties will open the System Properties window. This performs the same function as the System Properties icon; see HAPSITE Icons [▶ 90].

Sensor Properties opens the HAPSITE Sensor Properties window. This performs the same function as the HAPSITE Sensor Properties icon; see HAPSITE Icons [> 90].

Set Access Level... allows user to select Normal or Advanced access level.

6.2.1.2.1.3.1 System Properties

6.2.1.2.1.3.1.1 Port Settings Tab

Port Settings is the default tab in the System Properties window.

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



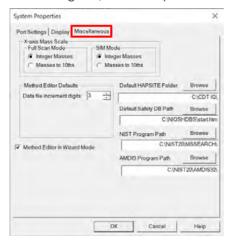
6.2.1.2.1.3.1.2 Display Tab

The **Display** tab is used to change the appearance of the CDT IQ settings, including the thickness of the chromatogram line, the fonts used, and the screen layout.



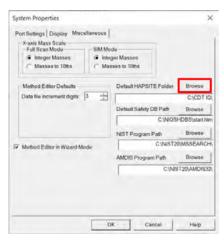
6.2.1.2.1.3.1.3 Miscellaneous Tab

The **Miscellaneous** tab displays the defaults, data file paths, the data file increment digits, the software, safety and library file paths, the scaling preferences for the chromatogram, and the option to select Wizard Mode for Method Editor.

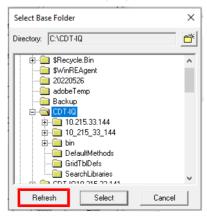


Four default software pathways are displayed. The **Browse** buttons access folders to reset the pathways, if necessary. However, the software installation should properly select these options. If a pathway requires resetting, follow the instructions below.

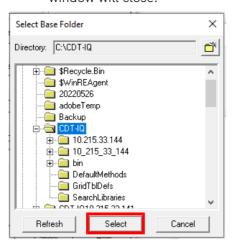
1 Click Browse for the Default HAPSITE Folder.



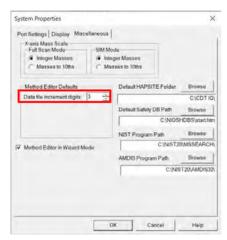
- 2 The Select Base Folder window will open.
- 3 Click to highlight the desired folder.
 - ⇒ Click **Refresh** to update the displayed folders if the desired folder is not displayed.



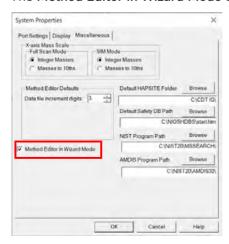
4 Once the desired file is highlighted, click **Select**. Once **Select** is clicked, the window will close.



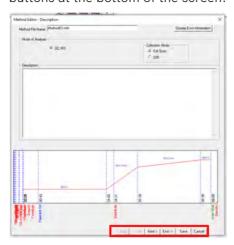
The Data file increment digits field is used to select the number of digits that are to be appended to a data file. For example, if 2 is selected, the file name would read Method_yearmonthday_01. If 3 is selected, the file name would read Method_yearmonthday_001. The data file increment digits can also be selected in Method Editor. See Data File Information [> 182] for instructions.



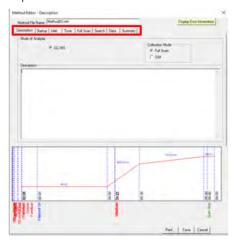
The Method Editor in Wizard Mode checkbox is the next option.



Wizard Mode guides the user through the Method Editor by using **Next >** and **< Back** buttons at the bottom of the screen.



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.



6.2.1.2.1.3.2 Set Access Level

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

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

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.

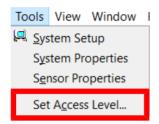
To restrict access to advanced functions, an advanced user password can be set. Once the password is set, it must be entered each time CDT IQ is opened, or whenever the access level is changed from Normal to Advanced. See Setting or Changing the Access Level Password [> 75].

6.2.1.2.1.3.2.1 Changing Access Levels



When the Normal access level is selected, a prompt will appear stating that some areas of the CDT IQ will have restricted access. Click "Yes" if continuing is desired.

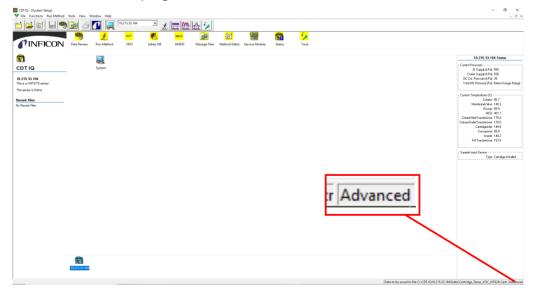
- 1 To change the access level, click on the Tools menu on the System Setup screen.
- 2 Select Set Access Level...



3 To select advanced access, click on the 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.



4 The current access level of the system is displayed at the bottom-right corner of the CDT IQ program, in the Status Bar.



6.2.1.2.1.3.2.2 Setting or Changing the Access Level Password

- 1 To change the Advanced password, first enter Advanced mode.
- 2 Press the Change Password button.
- 3 The window shown below will be displayed.



- 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.



CDT IQ maintains the last access level when closed. Upon reopening the program, the system will default to the last access level used. 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.

6.2.1.2.1.4 View Menu

The View menu is shown below. It is used to select the desired toolbars.



The Main Toolbar is shown below. See HAPSITE Icons [▶ 90] for icon descriptions.



The **Sensor Toolbar** is shown below. See HAPSITE Icons [▶ 90] for icon descriptions.



The **Function Toolbar** is only available when the Data Review screen is open. See Data Review Menus and Toolbar $[\triangleright 95]$ for icon descriptions.



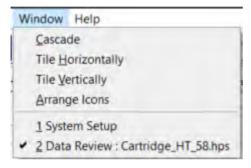
Toolbars Use Large Icons increases the size of the toolbar icons.

Sensor Status Grid will open the Sensor Status Grid, which shows the current condition of various components.



6.2.1.2.1.5 Window Menu

The Window menu is shown below. This menu only appears when a window is open.



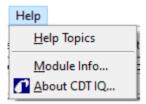
The first three options, Cascade, Tile Horizontally, and Tile Vertically, determine the arrangement of open windows on the screen.

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.

6.2.1.2.1.6 Help Menu

The Help menu is displayed below.



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 CDT IQ shows the installed software version.

6.2.1.3 Safety Database

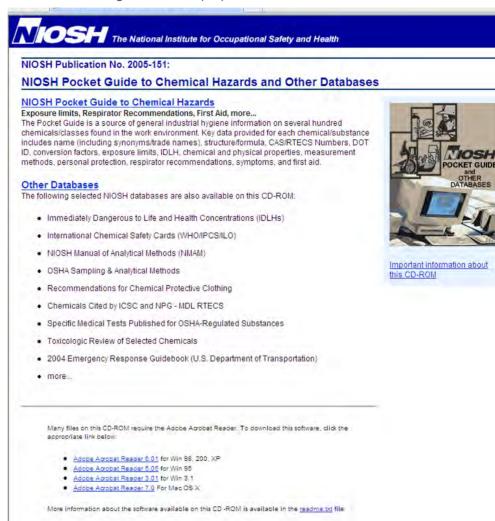
The **Safety DB** icon accesses the NIOSH Safety Database, which is used to locate NIOSH REL, OSHA PEL, CAS Numbers, synonyms, IDLHs, and safety recommendations. Follow the procedure below to access the Safety FB.

1 Double-click the Safety DB icon.



Safety DB

2 The following screen is displayed.



- 3 Click the NIOSH Pocket Guide to Chemical Hazards link or the link to the desired database.
- 4 If the NIOSH Pocket Guide to Chemical Hazards link is clicked, the following screen is displayed.



NIOSH Publication No. 2005-151:

NIOSH Pocket Guide to Chemical Hazards

The NIOSH Pocket Guide to Chemical Hazards (NPG) is intended as a source of general industrial hygiene information on several hundred chemicals/classes for workers, employers, and occupational health professionals. The NPG does not contain an analysis of all pertinent data, rather it presents key information and data in abbreviated or tabular form for chemicals or substance groupings (e.g. cyanides, fluorides, manganese compounds) that are found in the work environment. The information found in the NPG should help users recognize and control occupational chemical hazards.

Contents

- Introduction
- · Index of Chemical Names, Synonyms and Trade Names
- . Index of Primary Chemical Names
- Index of CAS Numbers
- . Index of RTECS Numbers
- Appendices

What's Inside

The Pocket Guide includes the following:

- Chemical names, synonyms, trade names, conversion factors, CAS, RTECS, and DOT numbers
- · NIOSH Recommended Expoure Limits (NIOSH RELs)
- . Occupational Safety and Health Administration (OSHA) Permissible Exposure Limits (PELs)
- NIOSH Immediate Dangerous to Life and Health values (NIOSH IDLHs) (<u>documentation for those values</u>)
- · A physical description of the agent with chemical and physical properties
- Measurement methods
- Personal protection and sanitation recommendations
- · Respirator recommendations
- Information on health hazards including route, symptoms, first aid and target organ information.
- 5 This screen displays 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. Click the Index of Chemical Names, Synonyms, and Trade Names link.



CD-ROM Start page

NIOSH Pocket Guide

- Introduction
- Index of Chemical
 Names, Synonyms and
 Trade Names
- Index of Primary Chemical Names
- Index of CAS Numbers
- Index of RTECS
 Numbers
- · Appendices

Other Databases Important Information

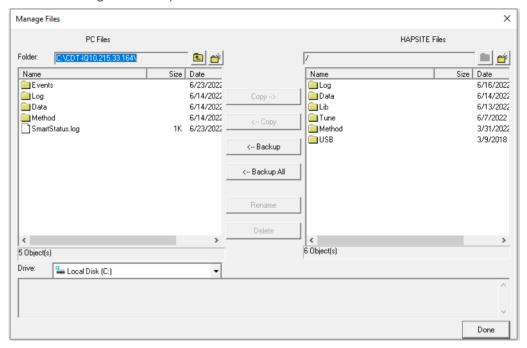
6.2.1.4 Manage Files

The Manage Files function transfers files between HAPSITE CDT and the laptop.



Manage Files

Double-clicking this icon opens the window shown below.



The **Copy** --> option allows methods only to be copied from the laptop to HAPSITE CDT. The <-- **Copy** option allows methods and data files to be copied from HAPSITE CDT to the laptop.



Data files can only be transferred from CDT IQ to the laptop; they cannot be transferred from the laptop to HAPSITE CDT. Method files can be transferred both from HAPSITE CDT to the laptop and from the laptop to HAPSITE CDT.

The <-- Backup option will back up the desired files from HAPSITE CDT onto the laptop. The <-- Backup All option will back up all of the Data, Method, and Tune files, along with a number of system specific configuration files from HAPSITE CDT onto the laptop. The Backup options will compress the files to a .tgz file, while the Copy option maintains the .hps or .mth file extensions.



Renaming and/or deleting files are Advanced user functions.

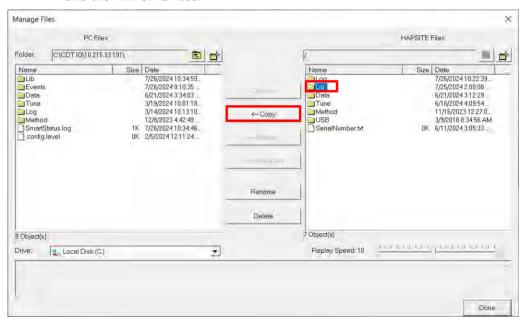
1 To rename a folder or file, click on the desired file and click Rename. A new window is displayed. The former name will be displayed on top and a box for typing in the new name will be displayed beneath it. Type in the new name and click OK.

2 The **Delete** option removes folders or files. To delete folders or files, highlight the desired folder or file and click **Delete**. After **Delete** is clicked, a confirmation window is displayed. Click **Yes** to delete the folder or file.

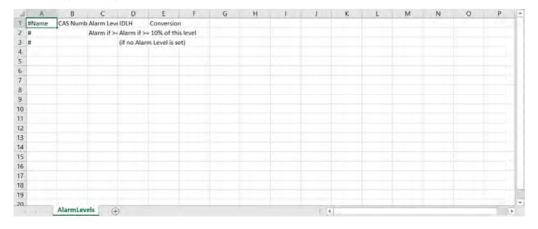
3 To exit the screen, click Done.

6.2.1.4.1 Set Alarm Levels

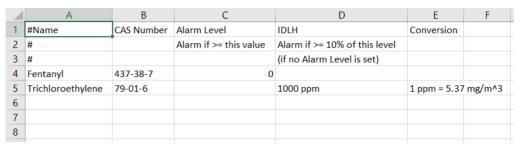
- 1 Open CDT IQ and make sure you are connected to the instrument. Confirm by clicking on the sensor at the bottom of the CDT IQ window.
- 2 Double-click the **Manage Files** icon to open the Manage Files dialog box. The PC files are listed on the left and the HAPSITE files are listed on the right.
- 3 Click on the Lib folder in the HAPSITE files and click <-- Copy to copy the folder to the PC files. When the Overwrite Files prompt opens, select Yes to All.
 - ⇒ The contents of the Lib folder should now be the same for both the PC files and the HAPSITE files.



4 Open Windows File Explorer and navigate to the directory on the C drive where the CDT IQ PC files are saved (for example, C:\CDT IQ\10.215.33.191\Lib). Double-click on the file AlarmLevels.csv to open the file in Excel.



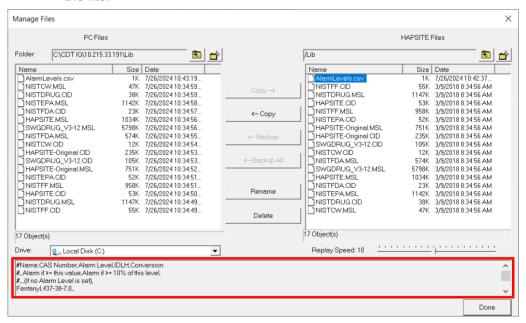
5 The columns show the compound name, CAS Number (with hyphens), Alarm Level, IDLH (Immediate Danger of Life and Health), and Conversion. Enter the desired compounds and alarm levels. To set an alarm when any amount of a compound is detected, enter 0 (zero) in the Alarm Level column for that compound.



- **6** After entering the desired compounds and alarm levels, save and close the file.
- 7 Return to the Manage Files dialog box and select AlarmLevels.csv from the PC files. Click Copy --> to copy the file over to the HAPSITE files. When the Overwrite Files prompt opens, select Yes.



⇒ The contents of the Lib folder should now be the same for both the PC files and the HAPSITE files. You can view the contents of the AlarmLevels.csv file by selecting the file in the HAPSITE files column. The preview window at the bottom of the Manage Files dialog box will display the contents of the file.



6.2.1.5 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.



6.2.1.5.1 Status

After double-clicking the **Status** icon, the Properties window opens on the **Status** tab. This screen displays the current temperatures and pressures of the key components in HAPSITE CDT. The battery status and internal standard canister status are also displayed.

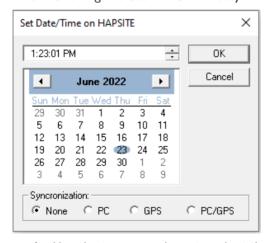


6.2.1.5.2 HAPSITE Time Zone

The **HAPSITE Time Zone** tab allows the user to set the time on HAPSITE CDT. Setting this parameter ensures that the data files are stamped with the proper date and time.



- 1 To set the time, select the desired time zone from the drop-down menu.
 - ⇒ Click **Select GMT** if Greenwich Mean Time is desired.
- 2 Clicking Set HAPSITE Date/Time to PC Date/Time automatically synchronizes HAPSITE CDT to the laptop date and time.
- 3 Clicking the **Set HAPSITE Date/Time** button displays a date/time window.



- 4 Use the top arrow keys to select the correct time.
- **5** To select the proper date, use the arrow keys below the time to scroll to the current month. Click on the current date.
- **6** The **Synchronization** option synchronizes the time on HAPSITE CDT to the PC, GPS, or both. If synchronization is not required, click **None**.
- 7 When all the parameters have been set, click **OK**.

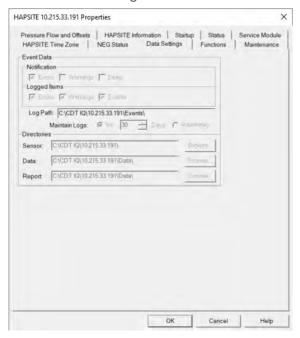
6.2.1.5.3 NEG Status

The NEG is a consumable item. **NEG Status** reports the number of hours that have been consumed. Refer to NEG Info $[\triangleright 35]$ and see the warnings and cautions in Maintenance $[\triangleright 219]$.



6.2.1.5.4 Data Settings

The Data Settings tab displays the Event Data and the Directories. The Event Data allows the user to set the type of Notifications that will be displayed on the HAPSITE CDT front panel and laptop. An error occurs when a warning has been displayed but the warning has been ignored. If Error is checked, an error message is displayed. If Warning is checked, a warning message is displayed, when a problem, such as high pressure, arises. If Beep is checked, HAPSITE CDT makes an audible sound when an error or a warning occurs.



When an error, warning, or event occurs, HAPSITE CDT stores information about the occurrence and date it occurred. The pathway where this data are stored is displayed. The desired number of days for log storage can be set or the logs can be stored indefinitely.

The **Directories** folder allows the file pathway for HAPSITE CDT to be set. All data and information that have been created by HAPSITE CDT are stored in the folder that was selected in the **Sensor** pathway. All data files that have been created by HAPSITE CDT are stored in the folder that was selected by the **Data** pathway. All report files, which are text files of the quantitative, qualitative, and summary reports, are stored in the **Report** pathway.

6.2.1.5.5 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**.



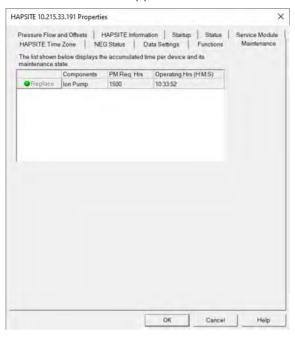
For information on the **ID Unknowns** function, see ID Unknowns [> 203]. For information on the **Overlay** function, see Chromatogram Overlay [> 103].



Entering the advanced access level will provide additional function options.

6.2.1.5.6 Maintenance

The **Maintenance** tab displays the number of hours that the ion pump has been running. It also displays the recommended preventive maintenance guideline of 1500 hours. If it needs to be replaced, the **Replace** button activates. See How to Contact Customer Support [\triangleright 224].



6.2.1.5.7 Pressure Flows and Offsets

The **Pressure Flows and Offset** tab displays various pressures that have been set by the factory.



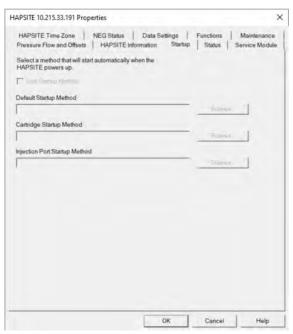
6.2.1.5.8 HAPSITE Information

The HAPSITE Information tab provides general information regarding the HAPSITE CDT 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 Software Version, HAPSITE Serial Number, GC Firmware Version, MS Firmware Version, and the HAPSITE name.



6.2.1.5.9 Startup

The **Startup** tab allows the user to select startup methods for the instrument to automatically prepare upon startup with appropriate sampling configuration installed.



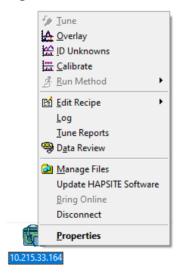
6.2.1.5.10 Service Module

The Service Module can be used as an alternate vacuum source or as a troubleshooting accessory. For more information on using the Service Module, see Maintenance [> 219] or refer to the Service Module Operating Manual, available from the INFICON website.



6.2.1.6 HAPSITE CDT Sensor Icon

Right-click on the HAPSITE CDT Sensor icon to display the following menu.



The first five options perform the same functions as their counterparts located in the System Setup screen. The **Edit Recipe** option performs the same functions as Method Editor. Refer to HAPSITE Icons [> 90] for more information.

The **Log** and **Tune Report** options can also be accessed through the **File** menu. Refer to File Menu [> 67] 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 HAPSITE Icons [▶ 90] for more information.

6.2.1.6.1 Update HAPSITE Software

Periodically, a software update for HAPSITE CDT 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 released with each software update, as instructions for each update may vary.



All update files will have the .swu extension.

For more information about software updates, please contact INFICON for additional information.

6.2.1.6.2 Bring Online

If HAPSITE CDT is not communicating when connected through the Ethernet cable, clicking on the **Bring Online** option will attempt to reestablish communication. If the connection has been manually disabled, clicking **Bring Online** will reenable the connection. When the connection is active, the **HAPSITE Sensor** icon will not be overlaid with an *X*.

6.2.1.6.2.1 Communication Messages

If the laptop is not communicating with HAPSITE CDT, there are three types of X's that may be displayed.



10.215.33.202

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



10.215.33.19

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



10.215.33.202

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

6.2.1.6.3 Disconnect

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

NOTICE

The laptop and HAPSITE CDT should always have the most current version of the software installed. Verify that the unit software and CDT IQ software have the same version number. Do not try to run incompatible versions of software together (for example, CDT IQ 1.05 and HAPSITE CDT Analytical Module software 1.16). CDT IQ will detect a version mismatch and display an error message.

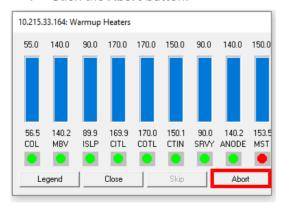
6.2.1.7 HAPSITE Icons

Icon	Description
ĪQ	Start CDT IQ software from the desktop.
System	System properties (Communications, Display, Miscellaneous).
10.215.33.137	HAPSITE CDT sensor properties. Right-click to access menu. Icon name will show IP address of the sensor.
Data Review	Accesses all saved data files.
Run Method	Accesses methods to initiate a run.
NIST NIST	Accesses the NIST software and library.
Safety DB	Accesses the NIOSH database.
AMDIS	Accesses the AMDIS software and library.
Manage Files	Allows transfer of files between HAPSITE CDT and laptop.
Method Editor	Allows editing and creating methods.
Service Module	Accesses the Service Module when attached.

Icon	Description
Status	Accesses HAPSITE CDT properties.
Tune	Accesses the HAPSITE CDT tune program.
<u>Li</u>	Accesses Data File information.
	Returns the current screen to the System Setup screen.
T	Displays the software version of CDT IQ software that is installed on the laptop.
44444	Accesses the Calibrate function.
MAN I	Accesses the ID Unknowns function.
Liludi.	Accesses Chromatogram Overlay function.
FILE FILE	Navigates through files in Data Review.
PEAK PEAK	Navigates through peaks in Search for Peaks.
PEAK	Returns to the complete full chromatogram (TIC) display in Search for Peaks.

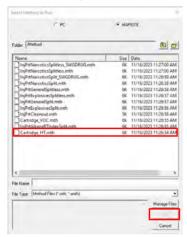
6.2.2 Select a New Method

1 Click the Abort button.

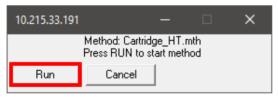


2 Double-click on the Run Method icon. A dialog is displayed for selecting the desired method.

- 3 Double-click the desired folder.
 - ⇒ Use the buttons at the top of the dialog box to choose the methods on HAPSITE CDT.
- 4 Choose and click the desired method that matches the sampling configuration, then click OK.



- 5 The software will check the pressure in the gas canisters and heat up all necessary components.
- **6** When it is finished heating, a prompt appears to indicate HAPSITE CDT is ready to run a sample. Click **Run**. For detailed instructions, see Quick Reference SOP: Cartridge Analysis [> 208].



6.2.3 Data Review

This section provides information regarding the analysis of data samples. Topics include chromatogram overlay, opening data files, compound identification using the AMDIS and NIST Libraries, overviews of all data review menus, and chromatogram subtract.

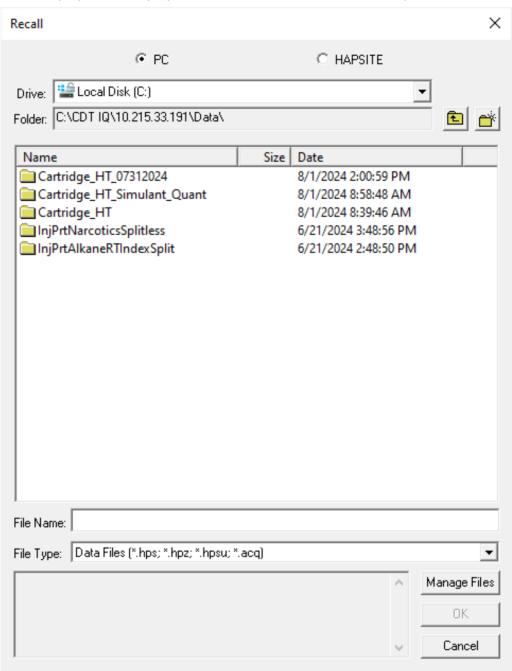
6.2.3.1 Accessing the Data Review Feature

The Data Review feature can be accessed as follows:

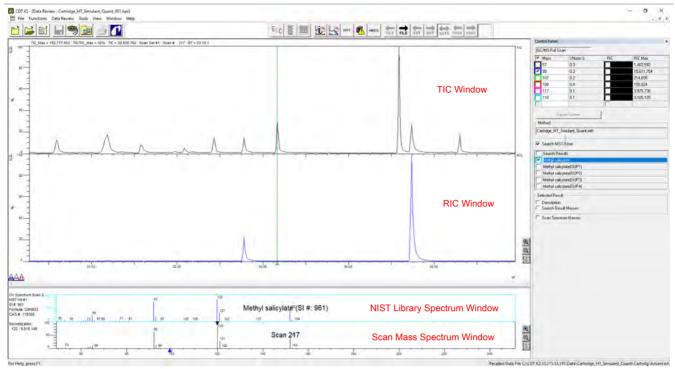


- 1 Double-click the Data Review icon.
- 2 Alternately, right-click the HAPSITE Sensor icon. Click Data Review.

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 CDT front display and the laptop was not connected at the time of sample collection.



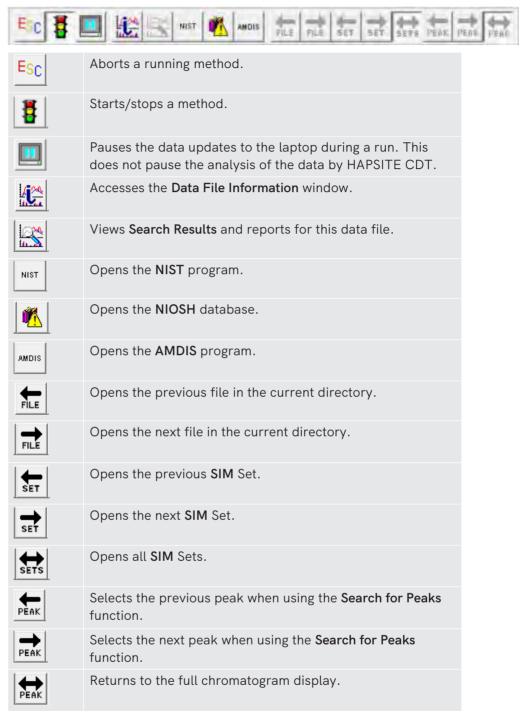
- 4 Navigate to the desired data file and double-click on the data file.
 - ⇒ HAPSITE CDT data file extensions end in .hps.
- 5 The Data Review window with the selected data file will be displayed. The Data Review window is divided into four sections, as shown below.



TIC window	The total ion chromatogram, which is the total intensity of the mass fragments, is plotted in this window. Basic data analysis, such as background subtraction and peak identification, is also conducted here.
RIC window	The reconstructed ion chromatogram, which is the intensity of a specific mass fragment, is plotted in this window.
NIST Library Spectrum window	This window will display NIST matches if Search NIST/User is checked in the Control Panel .
Scan Mass Spectrum window	The mass spectrum generated from the sample, where the cursor is located, is displayed in this window.

6.2.3.2 Data Review Menus and Toolbar

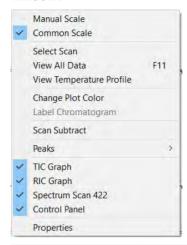
The Data Review toolbar is shown in the figure below.



6.2.3.2.1 Right-Click Menus within Data Review

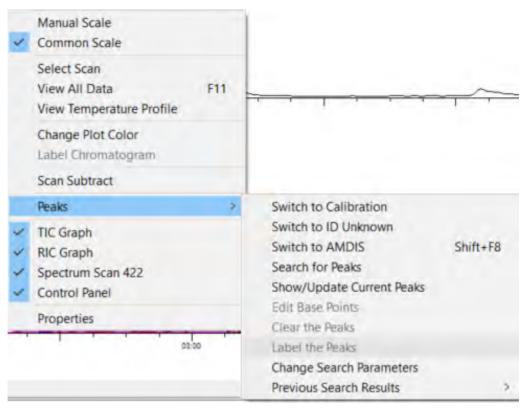
6.2.3.2.1.1 Right-Clicking in the TIC Window

The figure below shows the functions available when 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 pressing F11 .
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	See Peaks Menu [▶ 97].
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 Properties Menu [> 98].

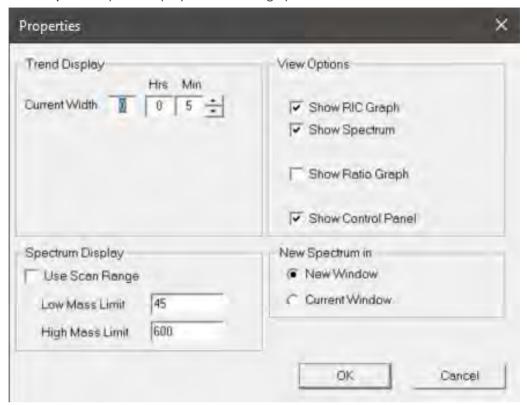
6.2.3.2.1.1.1 Peaks Menu



Switch to Calibration	Opens the Calibrate function. See Calibration [▶ 188].
Switch to ID Unknowns	Opens the ID Unknowns function. See ID Unknowns [> 203].
Switch to AMDIS	Opens the AMDIS program. Refer to Analyzing Data Using AMDIS [\triangleright 119].
Search for Peaks	Searches the chromatogram for peaks. Performs the same function as Show/Update Current Peaks . Refer to Show/Update Current Peaks [> 129].
Show/Update Current Peaks	Searches the chromatogram for peaks. Refer to Show/Update Current Peaks [\triangleright 129].
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. See Set Up a Quantitative Search [▶ 171].
Previous Search Results	View results from a previous search (menu of previously opened data files).

6.2.3.2.1.1.2 Properties Menu

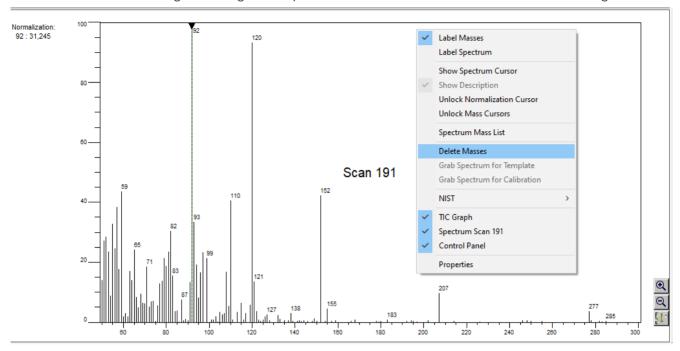
The **Properties** option displays the following options:



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 CDT will display masses in the spectrum above this limit.
High Mass Limit	HAPSITE CDT will display masses in the spectrum below this limit.

6.2.3.2.1.2 Spectrum Window

Right-clicking in the Spectrum window accesses the menu shown in the figure below.



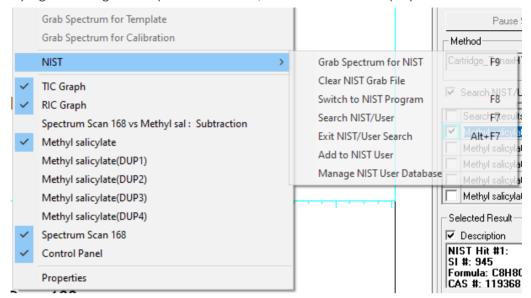
Label Masses	When checked, it displays the atomic weight of the mass fragments in the Spectrum window.
Label Spectrum	Displays a text box in order to manually label the spectrum.
Show Spectrum Cursor	Displays the spectrum cursor in the spectrum window.
Show Description	This displays the SI number, the NIST hit number, the formula, CAS number, and the normalization number next to the spectrum.
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 Calibration [> 188].
Grab Spectrum for Calibration	Used for Quantitative methods. See Calibration [▶ 188].
NIST	Allows the analyst to utilize the NIST database for qualitative identification of the displayed spectrum. Refer to Analyzing Data Using NIST [\triangleright 100].
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.



"Show Description" is only active if "Search NIST/User" is selected.

6.2.3.2.1.3 Analyzing Data Using NIST

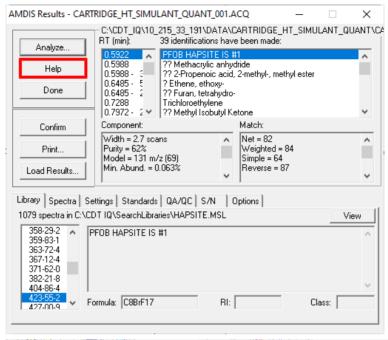
By right-clicking in the Spectrum window, the NIST menu is displayed.

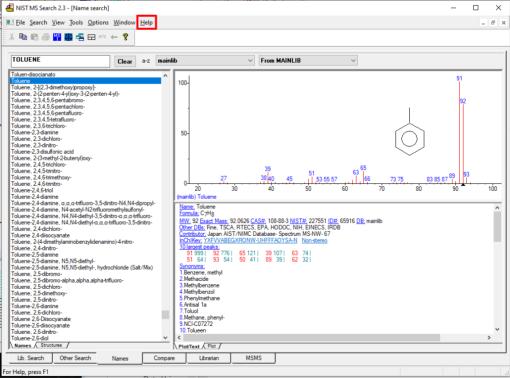


Grab Spectrum for NIST (F9)	This function will select a file to be exported into the NIST database program.
Clear NIST Grab File	Clears the list of previously selected files.
Switch to NIST Program (F8)	Starts the NIST database program and will export any selected files to NIST database program.
Search NIST/User (F7)	Starts the NIST Library search. Refer to NIST Library Searches [▶ 127].
Exit NIST/User Search (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.

6.2.3.2.1.4 NIST Database Program

The NIST database program is third-party software that is included with HAPSITE CDT. Instructions for using the software are located by selecting **Help** from the Menu selection in either the AMDIS or NIST program.

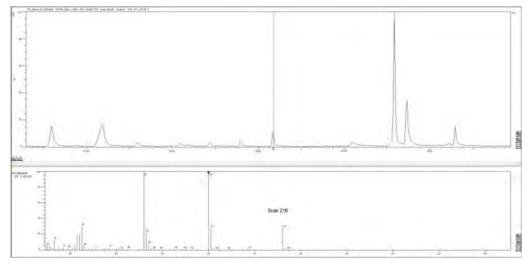




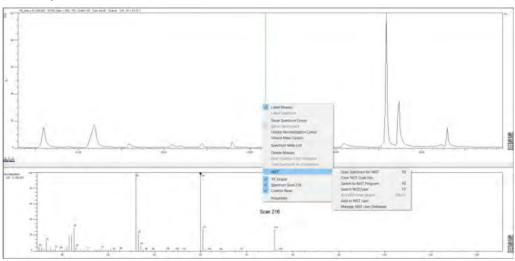
6.2.3.2.1.5 Grab Spectra for NIST

To export the spectrum to the NIST database:

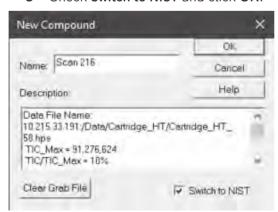
1 Double-click on the desired peak in the TIC/RIC window.



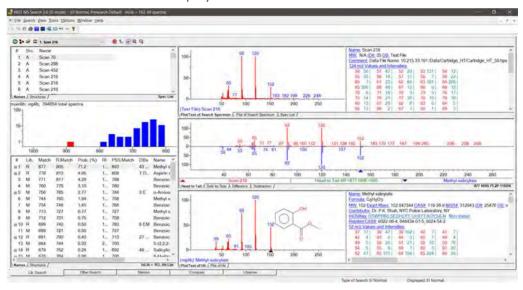
With the cursor in the Spectrum window, right-click and select NIST > Grab Spectrum for NIST.



3 Check Switch to NIST and click OK.



4 The identification is displayed on the screen.



6.2.3.3 Data Analysis Tools

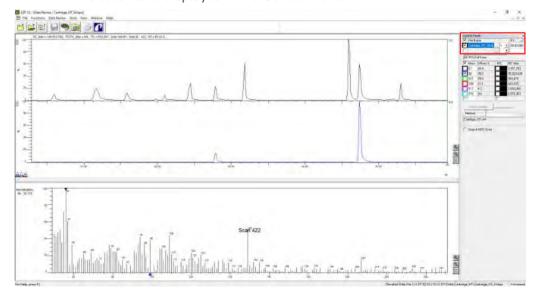
6.2.3.3.1 Chromatogram Overlay

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.



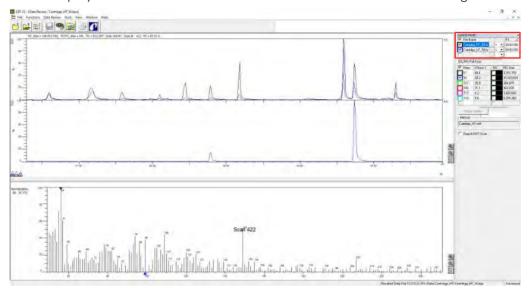
- **2** Follow the Data Review instructions in order to locate the desired file; see Accessing the Data Review Feature [▶ 92].
 - ⇒ The data file is displayed in the Control Panel.



3 Click the icon displayed below in the row below the data file.



- 4 Follow the file selection procedure that was used in Step 2.
- **5** Both chromatograms are displayed in the chromatogram window. The color displayed in the check box correlates with the color of the chromatogram.

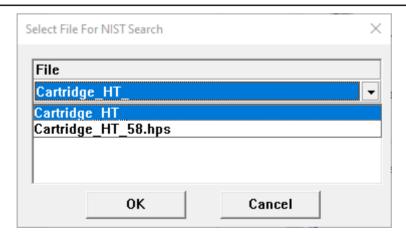




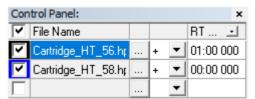
The mass spectrum is displayed for the highlighted file.



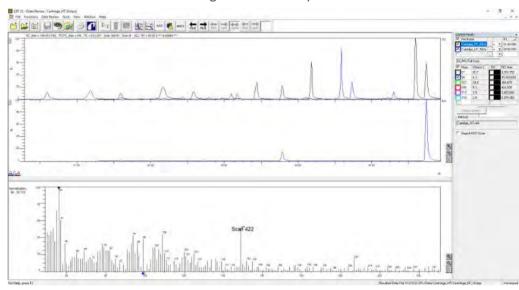
A NIST search can be performed on either chromatogram. Select "Search NIST/User" (refer to NIST Library Searches [127] for instructions) and select the desired file from the drop-down menu. The NIST identification is displayed for the highlighted file.



6 Peaks can be aligned by retention time for further comparison. Determine the time difference between the peaks being compared. The chromatogram is shifted the desired amount of time by selecting + or - and typing in the time difference.



7 Press Enter. The chromatogram will shift by the time selected.



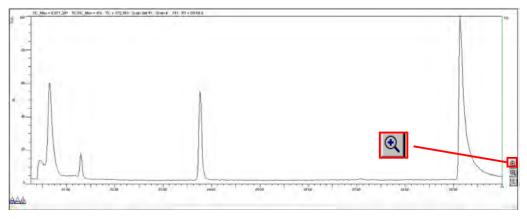
To close the **Chromatogram Overlay** feature, uncheck the box located to the left of the data file's name.

6.2.3.3.2 Zoom Function

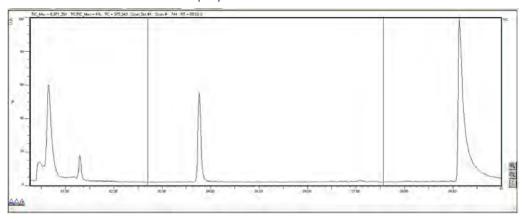
6.2.3.3.2.1 Using the Zoom Function in the TIC/RIC Window

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

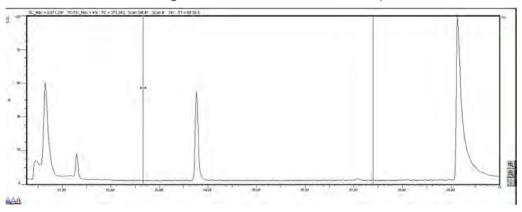
1 Click the **Zoom** icon.



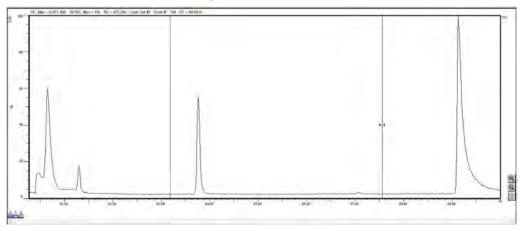
2 Two vertical lines are displayed.



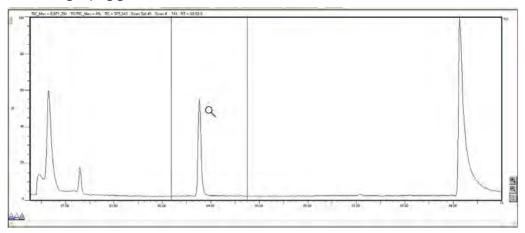
3 Hover the cursor over one of the lines. The cursor becomes a double-sided arrow. Click and drag the line to move it to the desired point.



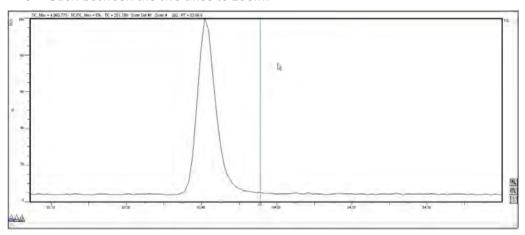
4 Hover the cursor over the other line. The cursor will again become a double-sided arrow. Click and drag the line to move it to the desired point.



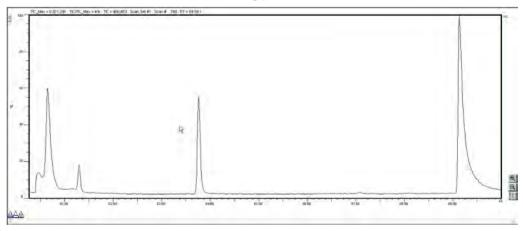
Move the cursor between the two vertical lines. The cursor will become a magnifying glass.



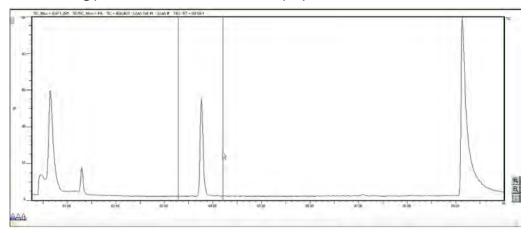
6 Click between the two lines to zoom.



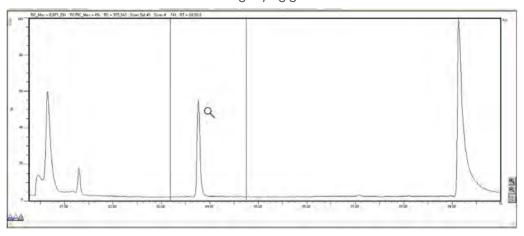
7 Alternately, a zoom can be completed by clicking and holding the left mouse button at the desired zoom starting point.



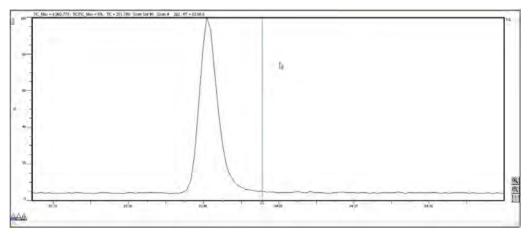
8 Continue to hold the left mouse and drag the mouse to the desired zoom ending point. Two vertical lines are displayed.



9 Release the left mouse button. Move the cursor in between the two vertical lines. The cursor becomes a magnifying glass.

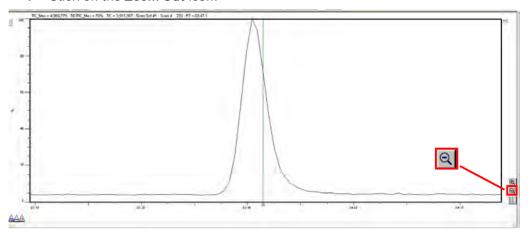


10 Click between the lines to zoom.

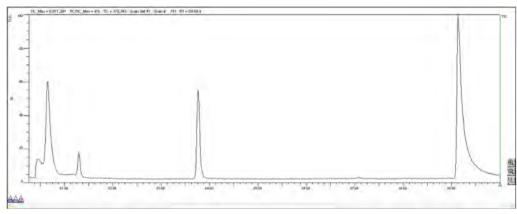


6.2.3.3.2.2 Zoom Out

1 Click on the **Zoom Out** icon.



2 The screen will return to the expanded view.

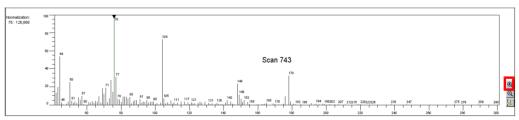


3 Alternately, press F11 to return to the expanded view.

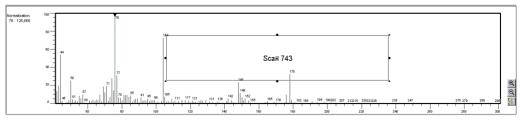
6.2.3.3.2.3 Spectrum Zoom

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

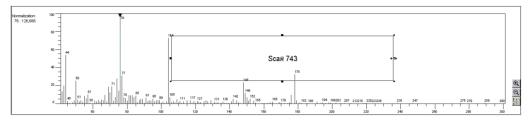
1 Click the Zoom In icon.



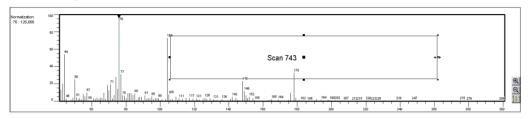
2 A rectangle is displayed in the **Spectrum** window.



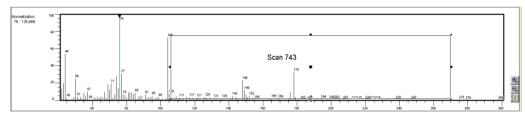
3 Hover the cursor over a side of the rectangle. The cursor becomes a double-sided arrow.



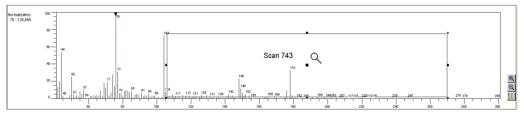
4 Drag the side to the desired end zoom point.



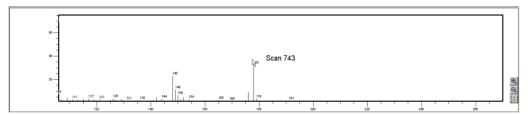
5 If necessary, repeat with the other sides of the rectangle in order to adjust the desired zoom area.



6 Move the cursor into the center of the rectangle. The cursor becomes a magnifying glass.



7 Click inside the rectangle to zoom.



6.2.3.3.3 Displaying Reconstructed Ion Chromatograms (RIC)

RIC plots are used to locate specific compounds in a chromatogram. An RIC plot of the top three or more mass fragments can help locate the peak of interest. Follow the instructions below to create an RIC plot.



The NIST program uses the term "peak" instead of "mass fragment." However, the terms are synonymous.

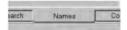
Alternately, double-clicking on a mass in the Scan window will automatically insert the selected mass in the Control Panel table and display the RIC for the selected mass.

When the box in the Control Panel labeled -RIC is checked, the TIC/RIC window displays the TIC minus the RIC selected.

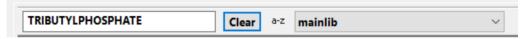
1 Either from the System Setup screen or the Data Review screen, double-click on the **NIST** icon.



2 Click on the Names tab at the bottom of the NIST screen.



3 Enter the name of the compound in the box on the top left of the screen (for example, tributyl phosphate).



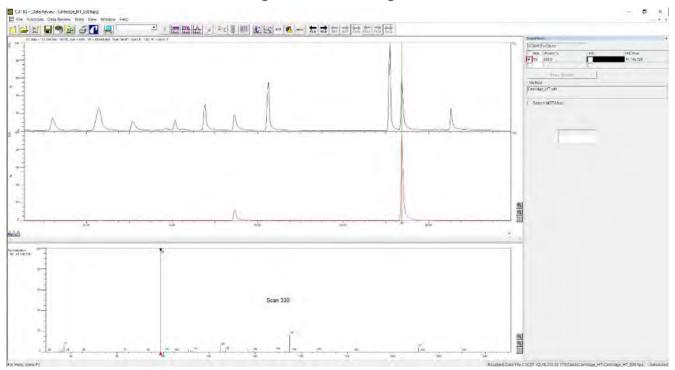
4 In the bottom-right box, in the Values and Intensities section, take note of the largest mass peaks that are in the scan range of the current method.



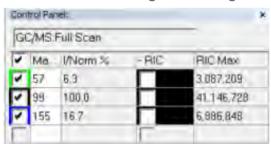


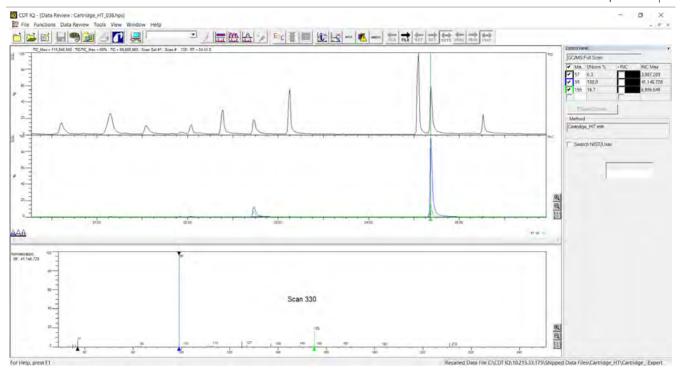
Mass fragments are listed in order from the smallest to the largest. For example, tributyl phosphate's largest mass fragments in the scan range of this method are masses 99, 155, and 57.

- **5** Minimize the NIST window and return to the **Data Review** screen displaying the chromatogram.
- 6 Enter the largest mass fragment, 99 for tributyl phosphate, into the Control Panel underneath the Mass column. Press Enter. The RIC plot is displayed underneath the TIC window. A new row will be created in the Control Panel for entering additional mass fragments.



7 Enter the next largest mass fragments into the Control Panel.

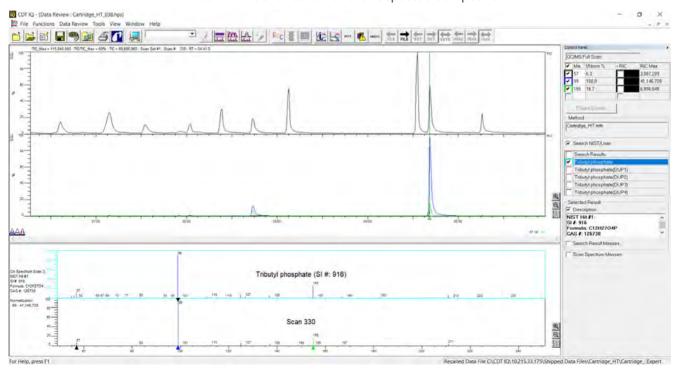






This RIC window can be closed by unchecking the masses selected in the Control Panel.

- 8 Alternately, click on the desired mass fragments in the Spectrum window to create a RIC plot.
- 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.





In this example, the largest mass fragment is 99. This is the highest RIC plot peak. The smallest mass fragment was 57. This is the lowest RIC plot peak.



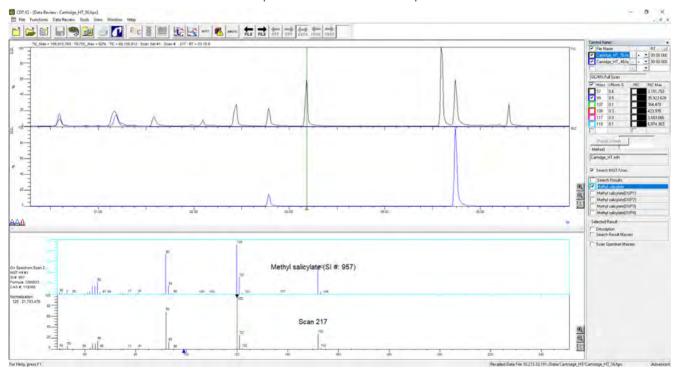
There may or may not be a peak present in the TIC window.

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.

6.2.3.3.4 Chromatogram Subtract

This feature shows the difference between two chromatograms' TIC. This is generally used to subtract the blank from the sample and verify the presence of a compound of concern.

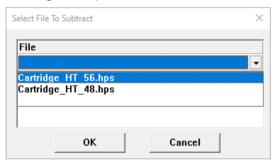
- 1 Overlay the desired chromatograms by using Chromatogram Overlay. Refer to Chromatogram Overlay [▶ 103].
- 2 Select the peak for the desired compound. Record the TIC.



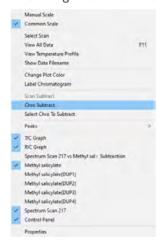
3 Right-click on the chromatogram. Click Select Chro to Subtract.



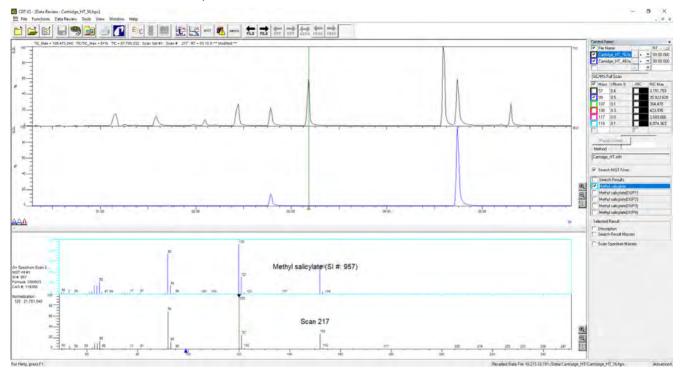
4 Select the desired file for subtraction from the drop-down menu. This will generally be the file for the blank.



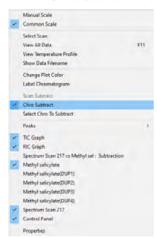
5 Right-click on the chromatogram. Click Chro Subtract.



6 The desired chromatogram is subtracted. Note the new TIC of the selected peak.



7 To return to the previous view, right-click on the chromatogram and click Chro Subtract from the menu to deselect.



6.2.3.4 Reports

1 To access data reports, double-click the View Search Results icon on the Data Review screen.



- 2 Alternately, View Search Results may be accessed from the Data Review menu.
- **3** There are a maximum of three reports available, depending on how the method was configured.
 - ⇒ The Summary report provides an overview of the Qualitative and/or Quantitative reports.

4 All three reports can be exported to Excel for further analysis by clicking on the Export to Excel button.

The Summary report includes:

- Date
- Time
- Method name
- · Method description
- · GPS info
- Analyte identification
- · Retention time
- Fit (see Analyzing Data Using AMDIS [▶ 119])



Concentration will be present if in the **Summary** report if using a calibrated library and those chemicals are detected.



The Qualitative report 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 Analyzing Data Using AMDIS [▶ 119])
- · CAS number



The Quantitative report 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
- · Scan number
- Internal standard
- · Retention time
- Number of hits (possible identifications)
- Area
- · Percent area
- Analyte identification
- Formula
- Fit (see Analyzing Data Using AMDIS [▶ 119])
- Purity

- CAS number
- · Concentration with units
- Response Factor Correction (RFC)

• The flag, which provides the reason that the compound was not identified.





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

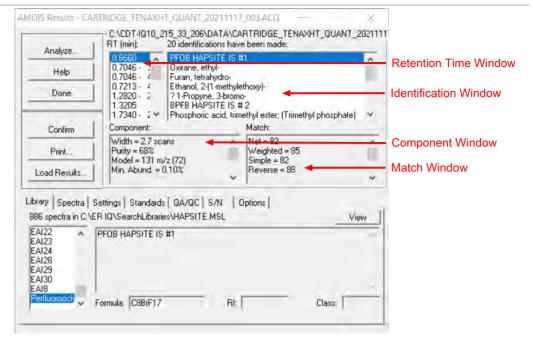
6.2.3.5 Analyzing Data Using AMDIS

AMDIS is an acronym for Automated Mass Spectrum Deconvolution and Identification System, a tool that was developed by the National Institute of Science and Technology (NIST). HAPSITE CDT uses an onboard library, **HAPSITE.msl**, and the AMDIS deconvolution algorithm to make identifications. The HAPSITE CDT onboard library contains approximately 1000 chemicals, and enables the identification of complex mixtures, including co-eluting chemicals. The onboard library is user configurable and can be updated to include several thousand compounds. The laptop AMDIS software can be accessed through CDT IQ, enhancing the quality of data analysis by including access to the NIST mass spectral library.

► Click on the AMDIS icon.



⇒ The following window is displayed.



The results screen includes:

Retention time window	AMDIS uses a decimal time format. Multiply the numbers after the decimal point by 60 seconds 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 fit is between 70 and 79. If two question marks are displayed, the fit is between 60 and 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 minimum abundance (min. abund). 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	Sets the library pathway, which may be necessary when reinstalling the CDT IQ program. See Setting the AMDIS Pathway [> 121].
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 Confirm Screen in AMDIS [> 126] 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 View Function in AMDIS [> 125].

6.2.3.5.1 Setting the AMDIS Pathway

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

- 1 Click on Analyze....
- 2 Click on Target Library.
- 3 Click **Select New** to change the library pathway.
- 4 The HAPSITE.msl is located at the following pathway:
 C:\CDT-IQ\SearchLibraries. If custom libraries are used, they must be located in this directory. Highlight the library and click Open.
- 5 Click Save.
- 6 Click Run.

6.2.3.5.2 Setting the AMDIS Scan Direction

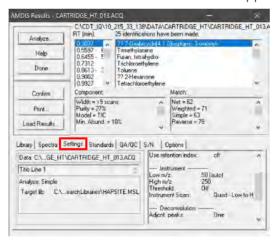
HAPSITE CDT mass spectrometer currently scans from low mass to high mass range. The default AMDIS scan direction for INFICON instruments is from high mass to low mass range. To optimize AMDIS search results with HAPSITE CDT, AMDIS scan direction should be set to scan from low mass to high mass range.

To check the selected mass spectrometer scan direction in AMDIS:

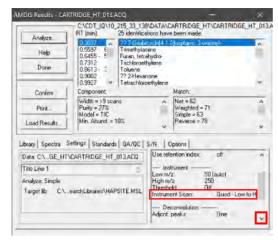
1 With a data file open, click on the AMDIS icon.



2 The AMDIS results window will appear. Navigate to settings tab.

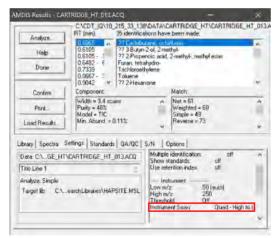


3 Scroll down and check that the Instrument Scan direction is low to high.

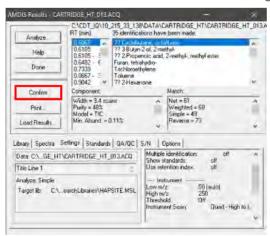


When switching between ER IQ and CDT IQ, the instrument scan direction in AMDIS may need to be switched to scan from the HAPSITE ER instrument scan direction (high to low) to the HAPSITE CDT instrument scan direction (low to high). To reset the scan direction:

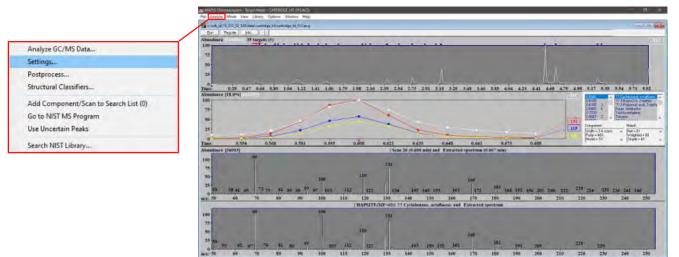
1 Confirm the Instrument Scan direction is set from high to low.



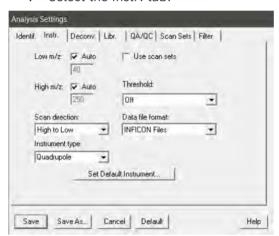
2 Click confirm. The AMDIS chromatogram target mode window will appear.



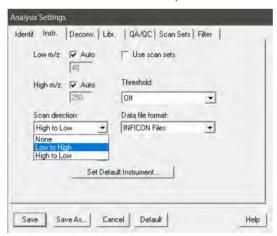
3 Navigate to the Analyze menu and select Settings.



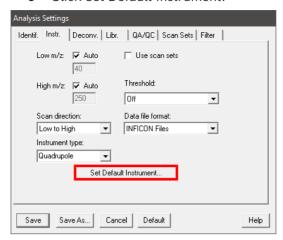
4 Select the Instr. tab.



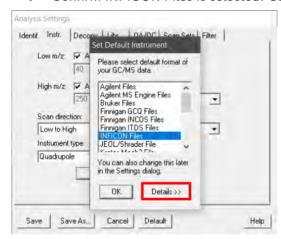
5 Under Scan direction, select Low to High.



6 Click Set Default Instrument.

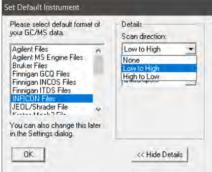


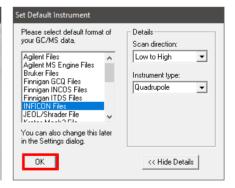
7 Confirm INFICON Files is selected. Click Details >>.



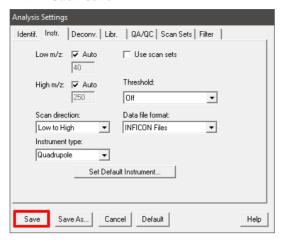
8 Under scan direction, select Low to High. Click OK.







9 Click Save.

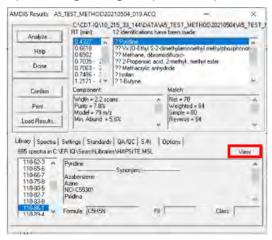


10 An AMDIS Analysis dialog window will appear. Click Yes.

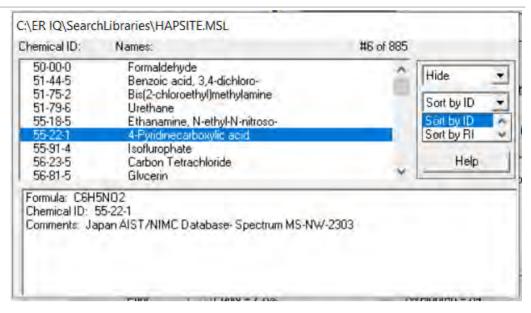


6.2.3.5.3 View Function in AMDIS

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**.



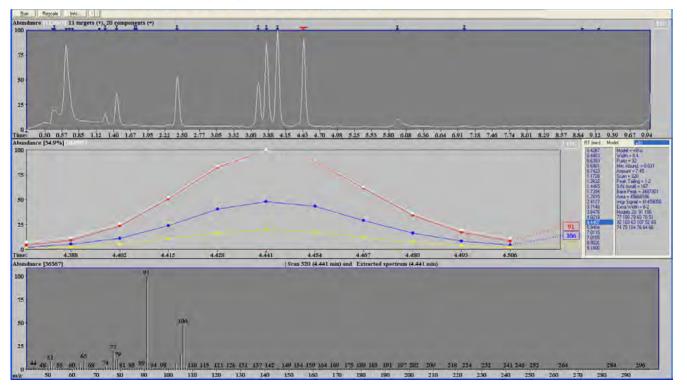
This function displays the components of the **HAPSITE.msl** library. This list can be sorted by retention index, name, or CAS number.



6.2.3.5.4 Confirm Screen in AMDIS

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

- 1 Click the **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.
- 3 If a peak has not been identified, click on the arrow above it. The arrow will turn red.



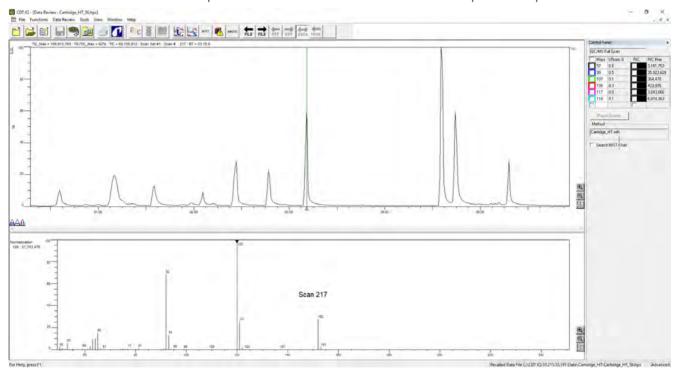
- 4 Click Analyze, then click Go to NIST MS Program.
- 5 The spectrum is exported to NIST. NIST will identify the unknown compound.

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

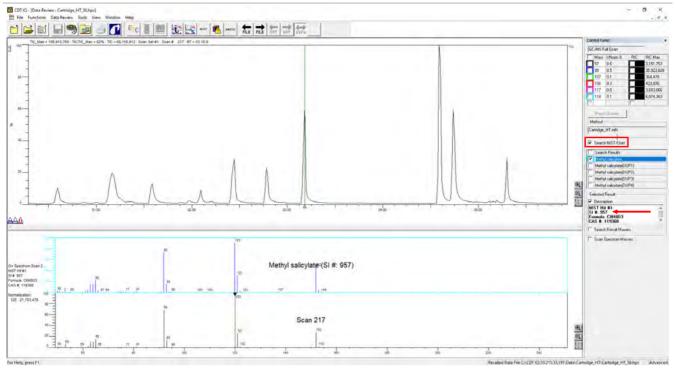
6.2.3.6 NIST Library Searches

The laptop will come preloaded with identification software from NIST's 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 similarity index (SI) number based upon purity and fit and the ratio of the intensities of the unknown spectra to the library spectra.

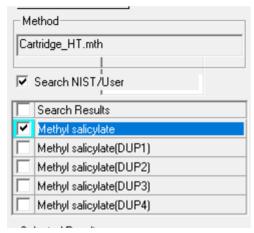
- ✓ Refer to Accessing the Data Review Feature [▶ 92] to open a data file.
 - 1 Double-click on the peak of interest. The green scan cursor will relocate to the peak. Use the arrow keys on the laptop to adjust the scan cursor. The optimal location of the scan cursor is at the apex of the peak.



- 2 Check the Search NIST/User box in the Control Panel. The library identification and the library spectrum will be displayed above the spectrum of the sample.
- 3 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.



The Search Results box shows 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 will be high.



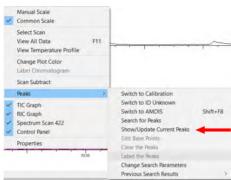
- **5** To view the spectrum for a different library identification, highlight the name of the desired compound.
- 6 If the **Description** box is checked, the highlighted hit, the SI, the formula, and CAS number are displayed.
- 7 If the Search Result Masses box is checked, the masses and relative intensities for the current scan are displayed as a table for the NIST library spectrum.
- 8 If the Scan Spectrum Masses box is checked, the masses and relative intensities are displayed as a table for the unknown spectrum.

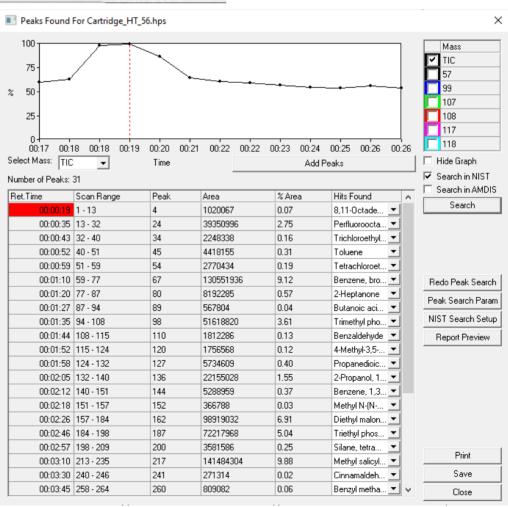
6.2.3.7 Current Peaks

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.

6.2.3.7.1 Show/Update Current Peaks

- 1 The Show/Update Current Peaks function is accessed by right-clicking on the chromatogram. Hover the cursor over Peaks and then click on Show/Update Current Peaks.
 - ⇒ The Show/Update Current Peaks window displays.





- 2 Check the Search in NIST box.
- 3 Click Search.
- 4 A NIST search is performed on the peaks that NIST has located. The **Hits** Found column is populated.
- **5** Each identification has a drop-down menu. Five hits are displayed in each menu.

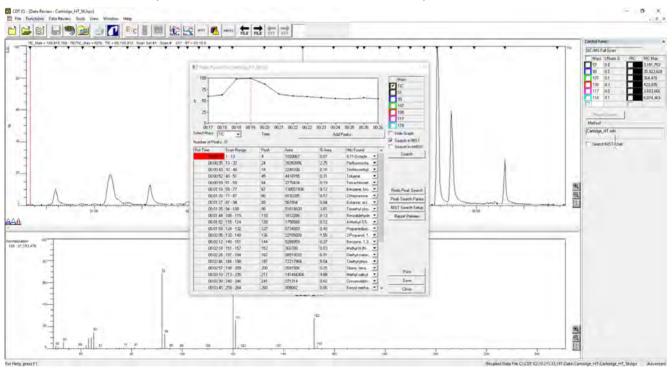
6 Check the Search in AMDIS box. The software will search the peaks using the AMDIS library. The AMDIS identification is located in the drop-down menu below the NIST hits.



This is not a true AMDIS search. AMDIS will not search the entire chromatogram. It will only search the peaks that NIST has located.

6.2.3.7.1.1 Show/Update Current Peaks Window Description

In the chromatogram beneath the **Show/Update Current Peaks** window, each detected peak is labeled with a black triangle. Pink dots appear at the base of each peak. These dots are used to determine the peak area.



On the **Show/Update Current Peaks** window, the highlighted peak is displayed with the dots along the peak representing each individual scan. The following is also 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 Range Tool [> 137].
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 Set Up a Quantitative Search [▶ 171] for more information.
NIST search parameters	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 NIST Search Setup [> 132] for instructions.
Report preview	The information in the Show/Update Current Peaks is displayed in a text format. See Show/Update Current Peaks [> 129] for instructions.

6.2.3.7.1.2 Peak Search Parameters

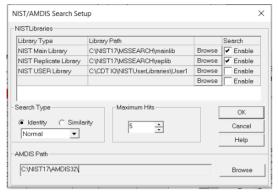
Some of the parameters for peak searching can be selected. These include the Min RIC Area, Min TIC Area, the Min and Max Width, the Mass Range, the Net Fit, the NIST library used for identification, and the number of identifications that are displayed by the NIST library.

Library name	The selected library will be used to make AMDIS identifications.
Maximum NIST hits	NIST will display the setpoint number of identifications.

6.2.3.7.1.3 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 the figure below.



To reset the NIST Main Library:

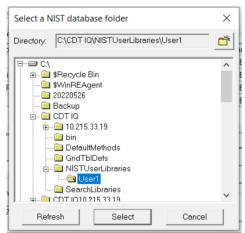
- 1 Click Browse....
- 2 Select the NIST Main Library from the folder displayed. Click Select to set the library.

To reset the NIST Replicate Library:

- 1 Click Browse....
- 2 Select the NIST Replicate Library from the folder displayed. Click Select to set the library.

To reset the **NIST USER Library**:

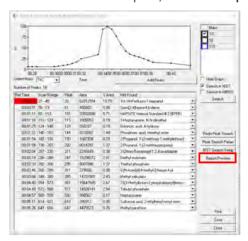
- 1 Click Browse....
- 2 Select the NIST USER Library from the folder displayed. Click Select to set the library.



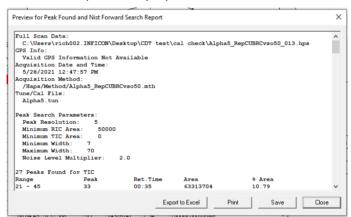
6.2.3.7.1.4 Report Preview

Report Preview reformats the Show/Update Current Peaks window into a text file.

1 To view the report, click the **Report Preview** button.



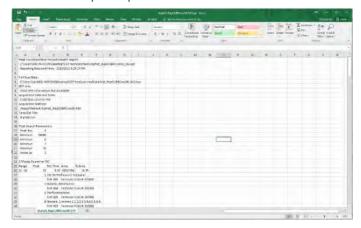
2 The report is displayed.



- **3** The report can be exported to Excel for further data analysis. Click **Export to Excel**.
- 4 The report will need to be saved before Excel will open. Click Save.



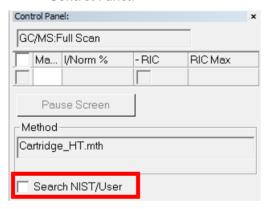
5 The report opens in Excel.



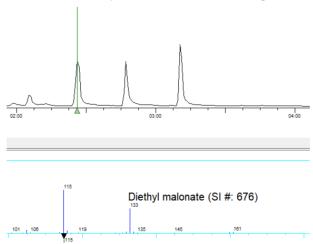
6.2.3.7.2 Background Subtract

Background Subtract will remove masses in the spectrum that are caused by background interference. Using Background Subtract will increase the Similarity Index (SI) number of the identification when the low SI number is a result of high background. An SI number below 700 is considered low, 700–800 is fair, 800–900 is good, and 900–1000 is excellent. Follow the instructions below to perform a Background Subtract.

Perform a NIST Library Search by checking the Search NIST/User box in the Control Panel.



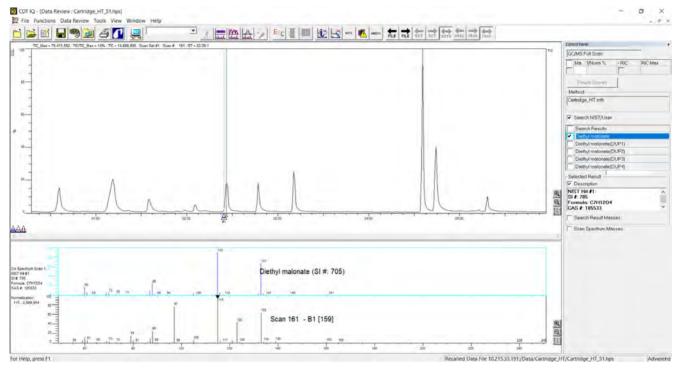
2 Select the peak of interest with the green cursor.



3 If the SI number is low and the background is high, select either of the blue **Background Select** triangles from the lower-left side of the chromatogram.



4 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.

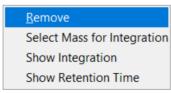


If the background on the opposite side of the peak differs from the subtracted background, a second background subtract can be used.



All background subtractions are indicated in the Spectrum window by the designation "Scan Number - B1(range) - B2(range)."

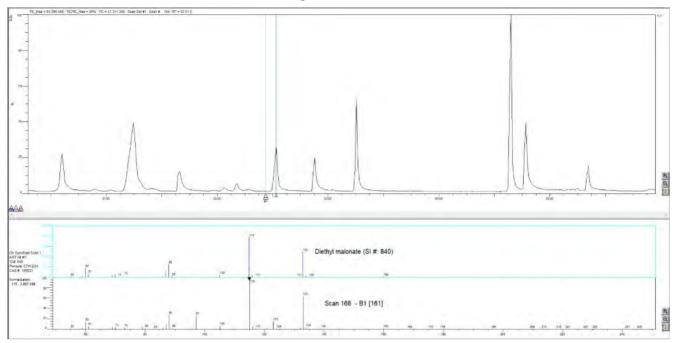
6 To remove Background Subtract from the chromatogram, place the cursor over the Background Select triangle, right-click, and select Remove.



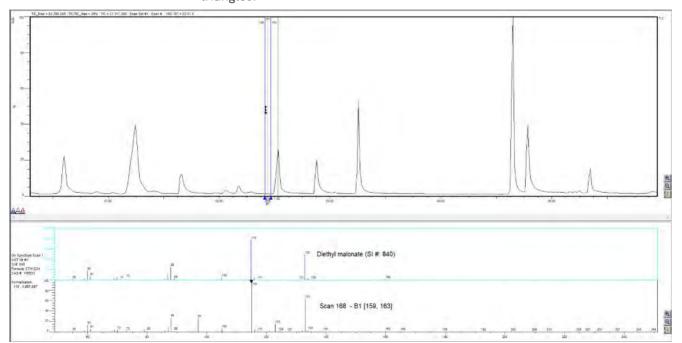
6.2.3.7.2.1 Background Subtraction Using a Range of Points

Background from a range of points can be subtracted, if desired.

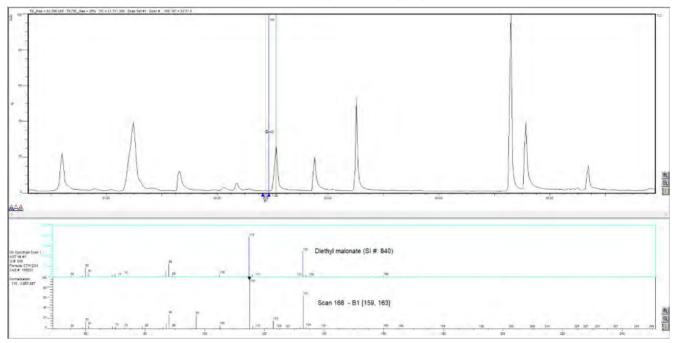
1 Click and drag the **Background Subtract** triangle near the peak of interest at the desired background location.



2 Hover the cursor 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 upward widens the background range. Moving the arrow downward narrows the range of the background. The width of the range is represented by two small blue triangles.



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.

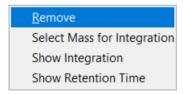




This procedure can be repeated by using the second "Background Subtract" triangle.

6.2.3.7.2.2 Additional Features of the Background Tool

By placing the mouse over a **Background Subtract** triangle and right-clicking, the following menu will be displayed:



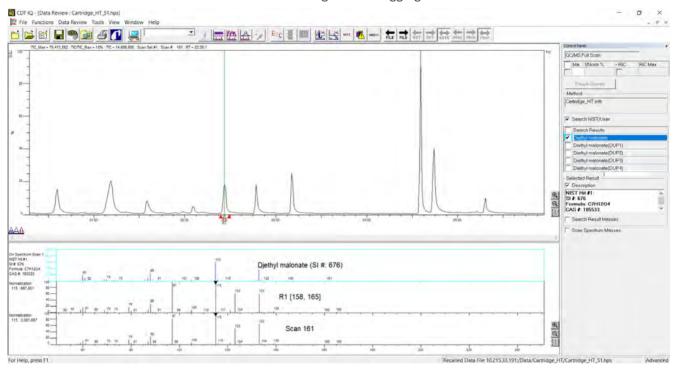
Remove	Removes the Background Subtract triangle.
Select Mass for Integration	Selects either the TIC or a mass fragment for integration for the range tool.
Show Integration	Displays the integration on the x axis for the range tool.
Show Retention Time	Displays the retention time on the x axis.

6.2.3.7.3 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**.

- Place the cursor on the red-striped triangle, which is the Range Tool. Leftclick, hold, and drag the triangle to the location where the scans should be averaged.
- 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 upward to widen a range. Moving the arrow downward narrows the range. The red range lines should intersect the peak sides at 50% of their height.
- 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.

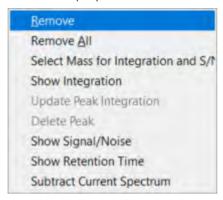




All ranges are indicated in the spectrum window by the designation "R1 [Range Start Scan, Range End Scan]."

6.2.3.7.3.1 Additional Features of the Range Tool

By moving the cursor over the **Range Tool** triangle and right-clicking, the following menu is displayed:



Remove	Removes the range cursor.
Remove All	Removes all of the range and background subtract tools in use.
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 Background Subtract [> 134].
Subtract Current Spectrum	Subtracts the spectrum at the point where the green scan cursor is located from the range.

624 Tune

6.2.4.1 Manual Tune Introduction

Manual tunes are a standard routine maintenance practice for HAPSITE CDT. During the manual tune process, known mass fragments are introduced into the mass spectrometer (MS). A passing tune will have these mass fragments at the proper mass positions, intensities, and ratios relative to each other.

The best practice is to tune HAPSITE CDT to ensure that the resulting spectra will match to what is expected in terms of mass assignment (m/z) and relative intensity (detector response) of the different fragments. A monthly manual tune check is recommended and will improve the accuracy of compound identifications. Performing a manual tune allows the user to check the health of the MS and adjust tune parameters as needed. Additional tune checks may be required if the system has been powered off for an extended period of time, been transported or moved, or experienced large temperature fluctuations.

HAPSITE CDT uses two gas-phase internal standards which contain mass fragments that span the mass range of interest. The internal standards are:

- 1-Bromoheptadecafluorooctane (perfluorooctyl bromide, PFOB)
- Bromopentafluoro benzene (BPFB)

6.2.4.2 Manual Tune Procedure

The following procedure outlines the steps in manually tuning HAPSITE CDT.

NOTICE

If performing this task for the first time, it is recommended to contact INFICON for support. See Service and Technical Support [> 224].

NOTICE

The Access Level must be set to Advanced to manually tune the instrument. Refer to Changing Access Levels [▶ 74].

- ✓ Confirm instrument is powered on and not in extended standby.
 - 1 Open HAPSITE CDT on the laptop.
 - 2 Click on the Tune icon in the toolbar.
 - 3 Select default.tun from the pop-up window.
 - 4 Click OK. It will take 10-20 seconds to initialize. During that time, the Emission and EM boxes turn green.



The NEG (non-evaporable getter) is consumed while Manual Tune is open.

5 Adjust the tune parameters until all values are within range. For additional guidance, see Manual Tune Variables [▶ 149].

6.2.4.3 Manual Tune Menus and Toolbars

6.2.4.3.1 Toolbar

Each Manual Tune toolbar icon is described below.



3 [‡]	Filament on/off	Turn the emission on or off.
ē×ē ē	Multiplier on/off	Turns the electron multiplier on or off.
ليليا	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.
Λ	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.

火	Mass calibration	Verifies and corrects the 10 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.
1	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	Save tune	Saves the tune file.
Load Tune	Load tune	Loads a new tune file and restarts tuning.

6.2.4.3.2 Tune Drop-Down Menu

The Manual Tune screen has an additional main drop-down menu, the Tune menu.

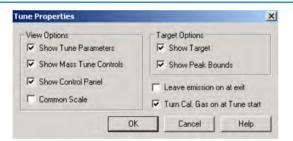


Mass Calibration	Verifies and corrects the 10 calibration masses for correct location within the mass range.
Noise Check	Scans a "quiet" mass range (no peaks) to determine the electronic baseline and threshold noise level.
Perform Tune Checkup	Runs a mass calibration and noise check.
Save Tune Parameters	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 .
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.
Auto Tune Tolerances	Sets the AutoTune Tolerance for mass resolution and mass axis position.

NOTICE

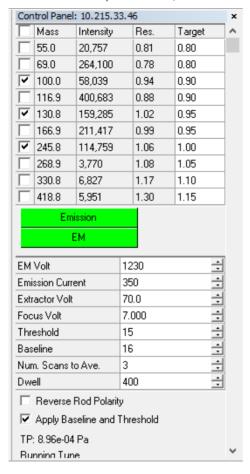
The Advanced tune functions should only be utilized under the direction of INFICON support personnel.



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 center 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.

6.2.4.3.3 Tune Control Panel

The **Tune Control Panel** is located on the right side of the screen and displays the individual mass peak scans, the measured intensity, and the resolution.

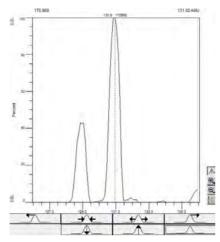


6.2.4.3.3.1 Tune Parameters

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.
Electron Multiplier (EM)	Turns the Electron Multiplier on and off. Green signifies that the electron multiplier is on.
EM Voltage	Increases or decreases the gain of the system. EM voltage should be set to a value between 1000 and 2000 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 300–400 (350 is typical).
Extractor Volt	Affects the efficiency of the ionizer. The Extractor Volt setting must be set to achieve maximum intensity for mass 117. Range is 70–90.
Focus Volt	Affects the efficiency of the ionizer. The Focus Volt setting must be set to achieve maximum intensity for mass 117. Range is -12 to 12.
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. Select the rod polarity that provides optimal performance at mass 117.
TP	The total MS pressure. Must be below 6×10^{-3} for instrument to operate.
Running Tune Base Peak Gain	Current measured Base Peak Gain (BPG).
Auto Resolve	Adjusts the resolution of all mass peaks to the target resolution.
Save Tune	Saves the tune file.
Mass Calibration	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.

6.2.4.3.4 Peak Scan Window

The **Peak Scan Window** can be used to manually tune the mass peak.



6.2.4.3.4.1 Peak Scan Window Control

	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.
Q	Zoom out	Returns the window to the original x -axis and y -axis scale.
10	Zoom out y axis	Returns the <i>y</i> axis to original scale.
×	y-axis scale	Increases or decreases the <i>y</i> -axis scale.

7	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.

6.2.4.3.5 Setting the Full Scan Range

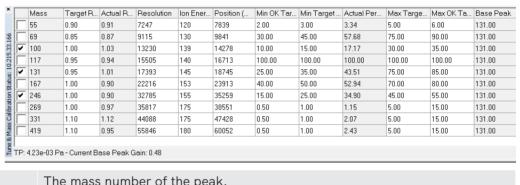
Placing the mouse cursor on the x axis of the full scan window and right-clicking displays the Set Full Scan Range window. This allows a custom scan range to be entered. The scan ranges can also be selected.



The EM voltage will automatically be decreased by 500 V (default) whenever a range below mass 45 is scanned.

6.2.4.3.6 Tune Status

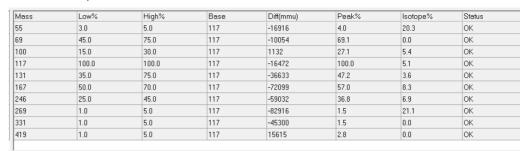
The **Tune Status** table located on the top-left portion of the manual tune screen shows the following parameters.



MassThe mass number of the peak.Target ResolutionTarget resolution at 10% peak height.Actual ResolutionMeasured resolution at 10% peak height.ResolutionResolution value; can be used to input a change in Resolution value.Ion EnergyIon Energy value; can be used to input a change in lon Energy value.Position (DAC Value)Current DAC setting for mass position.Scan WidthDisplays the points measured per amu.Min OK Target PercentageDisplays the minimum target percentage required for the mass peak to meet the OK LOW criteria.Min Target PercentageDisplays 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 PercentageDisplays the actual measured 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 PercentageDisplays the maximum percentage required for the mass peak to meet the OK High criteria.Base PeakDisplays the base peak, which is used to measure the mass peak percentage.		
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 maximum target percentage required for the mass peak to meet OK criteria. If the actual percentage required for the mass peak to meet OK criteria. If the actual percentage required for the mass peak to meet OK criteria. If the actual 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.	Mass	The mass number of the peak.
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 maximum target percentage required for the mass peak to meet OK criteria. If 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.	Target Resolution	Target resolution at 10% peak height.
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.	Actual Resolution	Measured resolution at 10% peak height.
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. 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.	Resolution	Resolution value; can be used to input a change in Resolution value.
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. 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.	Ion Energy	Ion Energy value; can be used to input a change in Ion Energy value.
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. 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.	Position (DAC Value)	Current DAC setting for mass position.
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. 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.	Scan Width	Displays the points measured per amu.
OK criteria. If the actual percentage is below the minimum percentage, the box will turn red. Actual Percentage Displays the actual measured 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.	Min OK 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.	Min Target Percentage	OK criteria. If the actual percentage is below the minimum percentage, the
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.	Actual Percentage	Displays the actual measured target percentage.
OK High criteria.	Max Target Percentage	OK criteria. If the actual percentage is above the minimum percentage, the
Base Peak Displays the base peak, which is used to measure the mass peak percentage.	Max OK Target Percentage	
	Base Peak	Displays the base peak, which is used to measure the mass peak percentage.

6.2.4.3.7 Mass Calibration Status

The dark gray Mass Calibration Status table displays the status of the last Mass Calibration. If the Mass Calibration is not displayed, select Mass Calibration from the Tune drop-down menu.

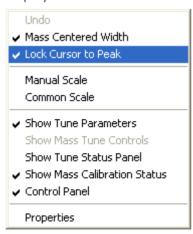


Mass Calibration from 2:26:32 PM 6/9/2022 - Base Peak Gain: 0.44

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 (menu)	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 locate mass peak within window.

6.2.4.3.8 Scan Window Menu

Place the mouse cursor in the **Peak Scan** or **Full Scan** window and right-click to display the menu shown in the figure below.



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.

6.2.4.3.9 Tune Status Window Menu

Place the cursor in the **Tune Status** panel or the **Mass Calibration Status** panel and right-click to display the menu shown in the figure below.



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.

6.2.4.4 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

6.2.4.4.1 Outputs

Base Peak Gain (BPG)

BPG is a measure of signal intensity. The ideal BPG value for HAPSITE CDT is 0.5 (ranging from 0.4 to 0.6).

55 69 100		0.91	7247	120	7839	2.00	0.00			1	
69	0.85			1.20	1000	2.00	3.00	3.34	5.00	6.00	131.00
100	0.00	0.87	9115	130	9841	30.00	45.00	57.68	75.00	90.00	131.00
100	1.00	1.03	13230	139	14278	10.00	15.00	17.17	30.00	35.00	131.00
117	7 0.95	0.94	15505	140	16713	100.00	100.00	100.00	100.00	100.00	131.00
	0.95	1.01	17393	145	18745	25.00	35.00	43.51	75.00	85.00	131.00
167	7 1.00	0.90	22216	153	23913	40.00	50.00	52.94	70.00	80.00	131.00
167 246 269	16 1.00	0.90	32785	155	35259	15.00	25.00	34.90	45.00	55.00	131.00
269	9 1.00	0.97	35817	175	38551	0.50	1.00	1.15	5.00	15.00	131.00
331	1.10	1.12	44088	175	47428	0.50	1.00	2.07	5.00	15.00	131.00
419	9 1.10 3e-03 Pa Current I	0.95	55846	180	60052	0.50	1.00	2.43	5.00	15.00	131.00

Ion Percentages

Actual percentages are listed in the **Tune Status** table, outlined in red. The range of acceptable values is presented in the four adjacent columns.

Example: The percentage of mass 55, first row, should fall within 3.0-5.0%, and must fall within 2.0-6.0%, for the mass spectrometer to be properly calibrated.

Boxes shaded with red indicate that the actual percentage is outside that range for that fragment (row).

×		Mass	Target R	Actual R	Resolution	Ion Ener	Position (Min OK Tar	Min Target.	Actual Per	Max Targe	Max OK Ta	Base Peak
		55	0.90	0.91	7247	120	7839	2.00	3.00	3.34	5.00	6.00	131.00
166		69	0.85	0.87	9115	130	9841	30.00	45.00	57.68	75.00	90.00	131.00
8	~	100	1.00	1.03	13230	139	14278	10.00	15.00	17.17	30.00	35.00	131.00
10.215.		117	0.95	0.94	15505	140	16713	100.00	100.00	100.00	100.00	100.00	131.00
	~	131	0.95	1.01	17393	145	18745	25.00	35.00	43.51	75.00	85.00	131.00
Status:		167	1.00	0.90	22216	153	23913	40.00	50.00	52.94	70.00	80.00	131.00
	~	246	1.00	0.90	32785	155	35259	15.00	25.00	34.90	45.00	55.00	131.00
Calibration		269	1.00	0.97	35817	175	38551	0.50	1.00	1.15	5.00	15.00	131.00
S		331	1.10	1.12	44088	175	47428	0.50	1.00	2.07	5.00	15.00	131.00
& Mass		419	1.10	0.95	55846	180	60052	0.50	1.00	2.43	5.00	15.00	131.00
<u>ھ</u>													
,≧.	TP:	4.23e-03 Pa	a - Current Ba	ase Peak G	ain: 0.48								

Status Column

The status column provides a categorical view of the actual percentages. 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.

6.2.4.4.2 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 1.15. Adjusting Resolution influences the Actual Percentages.

	Mass	Target R	Actual R	Resolution	Ion Ener	Position (Min OK Tar	Min Target	Actual Per	Max Targe	Max OK Ta	Base Peal
	55	0.90	0.91	7247	120	7839	2.00	3.00	3.34	5.00	6.00	131.00
	69	0.85	0.87	9115	130	9841	30.00	45.00	57.68	75.00	90.00	131.00
~	100	1.00	1.03	13230	139	14278	10.00	15.00	17.17	30.00	35.00	131.00
	117	0.95	0.94	15505	140	16/13	100.00	100.00	100.00	100.00	100.00	131.00
~	131	0.95	1.01	17393	145	18745	25.00	35.00	43.51	75.00	85.00	131.00
	167	1.00	0.90	22216	153	23913	40.00	50.00	52.94	70.00	80.00	131.00
~	246	1.00	0.90	32785	155	35259	15.00	25.00	34.90	45.00	55.00	131.00
	269	1.00	0.97	35817	175	38551	0.50	1.00	1.15	5.00	15.00	131.00
П	331	1.10	1.12	44088	175	47428	0.50	1.00	2.07	5.00	15.00	131.00
П	419	1.10	0.95	55846	180	60052	0.50	1.00	2.43	5.00	15.00	131.00

Wider resolutions mean larger percentages (measuring over a wider mass range). 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 maximum target and the minimum target. If the masses cannot be brought into range by adjusting the target resolution, adjust the ion energies.

Ion Energies

Adjusting the ion energies 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.

Ideal Values

Displays the ideal values for ion energies for each of the 10 mass fragments.

Mass	IE Low	IE High
55	90	170
69	90	170
100	90	170
116.9	90	170
130.8	140	170
166.9	140	220
245.8	175	230
268.9	180	230
330.8	185	250
418.8	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 updates the Status column readings. Perform a mass alignment prior to and after making adjustments to the tune parameters.

Adjusting EM Voltage

The BPG is adjusted using EM (electron multiplier) voltage. Adjustments are made using increments of 25 V. The normal operating range is 1000–1600 V, with newer units typically showing lower values and older units showing higher values.

NOTICE

If the system requires an EM voltage of 1600–2000 V to reach a BPG of 0.5, please contact INFICON for support, as your unit may require service.

Observing Base Peak Gain (BPG) Properly adjusted base peak gain for a HAPSITE CDT is between 0.4 and 0.6, ideally at 0.5.

6.2.4.4.3 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, that is, raising amplification of larger ions and lowering smaller ions, or raising small ions and lowering larger ions. The ideal value is between 2 and 8.
- Emission current increases the power of the ionizer. Increasing this can help raise BPG, but can also increase noise. The ideal value is 300-400.

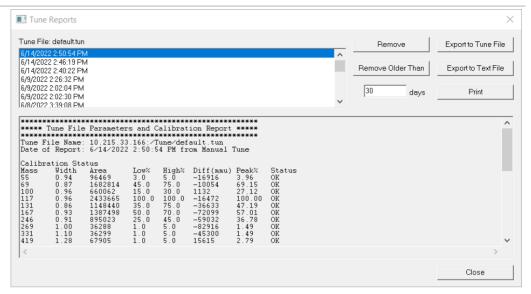
Baseline and Threshold are indicative of noise and should be less than 300 each.



6.2.4.5 View Tune Report

The most current tune report can be viewed from the laptop or the front display. Past tune reports can be viewed from the laptop.

- 1 To view the report from the laptop computer, select File.
- 2 Select View Tune Reports from the drop-down menu.
- 3 Highlight the default.tun file and press OK.
- **4** The Tune Reports are displayed. Tune Reports are stored, by default, for 30 days.



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.

6.2.4.6 Save Tune

- 1 Verify that "OK" is displayed in the Status Column.
- 2 Once you are satisfied with the quality of the tune, click the **Save Tune** icon in the toolbar. Save the tune as **default.tun**.
- 3 Close manual tune.

6.2.5 Methods

6.2.5.1 Default Methods

The methods found in the **Default Methods** window are general purpose methods for each of the HAPSITE CDT configurations.

Cartridge_VOC.mth*	General purpose GC/MS analysis for an air sample using a Tenax cartridge, <7 min analysis.
Cartridge_HT.mth*	High temperature GC/MS analysis for an air sample using a Tenax cartridge, <7 min analysis.
InjPrtAlkaneRTIndexSplit.mth	Split GC/MS analysis for alkane retention index using an injection port, <12 min analysis.
InjPrtCleanout.mth	Injection port cleanout analysis.
InjPrtExplosivesSplit.mth*	Concentrated explosives split GC/MS analysis for a liquid or solid sample extracted or dissolved in an organic solvent using an injection port, 2 min solvent delay, <7 min analysis.
InjPrtExplosivesSplitless.mth*	Trace explosives splitless GC/MS analysis for a liquid or solid sample extracted or dissolved in an organic solvent using an injection port, 2 min solvent delay, <7 min analysis.
InjPrtGeneralSplit.mth*	Concentrated general purpose split GC/MS analysis for a liquid or solid sample extracted or dissolved in an organic solvent using an injection port, ~2 min solvent delay, ~12 min analysis.
InjPrtGeneralSplitless.mth*	Trace general purpose splitless GC/MS analysis for a liquid or solid sample extracted or dissolved in an organic solvent using an injection port, ~2 min solvent delay, ~12 min analysis.
InjPrtNarcoticsSplit.mth*	Concentrated narcotics splitless GC/MS analysis for a liquid or solid sample extracted or dissolved in an organic solvent using an injection port, ~2 min solvent delay, ~12 min analysis.
InjPrtNarcoticsSplitless.mth*	Trace narcotics splitless GC/MS analysis for a liquid or solid sample extracted or dissolved in an organic solvent using an injection port, 2 min solvent delay, <11 min analysis.
* Identification is by AMDIS library.	

6.2.5.2 Method Editor

The Method Editor function in CDT IQ creates methods to identify and quantify volatile organic compounds. The Method Editor function is composed of the following screens:

- The Description screen for entering a description of the method.
- The Startup screen for selecting the type of method to be created. Temperature settings are also selected on this screen.
- The Inlet screen defines the temperatures, timing, inlet and valve states.
- The Collection Mode screen designates the mass spectrometer scanning parameters.
- The Search screen designates the calibration library for the method. This screen also sets the Library Search Parameters.

The Data screen 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\CDT IQ Software\System IP Address\Data\method name\file
name.file extension.

• A Summary screen is provided, at the end of the Method Editor, to review and print the method parameters.

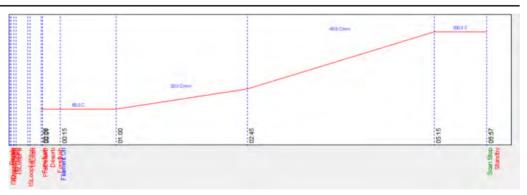


Methods cannot be viewed, created, or changed when the access level is set to Normal.

For questions relating to method development, please contact INFICON for application support. 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. It is a best practice to start with a similar default method and adjust settings as needed.



The bottom of each screen will display the inlet states (see Inlet States [> 158] for more information) and the temperature profile (see GC Temperature Profile [> 160] for more information).



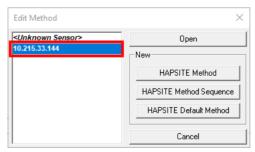
To access Method Editor:

1 On the System Setup screen, double-click on the **Method Editor** icon.



Method Editor

2 If more than one system is connected to the laptop, click on the name of the desired HAPSITE CDT.

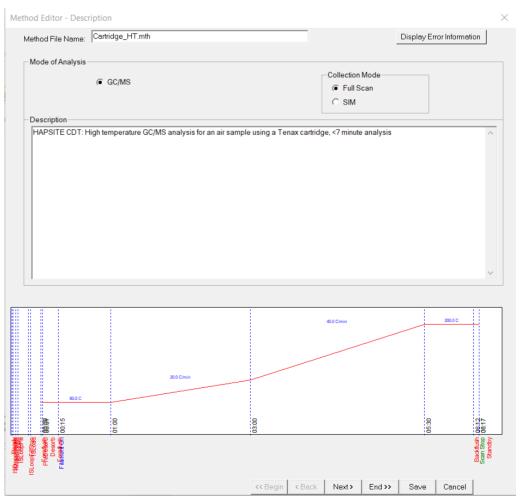


There are four options for accessing a method:

Open	Opens an existing HAPSITE CDT method for modification.
Method	Open 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 [> 185].
Default Method	Selects a default method. See Loading Default Methods.
Cancel	Closes the Edit Method window.

6.2.5.2.1 Description

The first screen displayed in the Method Editor is the Description screen. This screen 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 Editor screens.

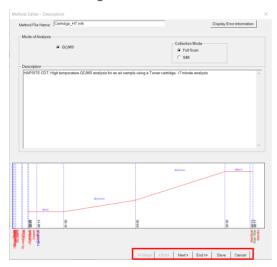




A method file ends with a file extension of .mth.

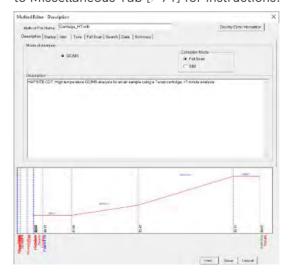
Mode of Analysis:	Analyze (GC/MS)	This analysis uses both the gas chromatograph (GC) and the mass spectrometer (MS) to separate and analyze compounds. Compounds are identified using a library search.
Collection Mode:	Full scan	This mode scans all the masses across a given range, which is 50–424 for default methods. It is used to identify unknown samples.
	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

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. The figure below shows the Wizard Mode navigation buttons.



known.

In Non-Wizard Mode, which is recommended only for experienced users, all screens are available through a tabbed window. To change the Wizard Mode settings, refer to Miscellaneous Tab [> 71] for instructions.

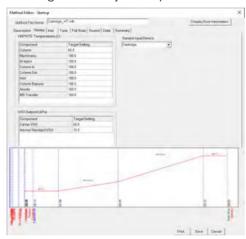




All method parameters on each screen of the Method Editor are checked for synchronization and correctness. The Method Editor function will highlight all questionable parameters in yellow when a discrepancy occurs. The Method Editor permits movement from screen to screen, even when errors are present.

6.2.5.2.2 Startup

The Startup screen, shown in the figure below, displays the initial settings for the HAPSITE CDT system heaters. The initial temperature setpoints for the components described in HAPSITE Temperatures (°C) can be modified on this screen. The initial pressure settings for internal standard and carrier gas valves are described in Voltage Sensitive Orifice® (VSO) Setpoints (kpa). The **Sample Input Device** (the cartridge or the injection port) can be selected on this screen.



The parameters on the Startup screen are:

HAPSITE Temperatures (°C)

Heater ID	Temperature Range (°C)
Column	60-225
Membrane	100-190
IS inject	70-110
Column in	170-200
Column out	170-200
Inlet	170-200
Column bypass	70-110
Anode	170-190
MS transfer	170-190



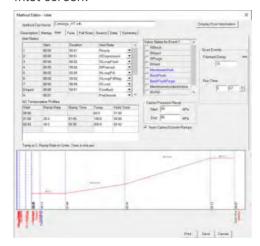
GC/MS methods do not use the column bypass heater.

VSO Setpoints (kpa)

Valve ID	Pressure Range (kPa)
Carrier VSO	35-200
Internal Standard VSO	5-25

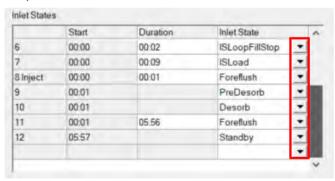
6.2.5.2.3 Inlet

The Inlet screen displays the default settings for the Inlet States, GC Temperature Profiles, and Valve States. Adjusting settings on the Inlet screen 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 screen.



6.2.5.2.3.1 Inlet States

Inlet States control the HAPSITE CDT and accessory valve settings for sampling, analysis, and purging of the HAPSITE CDT. The figure below shows the grid used to program the Inlet States. To edit the Inlet States grid, select an **Inlet State** from the drop-down menu.



The following choices are available for all method types in the Inlet States column:

Inlet State	Description
Ready	Checks that all initial heater conditions are met and cartridge is docked on system accessory deck.
Foreflush	Directs the carrier gas to push the sample onto the column.
Backflush	Directs the carrier gas from the back to the front end of the column. This state protects the column by keeping it purged with nitrogen carrier gas when there is no accessory installed.
IS Tune	Directs the internal standard to the MS for tuning.
Other	Allows for customized GC valve states. Contact INFICON personnel for support.
Standby	Standby is the last state of every method. Standby closes the Membrane Isolation valve and turns off the MS filament.

The following additional Inlet States are available in the Inlet States column when the **Cartridge Sample Input Device** is selected on the Startup Screen:

Inlet State	Description
ISDepressure	Vents all gas built up in the IS loop.
ISLoopFlush	Directs carrier gas through the IS loop.
ISPreload	Directs carrier gas back through the IS loop in reverse.
ISLoopFill	Directs IS gas into the IS loop.
ISLoopFillStop	The IS loop is closed, containing a known volume of IS gas equilibrated to atmospheric pressure.
ISLoad	Directs the carrier gas to load the volume of IS gas in the IS loop onto to the cartridge.
PreDesorb	PreDesorb starts the thermal desorption of analytes from the cartridge.
Desorb	Completes the thermal desorption process. This state directs the sample to the GC column.

The following additional Inlet States are available in the Inlet States column when **Injection Port Sample Input Device** is selected on the Startup screen:

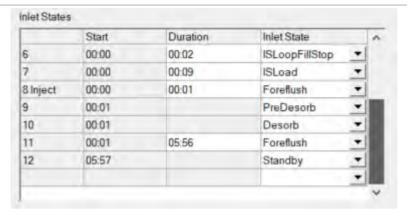
Inlet State	Description
SplitlessForeflush	Directs the sample and carrier gas to the GC column.
SplitForeflush	Vents a portion of the sample and carrier gas through the injection port exhaust while directing the remaining sample and carrier gas to the GC column.
InjectNow	This indicates when the user should inject the sample.

After selecting the Inlet State, enter the desired time period for the event in the Duration column. The following order and duration of each Cartridge Inlet State should be used when creating a cartridge method:

Event Order	Inlet State	Duration
1	Ready	0:01
2	ISDepressure	0:01
3	ISLoopFlush	0:02
4	ISPreload	0:02
5	ISLoopFill	0:09
6	ISLoopFillStop	0:02
7	ISLoad	0:09
8 (Inject)	ForeFlush	0:01
9	PreDesorb	0:11
10	Desorb	2:00
11	Foreflush	Application specific
12	Standby	N/A



The inject event initializes the start of MS data collection.



Upon entering the Duration settings, the Start time is automatically calculated for the next Inlet State.

Events can be deleted from the template. Click inside the desired cell in the grid and press **Delete** on the laptop keyboard.

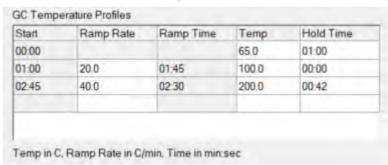
Events can be inserted into the template. Click inside the cell that will precede the desired event and press the **Insert** key on the laptop keyboard to insert a row.



Rows cannot be inserted after the Standby event.

6.2.5.2.3.2 GC Temperature Profile

GC Temperature Profiles specify the column temperature, ramp rate, and hold settings for the HAPSITE CDT method. Adjusting the temperature program changes the retention times of the target analytes and internal standard peaks.



Adjustments to the Hold Time, Ramp Rate, and Temp columns automatically update dependent parameters. For example, increasing the Temp increases the Ramp Time, and increasing the Hold Time adjusts the Start time of the next parameter.



A maximum of four lines is permitted in this section.

6.2.5.2.3.3 Scan Events

The items displayed in the **Scan Events** field are dependent upon the type of method.



The **Filament Delay** delays the turning on of the filament until after the inject event. This protects the filament by allowing the components of the air peak or solvents to pass through the MS.

The **Run Time** is the amount of time that the method will run after the inject event.

A CAUTION

If the Filament Delay is too short, the high-pressure burst caused by a solvent peak may damage the filament.

6.2.5.2.3.4 Scan Events for SIM Methods

When creating SIM methods, the beginning and end time for each scan set will be displayed. Adjustments to these times can be made on the SIM page. See SIM [> 163] for more details.



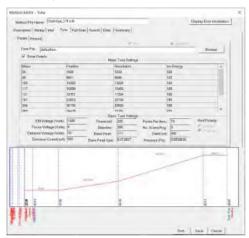
6.2.5.2.4 Tune

The Tune screen contains two tabs, **Report** and **Param**. Each provide information about the Tune file.

6.2.5.2.4.1 Param

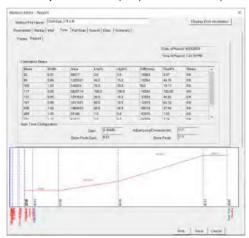
The **Param** tab displays the tune file name, which sets the MS tune parameters for the method. The default file name is **default.tun**. If a different tune file is desired, when connected to the instrument, the **Browse** button can be used to locate and specify the desired tune for the method.

This page also has a **Show Details** checkbox, which will produce a grid of tune parameters contained in the file. These parameters cannot be edited. If editing is desired, refer to Tune [\triangleright 139].



6.2.5.2.4.2 Report

The **Report** tab displays the tune report in a printable format.

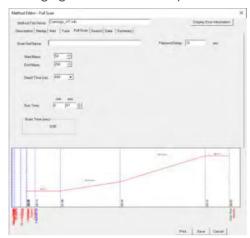


6.2.5.2.5 Collection Mode

Refer to the Description [155] screen to select a different collection mode.

6.2.5.2.5.1 Full Scan

The Full Scan screen 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 screen (refer to Scan Events [* 161]), is also shown on the Full Scan screen. Changing the Filament Delay on this screen may require changes to the Inlet screen.



The following mass spectrometer parameters can be programmed:

Start Mass	The mass at which the mass spectrometer will start to scan.
End Mass	The mass at which the mass spectrometer will end a scan. The end mass can be set from 50 to 424 amu. This value must be larger than the start mass.
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 mass fragment. A dwell time greater than 400 μs is recommended for a better signal-to-noise ratio.
Run Time	The time span of the method from start to finish.



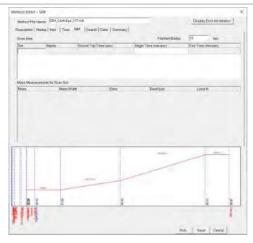
End the scan at least 2 amu above any mass used for compound identification. However, do not increase the end mass higher than necessary, as this will increase the scan time and a lower number of scans will be collected.

6.2.5.2.5.2 SIM

Selected Ion Monitoring (SIM) scans a set of specific masses to increase the sensitivity for known compounds. The figure in the following section displays the SIM screen.

6.2.5.2.5.2.1 SIM for Analyze

Each set has a **Begin Time** and an **End Time** that 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.



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.



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 to 10, for each mass. Extra scans lower the detection limits by increasing signal to noise ratio for that mass. Extra scans should be used when scanning for compounds with concentrations of parts per billion or lower.
Dwell	Dwell is the amount of time the detector will search for each selected mass. The Dwell can be set from 200 μs to 5000 μs . 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 μ s delay prior to collecting data. The delay is based on Lead In multiplied by the Dwell.



The Mass Width, Extra, Dwell, and Lead In values for a new entry are automatically populated based upon the entry listed above.

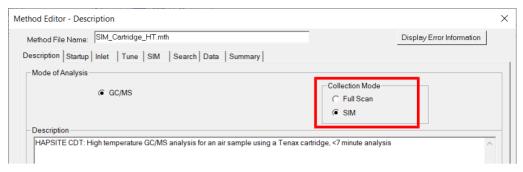


To fill any column with the entry listed above, click in the desired cell and press Ctrl + D.

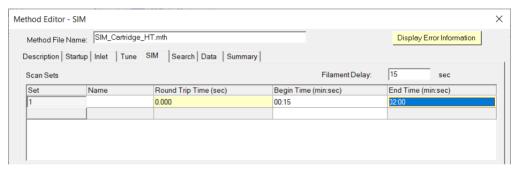
6.2.5.2.5.2.2 Creating a SIM Method

✓ Follow Step 1 through Step 4 of Reloading Default HAPSITE Methods.

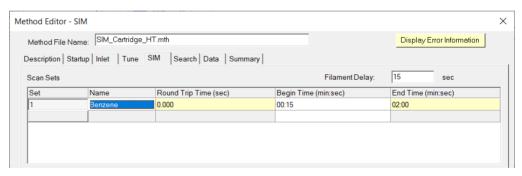
1 Change the Collection Mode to SIM.



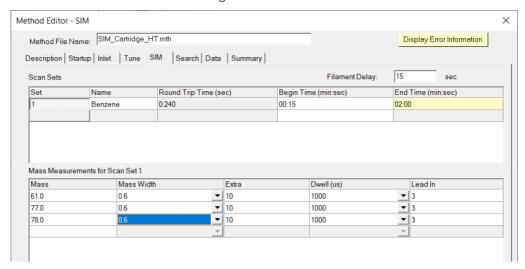
- 2 Select **Next** until the SIM page is displayed.
- **3** For the **Begin Time**, enter in the number displayed in the Filament Delay. For default methods, this is 15 seconds.
- 4 Enter the desired **End Time** so that the **Begin Time** and the **End Time** surround the expected retention time of the compound.



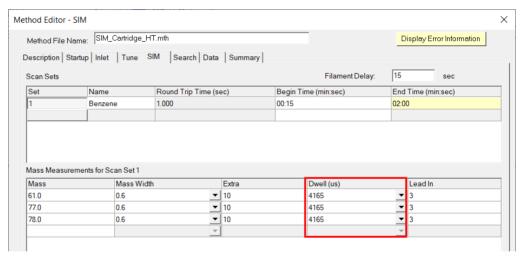
5 Enter the name of the chemical of interest.



6 Enter at least three mass fragments for the selected chemical of interest.



7 It is recommended that the Dwell Time is adjusted until the Round Trip is approximately one second.



8 Repeat Step 4 through Step 7 for additional target analytes.



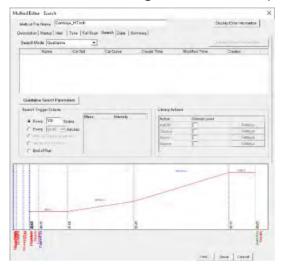
The End Time for the final SIM compound must be the same as the end run time for the method.



The AMDIS and Search NIST/User libraries are not available when using a SIM method.

6.2.5.2.6 Search

The Search screen sets the necessary parameters to qualify and quantify data. To quantify data, a calibration library must be created. See Calibration [** 188] for instructions on creating a calibration library.



There are four choices in the **Search Mode** drop-down menu.

SIM Methods only allow No Search as the search option.

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.
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.

6.2.5.2.6.1 Set 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 Parameters** button.



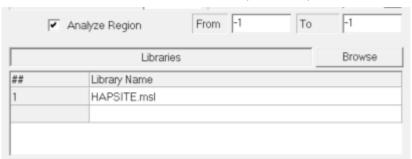


The table below lists the different analysis types available for the search.

Simple	The mass spectra data are used to identify the compounds. The calculated match factor is only based upon the quality of the match between the deconvoluted component spectrum and the target library spectrum.
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 Calibration Data + Internal Standard	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 CDT is properly identifying performance standards. The analysis does not perform a calibration.
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 how the algorithm interprets peak shape. Higher resolution will recognize sharper peaks while lower resolution will recognize broader peaks.

If Analyze Region is selected, AMDIS only searches in the selected scan range. When Analyze Region is off (i.e., unchecked), the software searches the entire range specified by Low Mass and High Mass.

HAPSITE.msl is the default AMDIS library for the system.

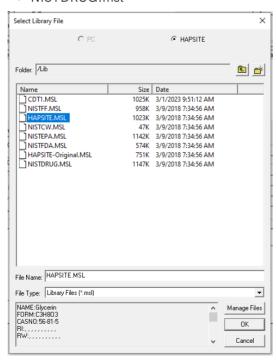


INFICON recommends using HAPSITE.msl

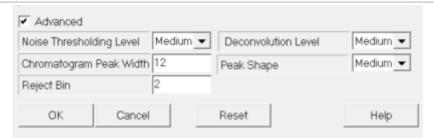
To view other library choices, select the **Browse** button. There are several small and specific libraries in addition to **HAPSITE.msl**. Many of the compounds found in these small libraries, which can be detected by the HAPSITE CDT, are incorporated in the **HAPSITE.msl** file.

AMDIS Libraries:

- HAPSITE.msl
- NISTEPA.msl
- NISTCW.msl
- NISTFDA.msl
- NISTFF.msl
- NISTDRUG.msl



Advanced Settings:

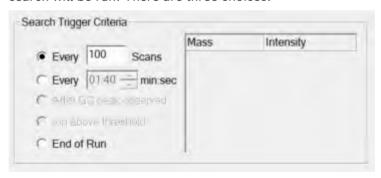


Noise Thresholding Level	Refers to the minimum signal recorded. Will filter out noise along the baseline.
Chromatogram Peak Width	Deconvoluted peaks will maintain same shape because the width, in AMUs, has been specified.
Reject Bin	Rejects peaks that have less than a set number of scans.
Deconvolution 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 parameter requires the deconvoluted peaks to have a similar shape. As the shape requirement increases, the shape of the individual ions will be more uniform.

NOTICE

INFICON does not recommend changing the Advanced Settings. Refer to the AMDIS operating manual for additional information regarding these advanced settings.

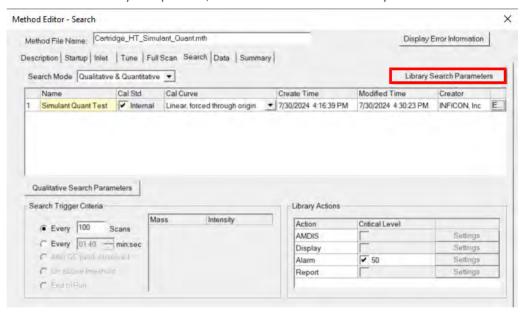
The **Search Trigger Criteria** section of the Search page determines when an AMDIS search will be run. There are three choices.



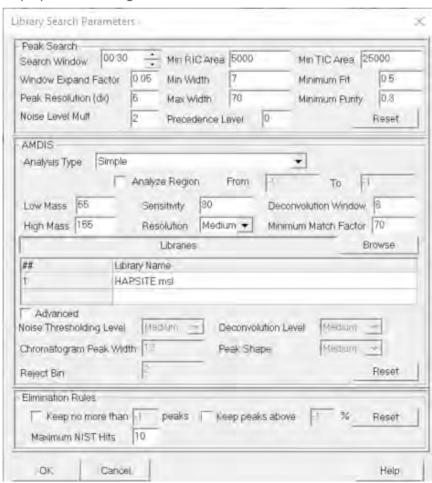
Every Scans	Determines the scan interval for running an AMDIS search. The default value for this is 100 scans.
Every min:sec	Determines the time intervals for running an AMDIS search.
End of Run	An AMDIS search will only be conducted at the end of a run.

6.2.5.2.6.2 Set Up a Quantitative Search

Once a calibration library has been created, the **Library Search Parameters** button is activated. The **Library Search Parameters** functions set the peak identification criteria of the library compounds, as well as the unknown analytes.



Clicking the **Library Search Parameters** button on the Method Editor - Search page displays the following window.

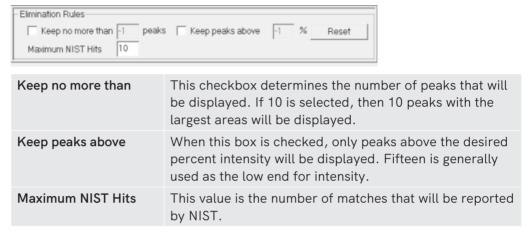


6.2.5.2.6.3 Peak Search

	The peak search section comprises 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 narrower 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 0.5–0.9 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 on the selectivity of the calibration, but typically 0.5–0.9 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 or compound-specific parameters. Leaving this set to zero allows the use of specific search parameters for individual compounds as discussed in Calibration.
Min. RIC Area	This number discriminates against low responses in the reconstructed ion chromatogram which are usually attributed to noise rather than analyte detection. Increase this number if false positives are encountered. Decrease this number if false negatives are encountered.

Min. TIC Area	This number discriminates against low responses in the total ion chromatogram which are usually attributed to noise rather than analyte detection. Increase this number if false positives are encountered. Decrease this number if false negatives are encountered.
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 **Elimination Rules** section gives you parameters for peaks to be reported. There are three options.

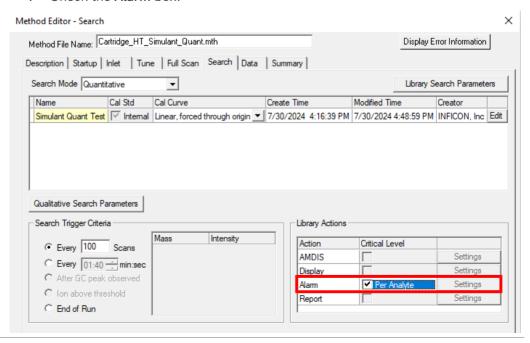


The **Reset** button resets the entered values to the default settings in the Peak Search window.

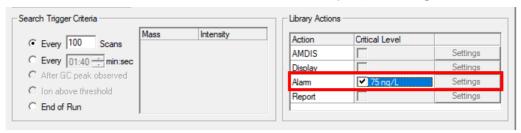
6.2.5.2.6.4 Alarm

On the main Method Editor - Search page, the **Alarm** option in the **Library Actions** box activates when a calibrated library has been saved to the method. To enable the **Alarm** option:

1 Check the Alarm box.



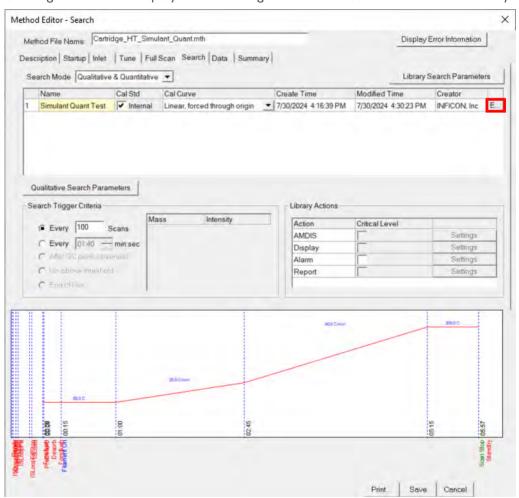
2 Enter the desired alarm level into the box with the units. The alarm is displayed when any analyte is detected at a concentration above the alarm level. To enter in alarm levels for individual analytes, see the figure below.



3 Click Yes on the dialog box to confirm that the alarm level is correct as entered.

6.2.5.2.6.5 Edit Options

Clicking the **Edit** box displays the following information about the calibration library.



Library Analyte List - Simulant Quant Test X Name CAS# Target Ion RT Time Standard Conc IS Ref. PFOB HAPSITE IS #1 00:36 180 ₩ 72.6 423-55-2 169.0 Internal PFOB HAPSITE IS #1 423-55-2 131.0 00:36 540 ₹ 72.6 Internal BPFB HAPSITE IS # 2 344-04-7 167.0 01:12 000 ₩ 35 Internal Phosphoric acid, trimethyl ester, (Trimethyl phosphate) 512-56-1 110.0 01:35 880 Analyte * 97.0 02:26 699 1445-75-6 Diisopropyl methanephosphonate Analyte 78-40-0 99.0 02:47 940 PFOB HAPSITE IS #1 Shift RTs Mass Peaks | Calibration | Search Parameters | Actions | Tolerance Template/Calibration Files 131.0 100 119.0 52 File Name File Saved Time Unit 129.0 41 /Certridge_HT_51.h 7/25/2024 12 13:41 25 na/L 169.0 40 /Cartridge_HT_56.h 7/30/2024 10:37:34... 50 ng/L 100.0 17 7/30/2024 10:47:21 /Cartridge_HT_57.h ng/L 181.0 13 219.0 9 179.0 231.0 Calibration Original View Report 58.0 162.0 13 1120 2 132 0 12 -1

The Library Analyte List is displayed.

The name of the compound is displayed in the name column, followed by the CAS number, the target ion, and the predicted retention (RT) time. In the **Standard** column, either **Internal** or **Analyte** is selected. If **Internal** is selected, the compound is an internal standard. If **Analyte** is selected, the compound is an analyte of interest.



The **Conc**. (concentration) column is populated for internal standards. It is blank if the compound is an analyte.



In the **IS Ref** column, all internal standards are given a number. For the internal standards, this is 1–6. The analyst, when creating a method, assigns a number (1–6 for the internal standard) to each analyte. The assigned number is based upon the closeness of the target ion of the analyte to 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.

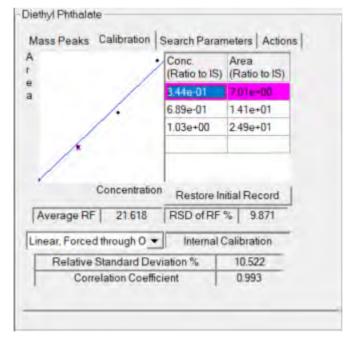
Cancel



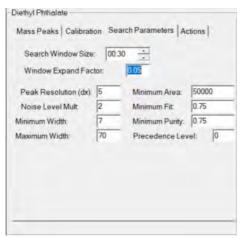
On the **Mass Peaks** tab, the mass fragments for the highlighted compound are displayed with their intensity.



On the **Calibration** tab, the calibration curve for the analyte is displayed. See Calibration $[\triangleright 188]$.

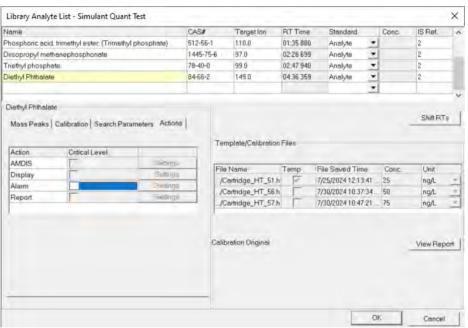


For information on the **Search Parameters** tab, refer to Peak Search [172].

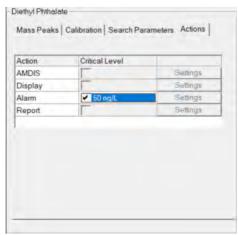


The **Actions** tab allows an alarm level to be entered for each individual compound. To enter an alarm:

1 Highlight the desired compound.

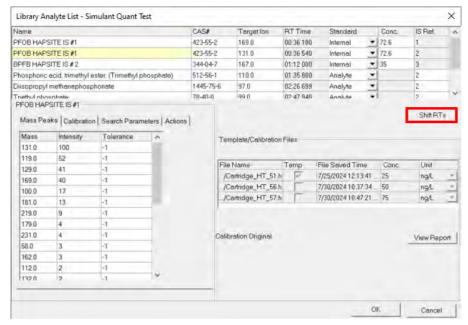


- 2 Check the Alarm box.
- 3 Enter the desired concentration followed by the desired units.



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:

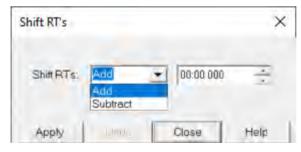
1 Click Shift RTs.



2 The Shift RTs window is displayed.



3 Select Add or Subtract from the menu.



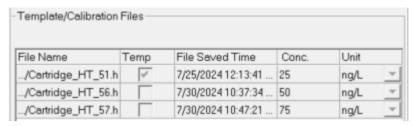
4 Type in the desired amount of time.



- 5 Click Apply.
- 6 Click Close.

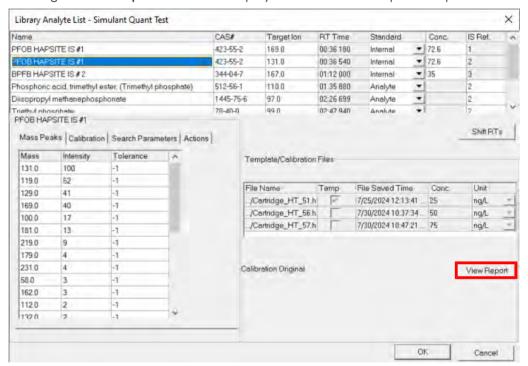
6.2.5.2.6.6 Template/Calibration Files

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.

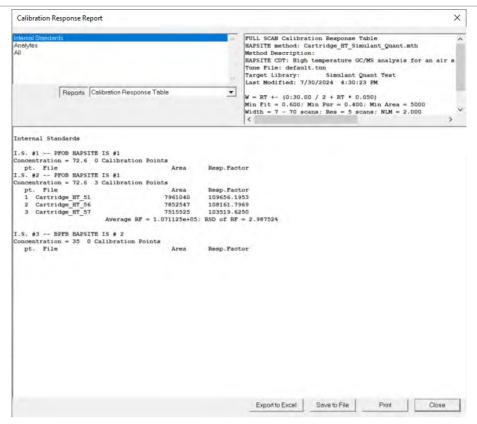


6.2.5.2.6.7 View Report

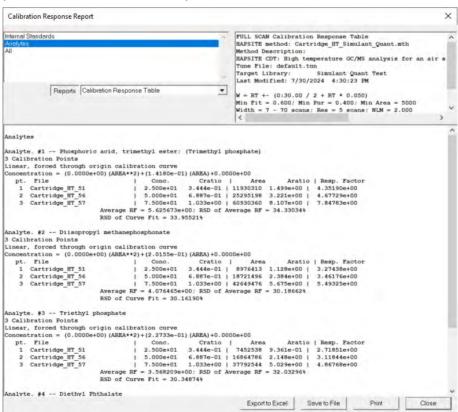
Clicking the View Report button will display the Calibration Response Report.



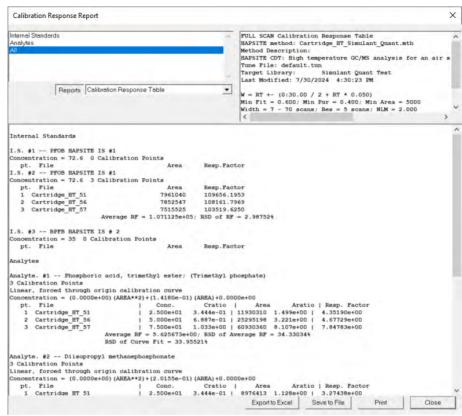
The default window that will be displayed is the Internal Standard Calibration Response Table. This table will display the file names, the area of the peak, and the response factor (the ratio between the signal produced by the analyte and the quantity of the analyte which produces a signal).



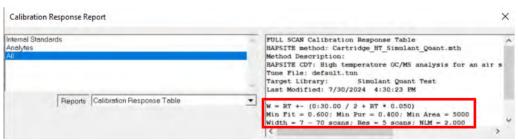
By selecting **Analytes** from the left-hand menu, the Analyte Standard Calibration Response Table will be displayed. The Analyte Standard Calibration Response Table contains the same information as the Internal Standard Calibration Table, but pertains to the calibrated analytes.



Selecting **All** will display the information contained in the Internal Standard Calibration Report and the Analyte Standard Calibration Report.

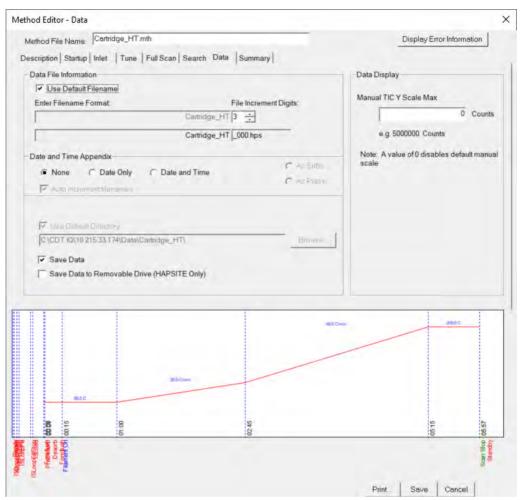


The Cal/Quant Report can be viewed by selecting **Calibration Report** from the drop-down menu. The Cal/Quant Report will display the same information as a Quantitative Report. Refer to Report [> 162] for more details. In the top-right corner, the peak search parameters are also displayed. Refer to Peak Search [> 172].



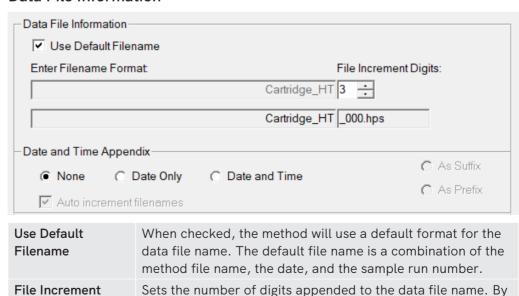
6.2.5.2.7 Data

The Method Editor - Data window customizes the names and the storage location of the data files for the method.



6.2.5.2.7.1 Data File Information

Digits



default, File Increment Digits is set to three digits.

6.2.5.2.7.2 Date and Time Appendix

If desired, the date and time can be added to the data file name using the following options:

None:

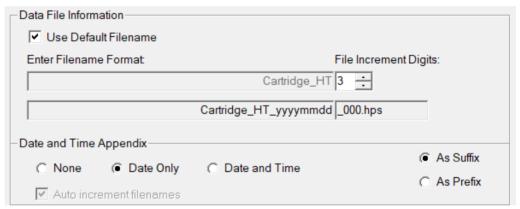
A date and time will not be added to the file name.



Date Only:

The date will be added to the file name.

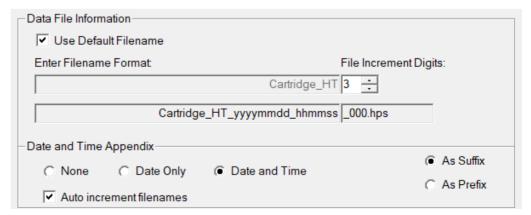
- yyyy is the year the data were collected
- mm is the month the data were collected
- dd is the day the data were collected



Date and Time:

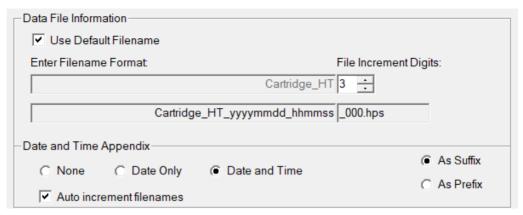
Both the date and time will be added to the data file name.

- hh is the hour data collection was started
- mm is the minute data collection was started
- ss is the second data collection was started



As Suffix:

When **Date and Time** is selected, the date and time are added to the end of the file name.



As Prefix:

When **Date and Time** is selected, the date and time are added to the beginning of the file name.

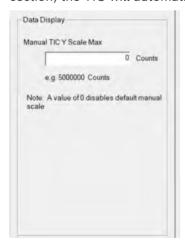


Save Data to Removable Drive:

Data are saved to the USB on the HAPSITE CDT as well as to the HAPSITE CDT hard drive in the folder (directory) shown immediately above this checkbox.

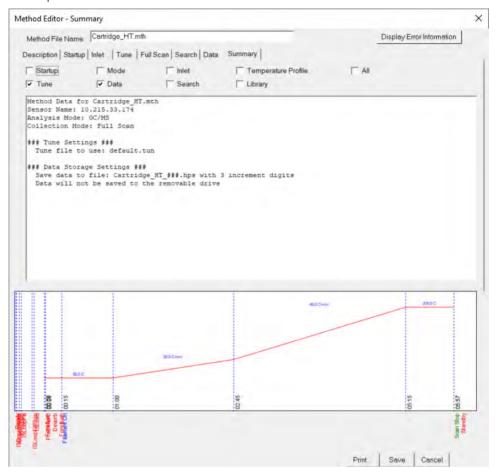
6.2.5.2.7.3 Data Display

A Manual TIC Response Y Scale Max 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.



6.2.5.2.8 Summary

The Method Editor - Summary window 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.



6.2.5.3 Method Sequence

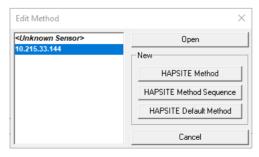
A series of methods can be run sequentially or at timed intervals. Follow the instructions below to create a method sequence.

1 Double-click the **Method Editor** icon.

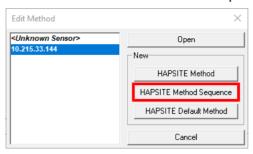


Method Editor

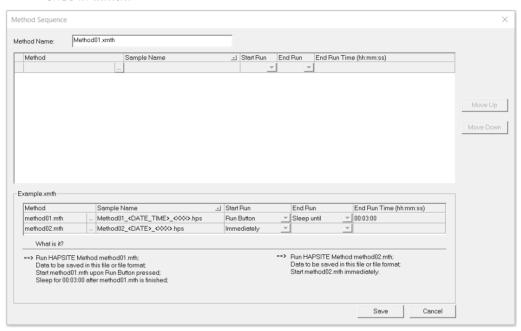
2 If more than one unit is connected to the laptop, click on the name of the desired HAPSITE CDT.



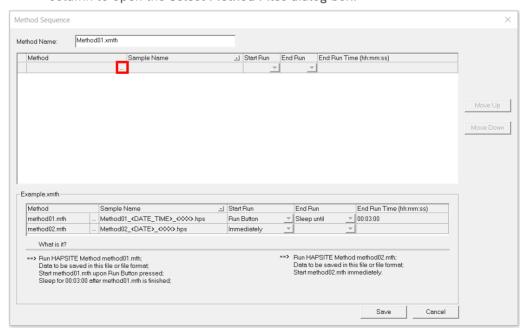
3 Click the HAPSITE Method Sequence option.



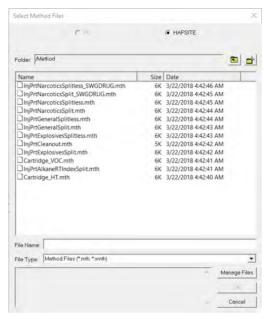
4 If desired, type in a new name for the method. Ensure that the file extension ends in .xmth.



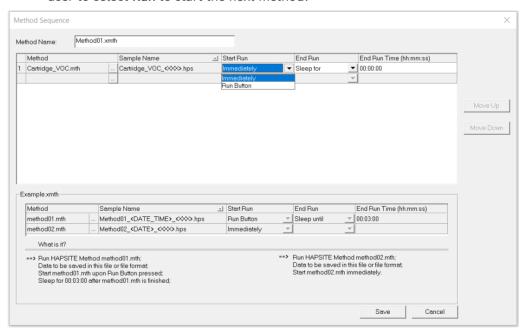
5 To select a method for your sequence, click the ellipsis button in the Method column to open the **Select Method Files** dialog box.



Select the desired method file and click **OK**.



7 Under the Start Run menu, select Immediately or Run Button from the drop-down menu to start the analysis. The Immediately option runs the method as soon as the previous method has finished. The Run Button option requires the user to select Run to start the next method.



8 Select the instructions and timing between sample runs under the End Run and End Run Times columns. Select **Sleep for** if a lapse in time is desired. For example, if 1:30:00 is entered, the second method will run an hour and a half after the first method finishes. Select **Sleep until** to enter a specific time. For example, if 1:30:00 is entered, the second method will start at 1:30 a.m.



"Sleep until" uses 24-hour notation.

9 Add multiple analyses by repeating steps 5-8. Alternately, right-click and select **Duplicate Row**.



- 10 Select Save to save the method sequence.
- 11 Select the desired location for saving the method sequence. The method can be saved to the laptop or the HAPSITE CDT by clicking the desired option at the top of the window.

6.2.6 Calibration

6.2.6.1 Introduction to Quantitative Analysis

A HAPSITE CDT 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.

6.2.6.2 Calibrating a Method



⚠ WARNING

Wear appropriate Personal Protective Equipment (PPE) as advised in the Safety Data Sheet (SDS) of the standard(s) being used.

- ✓ Prepare the standards as necessary to achieve the desired concentrations.
 - 1 Run each standard separately on HAPSITE CDT using the desired method. Each standard has its own separate run. The method used for HAPSITE CDT can be a default method or a custom method created with the Method Editor.

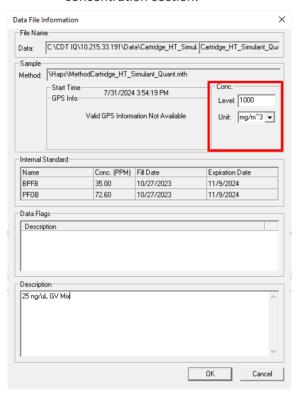


All other components of method development described in Method Editor must be made prior to running the standards.

- 2 Enter the concentration of the standard and a description in the **Data File Information** window during each sample run.
 - ⇒ Click the **Data File Information** icon to open the Data File Information window.



⇒ Enter the concentration and units into their respective fields under the concentration section.



⇒ Click **OK**.

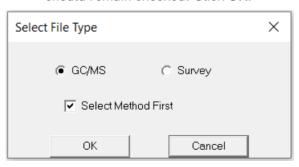


If desired, a description can be entered into the Description field.

When every standard has finished running, double-click the **Calibrate** icon.



4 Selecting the Calibrate function displays 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.



5 The Select Method File window is displayed if the Select Method First box remained checked.



6 If the Select Method First box was unchecked, select Browse to select a method file. Then click OK.



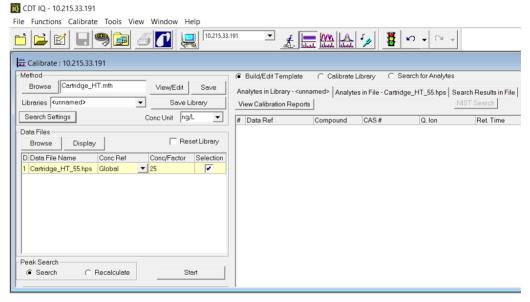
7 Click **Browse** under **Data Files**. Select the data file for library template creation.



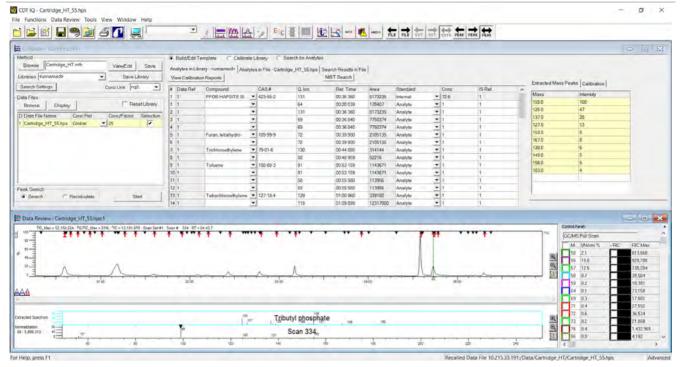


It is recommended to use a high or mid-range standard for calibration library development. Standards with low concentrations may have peaks too small to be detected with default Search Settings.

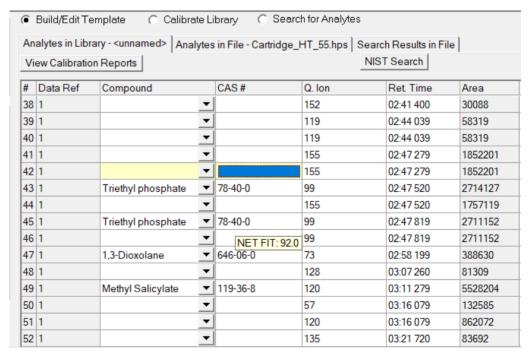
- 8 Select Build/Edit Template.
- 9 Select the units.
- 10 Set the Concentration Reference to Global or Analyte.
 - ⇒ Select **Global** for standards that contain analytes that have the same concentration.
 - ⇒ Select **Analyte** for standards that contain analytes with different concentrations.
- 11 If Global is selected, enter in the concentration of the standard. Step 12 is automatically completed if the information was entered in the Data File Information window when the sample was run. Refer to Steps 2–5.
- 12 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 is entered into the concentration column in Step 32.



- 13 Set Peak Search to Search.
- 14 Check Select.
- 15 Click Start.
- 16 All compounds that have been identified by AMDIS will be labeled with a red "T" over the apex of the peak and will have an associated compound entry in the Build/Edit Template table.

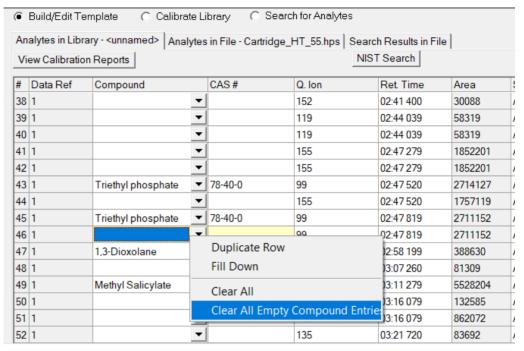


- 17 The highlighted compound in the library template corresponds to the peak with the red dotted line.
- Verify that all analytes have a **Net Fit** greater than 70 by hovering the mouse over the analyte name.

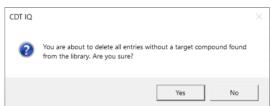


- 19 Verify that the retention times are correct.
- 20 If peaks are detected and loaded into the template without an identification, the NIST Search can be used to identify these compounds. See Reports [> 201] for information on NIST searches.

21 Unidentified compounds are indicated by a blank row. To remove remaining unnecessary unidentified compounds, right-click in the table and select Clear All Compound Entries.



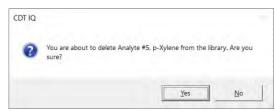
22 Click Yes to confirm the deletion of the unidentified compounds.



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.

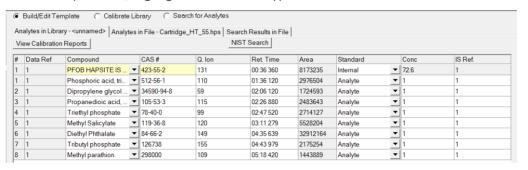


24 Click Yes to confirm the deletion of the undesired compounds.



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.

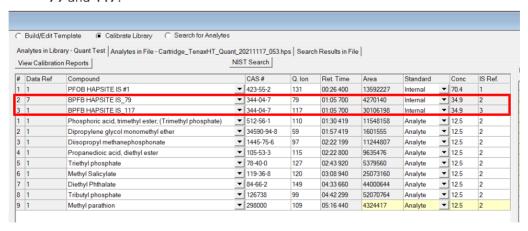
26 Set the IS Ref. (IS Reference). When using internal standards, the best practice is to use a quant ion from the internal standard that is closest in mass to the quant ion of the compound to be quantified. The software always selects the largest mass fragment in the spectrum as the quant ion. To change the quant ion, highlight the field and type in the new number.





The software automatically recognizes PFOB and BPFB. It automatically enters the concentration from the IS canister into the method for calibration and quantization.

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 HAPSITE IS_79 and BPFB HAPSITE IS_117. The quant ion is changed to 79 and 117.



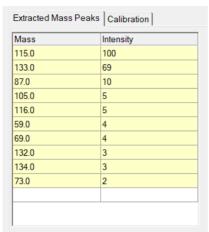


When adding more than one quant ion, the message shown below is displayed. Click "Yes" to allow the recalibration to continue.



28 Enter the lowest concentration of each analyte to the **Conc** column if **Analyte** has been selected. If **Global** is selected, this step can be skipped.

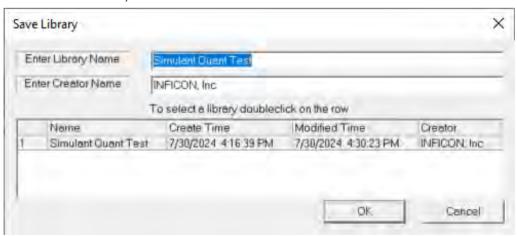
29 The Extracted Mass Peaks can also be edited to delete mass fragments. To delete unwanted mass fragments, highlight the field and press the Delete key. Unwanted mass fragments would be those with intensities below 15%, unless the fragmentation pattern is not very distinct.



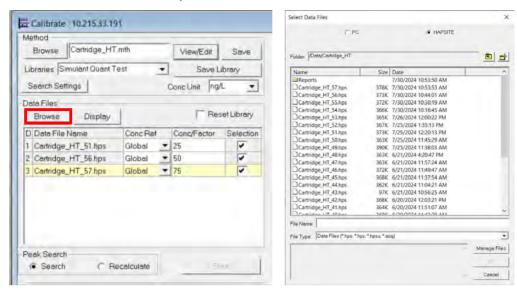
30 Save the template by clicking Save Library.



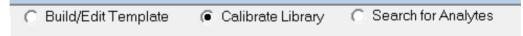
31 Enter a library name and a user name.



- 32 Click OK.
- 33 To calibrate the library, click **Browse** and select the desired data files.



34 Select Calibrate Library.



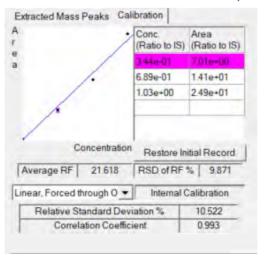
35 Check all of the data files and click Start under Peak Search.



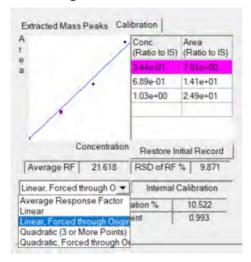
Additional calibration points can be added to the curve by following Step 10 through Step 39. Click "OK" when the "A calibration point exists already will not be added" message is displayed.



36 Review the curves for each analyte by clicking the Calibration tab.



37 Click each analyte to display the corresponding calibration curve. The curve should fit the data points. The menu provides four curve fit options: Linear; Linear, Forced through Origin; Quadratic; and Quadratic, Forced through Origin.





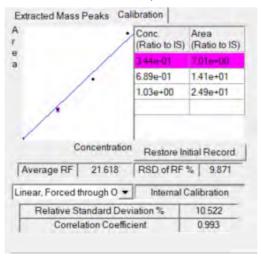
The RSD of the curve varies depending upon the curve fit selected.

- Verify that the RSD of RF% is acceptable. It is recommended that the RSD of RF% is 30% or lower.
- 39 It is possible to delete points from the calibration curve.



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 is overlaid with a pink X.



- 41 Use the up and down arrows to select the outlying point.
- 42 Click Delete.

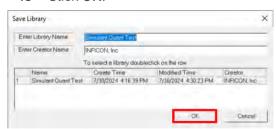


If a point was inadvertently deleted, the original calibration points can be restored by clicking "Restore Initial Record."

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.



- 44 To recalibrate the library with new parameters, check the Reset Library box.
- 45 Verify that the Peak Search is set to Search.
- 46 Repeat Step 16 through Step 41.
- 47 When the method is satisfactory, click Save Library.
- 48 Click OK.

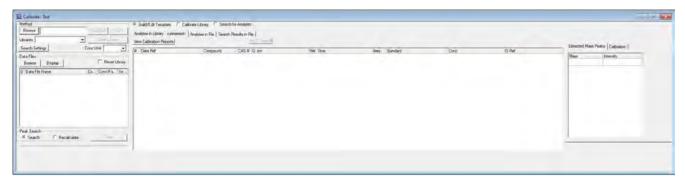


49 Save the library to the method by clicking Save.



50 Click OK.

6.2.6.3 Definition of Terms in the Calibrate Window



6.2.6.3.1 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. Refer to Methods [> 153].
Save	Saves the current method.
Libraries	A 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. Refer to Peak Search Parameters [> 131].
Concentration Unit	Used to select the concentration units.

6.2.6.3.2 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:
Data Ref	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.

6.2.6.3.3 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 for 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 them to the library template.



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.

6.2.6.3.4 Analytes

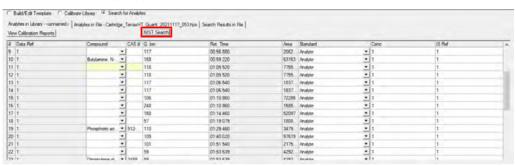
selected, a review of the analytes de	Search for Analytes tected in the file is to be added to the	
selected file. Search Results in File If a search has been performed with selected, a review of the analytes decrease.	Search for Analytes tected in the file is to be added to the	
selected, a review of the analytes de	tected in the file is note added to the	
, , ,	_20211117_0637ps Search Results in Rie	
# Date Ref Compound CAS # Q Ion Ref. Time Area Standard Conc	IS Ref.	
1 1 PPOB HAPSI ▼ 225. 131 0036 239 4324 Internal ▼ 170.4	1	
1 1 219 00:35 639 4415. Analyte 1	1	
2 1 • 219 00:35 639 4415. Analyte • 1	1	
3 1 • 131 00:35:239 4334 Analyte • 1	1	
4 59 00:35 540 9561 Analyter 1	1	
5 1 Add to Template 59 00:35 540 9551 Analyte 1	1	
6 1 760 95 00-44 040 1124 Applies V 1	1	
7 1 Add All 109 91 0051300 4131 Analyte 1	1	
8 1 • 117 00.56.880 2062 Analyte • 1	1	
9 1 v 117 00.56.880 2052 Avaide v 1	1	
10 1 168 00.59.20 53163 Analyte T 1	1	
11 1 V 118 01.05.520 7755 Analyte V 1	1	
12 1 ▼ 118 01:05:520 7755 Analyte ▼ 1	1	
13 1 v 117 01.95 540 1837, Anarde v 1	1	

6.2.6.3.5 Reports

To view Calibration Reports, refer to View Report [▶ 179].

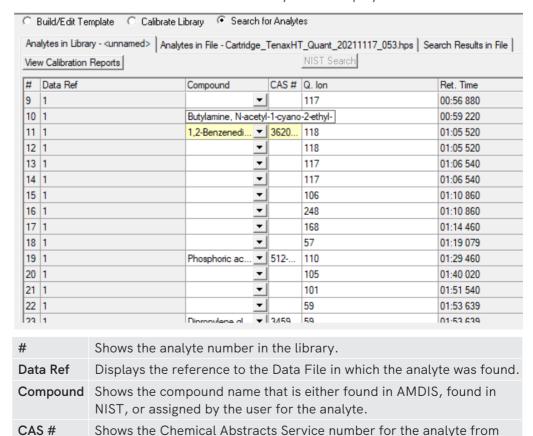
Calibration Response Table	Report that displays the response factor and curve statistics based on the selected curve type.
Calibration Report	Report that displays the area fit and purity for the calibration standards.
NIST Search	The initial search when building a template/library is performed using 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.
- 2 Click the NIST Search button.



3 The identification from the NIST library will be displayed.

the AMDIS or NIST library.



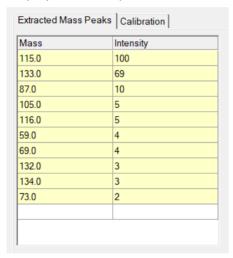
Q ion	Shows the quantization ion for the analyte.
Ret. Time	Shows the retention time for the analyte.
Area	Displays the integrated area of the quant ion.
Standard	Designates the compound as an analyte or an internal standard.
Conc	Shows the concentration of the analyte or internal standard in the displayed file.
IS Ref.	Displays the internal standard reference number for analyte quantization.



The Conc column is not used if the concentration flag is set to Global.

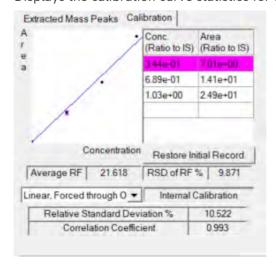
6.2.6.3.6 Extracted Mass Peaks

Displays the mass peaks and relative percentages for the selected analyte.



6.2.6.3.7 Calibration

Displays the calibration curve statistics for the selected analyte.



6.2.6.4 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.

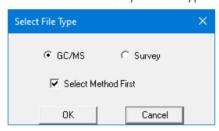
6.2.6.5 ID Unknowns

The **ID Unknowns** function allows the user to determine if all of the peaks in the chromatogram have been identified.

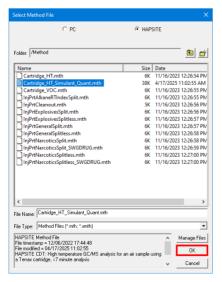
1 Double-click on the **ID Unknowns** function.



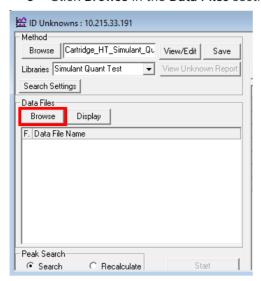
2 Select the GC/MS file type.



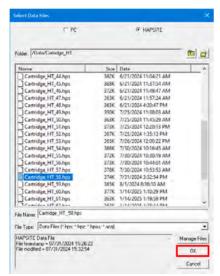
- 3 Verify that the **Select Method First** box is checked.
- 4 Click OK.
- 5 Select the desired method file. The data file that will be analyzed by ID Unknowns should have been generated from this file. Click OK.



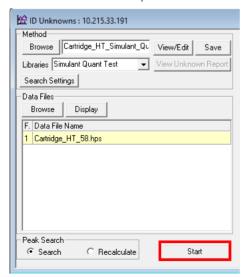
6 Click Browse in the Data Files section for the desired data file.



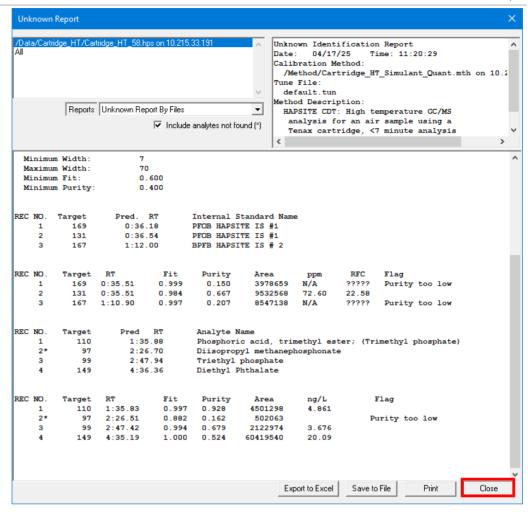
7 Select the desired data file and click **OK**.



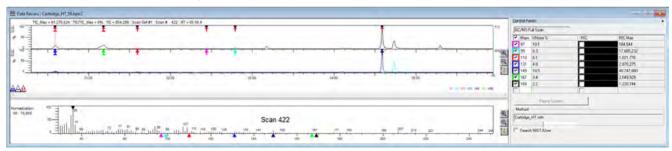
8 Click Start to open the Quant Report and the chromatogram.



⇒ For information on reading the **Quant Report**, refer to View Report [▶ 179].

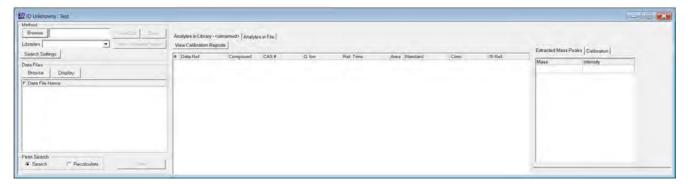


- 9 Click Close to exit the Quant Report.
- 10 If the compound is part of the calibration library, ID Unknowns will label the peak with a "T."



11 If the compound is not part of the calibration library, it is necessary to use AMDIS (refer to Analyzing Data Using AMDIS [▶ 119]) or NIST (refer to NIST Library Searches [▶ 127]) to make an identification.

6.2.6.6 Definition of Terms in the ID Unknowns Window



6.2.6.6.1 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. Refer to Methods [> 153].
Save	Saves the current method.
Libraries	A 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. Refer to Peak Search Parameters [> 131].
View Unknown Report	Gives the option to display the report by file or by analyte.

6.2.6.6.2 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. See Display Function [▶ 207].
File Entry	Lists the reference number for the file.
Data File Name	Displays the data file name and pathway.

6.2.6.6.3 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.

6.2.6.6.4 Analytes

Analytes in Library	Displays the analytes in the library.
Analytes in File	Displays the analytes in the currently displayed or selected
	file.

6.2.6.6.5 Reports

Calibration Response Table	Displays the response factor and curve statistics based on the selected curve type.
Calibration Report	Displays the area fit and purity for the calibration standards.
View Report	Displays the selected calibration report.
#	Shows the analyte number in the library.
Data Ref	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.
IS Ref	Displays the internal standard reference number for analyte quantization.



The Conc column is not used if the concentration flag is set to Global.

6.2.6.7 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.



6.2.7 Quick Reference SOP: Cartridge Analysis

Required Materials:

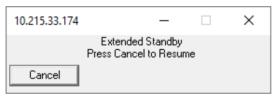
- HAPSITE CDT (analytical module)
- · Internal standard gas canister
- · Carrier gas canister
- · Charged battery
- · Power supply
- Cartridge
- · Laptop with CDT IQ installed

Procedure:

- ✓ For assembly instructions, refer to Basic Assembly [▶ 16].
- ✓ Verify that a clean cartridge is installed, refer to System Blank Analysis [> 55].
 - 1 Power on the laptop by pushing the **Power** button. Open CDT IQ software by double-clicking on the **CDT IQ** icon.



2 Connect to HAPSITE CDT through the sensor icon on the bottom of the screen. Touch Cancel on the dialog box to exit Extended Standby.



- 3 Select a desired cartridge method to prepare (refer to Select a New Method [> 91]). The system heats all necessary components and checks gas pressures. Progress of the heaters is indicated by a bar graph on the laptop screen.
 - ⇒ Once all temperature zones have reached their setpoints, a prompt is displayed to "Press RUN to start method."
- 4 Click Run on the window or from the Control Panel on the screen.



- **5** As the method runs, the chromatogram begins to appear on the laptop screen.
- 6 Review the results at the end of the analysis; for information on data review, refer to Data Review [▶ 92]. If red lines appear on the chromatogram, saturation has occurred. To clear saturation, run blank runs until the saturation has cleared.

6.2.8 Quick Reference SOP: Injection Port Analysis

Required Materials:

- HAPSITE CDT (analytical module)
- · Internal standard gas canister
- · Carrier gas canister
- · Charged battery
- · Power supply
- Injection port
- 10 µL glass syringe
- Laptop with CDT IQ installed

Procedure:

✓ For assembly instructions, refer to Basic Assembly [▶ 16].

✓ Verify that the injection port is installed.



If desired and equipped, HAPSITE CDT can be used with the laptop computer via the wireless connection. Refer to Wireless Connection [29] for additional information on setup and usage.

1 Power on the laptop by pushing the **Power** button. Open CDT IQ software by double-clicking on the **CDT IQ** icon.



2 Connect to HAPSITE CDT through the sensor icon on the bottom of the screen. Touch Cancel on the dialog box to exit Extended Standby.



- 3 Select a desired injection port method to prepare (refer to Select a New Method [▶ 91]). The system heats all necessary components and checks gas pressures. Progress of the heaters is indicated by a bar graph on the laptop screen.
- 4 Prepare sample and syringe while system is preparing (see Quick Reference SOP: Sample Preparation for Surface Wipes of Unknown Powder Residue [▶ 210]).
- Once all temperature zones have reached their setpoints, a prompt is displayed to "Press RUN to start method."



To avoid any timing errors, only press "Run" if sample and syringe are prepared and ready for analysis.

6 Once system is ready for analysis, click on the Run prompt in CDT IQ, wait for the Inject Now window to display on the front panel before inserting the syringe and injecting the aliquot into the injection port.

7 As the method runs, the chromatogram begins to appear on the laptop screen.

8 Review the results at the end of the analysis; for information on data review, refer to Data Review [> 92].

↑ CAUTION

Injection of any substance other than the diluted or extracted sample in organic solvents may damage HAPSITE CDT.

6.3 Sample Preparation

6.3.1 Injection Port Sample Preparation

The Injection Port Accessory enhances the capabilities of HAPSITE CDT (GC/MS) to provide on-site analysis of semi-volatile organic compounds (SVOCs) and narcotics extracted from various sample matrices, including liquid, solid, and wipe samples. With its fast and easy sampling, the system ensures immediate results in the field, allowing for quick decision-making.

HAPSITE CDT with the Injection Port Accessory provides emergency responders and environmental testing professionals with powerful analysis and confirmatory results, ease of use, and economy under a broad range of field conditions.

6.3.1.1 Surface Wipe Sample Preparation

6.3.1.1.1 Quick Reference SOP: Sample Preparation for Surface Wipes of Unknown Powder Residue

Required materials:

- HAPSITE CDT (analytical module)
- · Internal standard gas canister
- Carrier gas canister
- · Charged battery
- · Power supply
- Injection port
- 10 μL glass syringe
- Surface wipe kit

Procedure:

- ✓ Ensure the injection port is properly installed; refer to Injection Port Information and Installation [▶ 26]
- ✓ Prepare HAPSITE CDT with preferred injection port method; refer to Quick Reference SOP: Injection Port Analysis [▶ 209]
 - 1 Use a new set of clean, non-powdered impervious gloves for each sample collected.

2 Using a transfer pipet, wet the sample media with solvent.



- 3 Press firmly with the sample media, using caution to avoid touching the surface with gloved hands. Smooth surfaces should be wiped; rough surfaces should be blotted.
- 4 When wiping the sampling area, two methods may be used:
 - ⇒ The square method involves wiping in a square around the outside edge of the sample site and wiping in concentric squares towards the center.



- ⇒ The "S" method involves wiping from side to side in an overlapping "S" motion until the entire sample surface is covered.
- **5** Fold the sample media with the sampled side in without allowing the media to contact any other surfaces.



6 Repeat the wiping method with the folded sample media. If using the "S" method, wipe from top to bottom on the second pass.

7 Fold the media in half with the sampled side in. Seal the sample media in a sample vial and label with the sample number and location.



- 8 Collect at least one sample media blank for every 10 samples collected. This media should be treated with solvent and folded but not wiped.
- 9 Add solvent to cover the sample media with transfer pipet.



10 Shake the sample for up to two minutes. Allow insoluble material to settle to the bottom of the vial.



11 Check that the HAPSITE CDT system status is "Ready To Run." Do not press Run until the syringe is prepared with sample.

Once insoluble material has settled to the bottom of the vial, transfer 1–2 mL of liquid sample to a smaller 4 mL vial.



- 13 Rinse a Hamilton® 80395 conical syringe three times with 10 μ L of the rinse solvent. Pull syringe plunger back to 1 μ L to provide a small solvent plug and air gap.
- 14 Pull 1 μ L of the prepared sample into syringe, being sure to only pull in the liquid extract and avoiding any insoluble material at the bottom of the vial.





- 15 Once the system is ready for analysis, click on the Run prompt in CDT IQ and wait for the "Inject Now" window to display on the front panel before inserting the syringe and injecting the aliquot into the injection port.
- 16 As the method runs, the chromatogram begins to appear on the laptop screen.
- Review the results at the end of the analysis; for information on data review, refer to Data Review [> 92].

A CAUTION

Injection of any substance other than the diluted or extracted sample in organic solvents may damage HAPSITE CDT. Acceptable solvents include: methanol, ethanol, acetonitrile, methylene chloride, and hexane.

Unacceptable liquids include: water, aqueous solutions, undiluted fuel and fuel oils, etc.

6.3.2 Remote Sample Collector Operation



NOTICE

Calibrate Sample Pump

Calibrate the sample pump prior to use. Refer to the GilAir Plus Operation Manual, available online at https://sensidyne.com/product/gilair-plus/.

6.3.2.1 Key Pad Overview



6.3.2.2 Power Controls

Power pump on P

Power the pump on. Press and hold the **Power/Enter** key until the pump displays the startup screen.

Power pump off

When the pump is not running or is in a program pause, press and hold the **Power/ Enter** kev.

Continue to hold **Power/Enter** until the power-down window appears and the countdown completes.

6.3.2.3 Remote Sample Collector Assembly

NOTICE

The remote sample collector comes preassembled from the factory.

6.3.2.3.1 Sample Pump Removal

1 To remove the tubing from the sample pump inlet along the right side, pull the tubing straight up, off of the hose barb.



2 Grasp the handle with your left hand, apply pressure forward and up to the pump with your thumb while squeezing the clip fastener tab together and pulling it to the right, out of the sample pump clip.



3 Once the clip fastener is removed from the sample pump clip, the sample pump should slide free of the remote sample collector.



⇒ The sample pump can now be docked onto its charging station.

6.3.2.3.2 Remote Sample Collector Reassembly



1 Attach the handle to the sample pump mount.



2 Attach the cartridge holder to the sample pump mount.



3 Install the sample pump into the sample pump mount. Press the pump into the mount while installing the clip fastener into the sample pump clip along the front side of the sample pump mount.



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4 Attach the tubing to the sample pump inlet and the holder outlet.



6.3.2.4 Flow Set

Flow Set allows the flow rate at which the pump will operate in constant flow control mode to be set.

6.3.2.4.1 Flow Rate Selection

NOTICE

This operation is required only if the pump flow rate is changed. If a previously set flow rate it being used, it is only necessary to verify it using a calibrated reference flow meter.

- 1 At the main menu screen, use the Navigation buttons to move the cursor to Flow Set.
- 2 Use the Increase/Decrease buttons to set the desired rate of flow.
- 3 Press the Power/Enter button to accept the flow rate.
- ⇒ Flow set is now complete.

NOTICE

Flow rates between 20 and 445 cc/min require the flow control valve to be set for low flow operation (the **Lo** indicator is displayed in the bottom status line). For Tenax cartridges, flow settings from 20 to 150 cc/min. are recommended. Higher flow settings may result in a pump error.

Above 445 cc/min the flow control valve must be set for high flow operation (the **Hi** indicator is displayed in the bottom status line).

The pump will not operate unless the flow control valve is in the correct **Hi** or **Lo** position for the corresponding flow rate setting.

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6.3.2.4.2 Flow Rate Range Adjustment

The flow rate range is set by using the hex key (provided with pump, standard 2 mm or 5/64 in. size) to change the position of the flow control valve.



For cartridge sample collection, the flow rate range should be set to the **Lo** position.

6.3.2.5 Cartridge Sample Collection

- ✓ The sample pump should be fully charged prior to use.
- ✓ Ensure the remote sample collector is properly assembled prior to use. Follow the directions in Remote Sample Collector Assembly for proper assembly.
 - 1 Power on the pump by pressing the **Power/Enter** button.
 - 2 Set Flow to the desired sampling flow rate. Follow the directions in Flow Set to adjust the flow rates.
 - **3** Open the cartridge storage cap and install the cartridge into the remote sample collector.
 - 4 Begin sampling by navigating to Run, then pressing the Power/Enter button.
 - Once the desired volume is reached, stop sampling by pressing the Power/ Enter button. Navigate to Stop and then press the Power/Enter button again.
 - **6** Remove the cartridge and close the cartridge storage cap.

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7 Maintenance

7.1 Service Module Attachment Procedure



⚠ WARNING

Venting HAPSITE CDT with a NEG above ambient temperature causes total NEG consumption and may possibly result in severe damage to the HAPSITE CDT mass spectrometer components. It may also result in physical injury since extreme heat generation from the NEG consumption creates hot surfaces.

⚠ CAUTION

If HAPSITE CDT NEG is above ambient temperature, then the NEG must be cooled before proceeding. Turn off HAPSITE CDT and allow NEG to cool for approximately 24 hours or until the NEG is at ambient temperature.

A CAUTION

Prior to attaching HAPSITE CDT to the Service Module, ensure the NEG is at ambient temperature and unplug the black NEG cable inside the HAPSITE CDT front display panel. This will ensure that the NEG will not heat when using the Service Module to provide vacuum.

⚠ 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.

NOTICE

If the Service Module has been in storage, refer to the HAPSITE Service Module Operating Manual.

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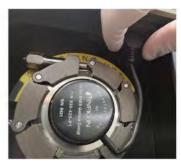
7.1.1 Laptop Operation Attachment Procedure

✓ Review all Service Module attachment cautions and warnings. Install two spacer blocks (PN 937-3087-P1) on the Service Module to adjust to the HAPSITE CDT width. Refer to the installation guide included with the latch extenders kit (PN 937-400-P1).

1 Remove front display screws (2) with a 2.5 mm hex driver. Drop front display screen. Unplug NEG cable.







- 2 Replace front display screen and reinstall the front panel screws.
- 3 Remove the Service Module cover and inspect the opening for damage to the O-ring, dust, or debris. Clean with a lint-free wipe and methanol or replace O-ring if needed.





MARNING

Wear nitrile gloves and safety glasses when handling methanol

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4 Remove HAPSITE CDT load lock cover; use a 3 mm hex driver to rotate the four socket head screws a quarter turn. Inspect the manifold connection and clean with a lint-free wipe and methanol.





- **5** Orient the Service Module facing backward. Carefully place HAPSITE CDT on top of Service Module; be sure to align the interconnect valves.
- 6 Once system is set in place, latch down both sides.

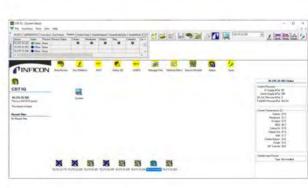






- 7 Power on Service Module and power on HAPSITE CDT from Service Module.
- 8 Once HAPSITE CDT is powered on, connect HAPSITE CDT to the computer using wireless communication or the Ethernet crossover cable to establish communication with CDT IQ.
- 9 Open CDT IQ.
- 10 Double-click the IP address for the desired unit. The green dot in the Status column will indicate that you are connected.





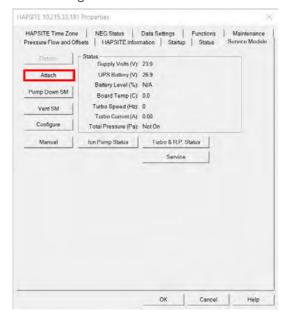
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11 Double-click the Service Module icon.



Service Module

12 The system properties window will appear, displaying the Service Module navigation tab. Click the **Attach** button.



13 Click Yes to attach the Service Module.



14 A window will appear while the Service Module is attaching. The attachment procedure usually takes about five minutes.



15 Wait for the HAPSITE is Attached message to appear, then click **OK**. The turbo speed will be at 1500 Hz, and the load lock will open. Allow system to pump down for at least two hours.



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7.1.2 Front Panel Operation Attachment Procedure

- ✓ Review all service module attachment cautions and warnings. Orient the Service Module facing backward. Install two spacer blocks on the Service Module to adjust to the HAPSITE CDT width.
 - 1 Follow Steps 1 through 7 of Laptop Operation Attachment Procedure [▶ 220].
 - 2 Touch the Accessories/Devices navigation tab (refer to Accessories/Devices [> 37]).
 - 3 Touch the Service Module icon.
 - 4 Touch the Attach SM button at the bottom of the screen.
 - ⇒ A status bar displaying the progress of the attachment procedure will be displayed and the **Attach SM** button will become unavailable.
 - **5** When the attachment procedure has successfully been completed, the "Service Module Attached" message will be displayed.
 - 6 Wait for the HAPSITE is Attached message to appear, then click **OK**. The turbo speed will be at 1500 Hz, and the load lock will open. Allow system to pump down for at least two hours.



Both the **Attach SM** and **Detach SM** buttons will be temporarily unavailable immediately after a successful attach while the system prepares.

8 Service and Technical Support

8.1 How to Contact Customer Support

Worldwide customer support information is available under **Contact** at www.inficon.com:

- · Sales and Customer Service
- · Technical Support
- Repair Service

When reporting an issue with HAPSITE CDT, please have the following information readily available:

- HAPSITE CDT part number and serial number
- a description of the problem
- an explanation of any corrective action that may have been attempted
- · the exact wording of any error messages observed

For technical support, visit www.inficon.com and select **Contact** >> **Service & Support**. Select your region and product to obtain support contact information. To submit a repair request in North America, fill out a Service Request form at https://service.inficon.com/.

8.2 Returning a System to INFICON

Do not return any component of your instrument to INFICON without first obtaining a Return Material Authorization (RMA) number from a Customer Support Representative. To obtain an RMA, fill out and submit a Service Request form (refer to How to Contact Customer Support [> 224]). Service Request forms must be approved by INFICON before an RMA number is issued.

If you deliver a package to INFICON without an RMA number, your package will be held and you will be contacted. This will result in delays in servicing your instrument.

Prior to being given an RMA number, you may be required to complete a Declaration of Contamination (DOC) form if your instrument has been exposed to certain materials. DOC forms must be approved by INFICON before an RMA number is issued. INFICON may require that the instrument be sent to a designated decontamination facility, not to the factory.

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9 Replacement Parts

9.1 HAPSITE Part Numbers

Part Number	Product Feature Options	HSCDT
937-2100-G10	HSCDT green, standard column, USB-802, 11, without NEG	1
937-2100-G11	HSCDT green, standard column, USB-802, 11, with NEG	2
937-850-G1	CDT Universal Ship Kit	1
937-3417-G1	CDT Remote Sample Collector Kit	1
930-0371-G1	HAPSITE and NIST software only, no laptop	A
930-261-G6	Laptop with Windows	В
930-261-G7	Ruggedized laptop with Windows	С
930-262-G6	Laptop with Windows (Europe)	D
930-262-G7	Ruggedized laptop with Windows (Europe)	Е
930-263-G6	Laptop with Windows (UK)	F
930-263-G7	Ruggedized laptop with Windows (UK)	G
930-264-G6	Laptop with Windows (Australia)	Н
930-264-G7	Ruggedized laptop with Windows (Australia)	J
930-264-G8	Laptop with Windows (China)	N
930-202-G1	Service Module, 100-240 V	1
930-202-G3	Service Module, 24 V (DC)	2
937-0351-G1	CDT IQ Software, English (installed in laptop and AM)	A
937-0395-G1	Future INFICON Methods	В
937-464-P1	Ruggedized shipping case	1

9.2 Spare and Consumable Parts

CDT Accessories

Part Number	Description
930-202-G1	100/120/230 V (AC)
937-400-P1	CDT Latch Extenders Kit
937-3417-G1	Accessory, CDT Remote Sample Collector Kit
937-3418-G1	Accessory, CDT Injection Port Kit

9 | Replacement Parts INFICON

CDT Spare Parts

Part Number	Description
059-0329	Quick Disconnect Stem for N2
930-612-P1	USB Drive
070-1204	Sample Vials, Case of 100
600-1319-P2	Ethernet Communication Cable (Crossover)
937-3402-G1	Accessory Deck Maintenance Kit
937-3403-G1	Accessory Deck Plugs Kit
937-3401-G1	Maintenance Tool Kit
937-3416-G1	CDT Torque Wrench Kit
937-3417-G1	Remote Sample Collector Kit
937-3418-G1	Injection Port Kit
937-3421-G1	Surface Wipe Kit
937-3420-G1	Surface Wipe Refill Kit
937-3427-G1	CDT Injection Port Maintenance Kit
937-3434-P1	Replacement Cartridge Labels
937-3445-G1	Cartridge to Sample Bag Adapter
937-3467-G1	Universal CDT Battery Charger Kit
930-4071-G1	NIST Version Upgrade
930-4081-G1	NIST (with AMDIS)
937-464-P1	CDT Instrument Shipping Case
937-465-P1	Injection Port Shipping Case
937-466-P1	CDT Spare Parts Shipping Case
937-469-G1	Universal 250 W CDT Power Supply Kit

CDT Consumables

Part Number	Description
930-432-P6	Canister, Carrier Gas, 6 each
930-432-P12	Canister, Carrier Gas, 12 each
930-432-P24	Canister, Carrier Gas, 24 each
936-2390-P6	Canister, Internal Standard, 6 each
936-2390-P12	Canister, Internal Standard, 12 each
936-2390-P24	Canister, Internal Standard, 24 each
930-730-G1	Extended Life Carrier Gas Deployment Kit (110 liter)
930-4611-P1	Extended Life Carrier Gas (110 liter)
937-3200-P1	Gas Combo Pack (4 Carrier Gas / 2 Internal Standard)
937-3090-P1S	HAPSITE CDT Battery - Spare, 1 each
937-3170-G6S	CDT Cartridge Pack, 6 each
930-425-P1	Spare NEG Pump

INFICON Replacement Parts | 9

Service Module Spare Parts

Part Number	Description
068-0002	Battery Charger/Service Module Power Cord
930-465-P1	Shipping Case, Service Module
930-734-G1	RS232 to USB Adapter Cable

9.3 Software and Computers

Part Number	Description
930-4071-G1	NIST Version Upgrade
930-4081-G1	NIST (with AMDIS)
930-261-G61	Replacement Standard Laptop with IQ Software and NIST
930-261-G71	Replacement Ruggedized Laptop with IQ Software and NIST

10 Declaration of Conformity



DECLARATION OF CONFORMITY

This declaration is issued under the sole responsibility of the manufacturer INFICON. The object of the declaration is to certify that this equipment, designed and manufactured by:

INFICON Inc.

Two Technology Place East Syracuse, NY 13057

USA

is in conformity with the relevant Community harmonization legislation. It has been constructed in accordance with good engineering practice in safety matters in force in the Community and does not endanger the safety of persons, domestic animals or property when properly installed and maintained and used in applications for which it was made.

Equipment Description: INFICON HAPSITE CDT with Sample Cartridge and Direct Injection Port

Applicable Directives: 2014/35/EU (LVD) Electrical Equipment (Safety) Regulations 2016 (UK)

2014/30/EU (EMC) Electromagnetic Compatibility Regulations 2018 (UK)
2015/863/EU (RoHS) Substances in Electrical and Electronic Equipment

Regulations 2012 (AS AMENDED)
2014/53/EU (RED) Radio Equipment Directive

CONTROL BUT CARLES

Applicable Standards:

Safety: IEC 61010-1:2010/AMD1:2016 3rd Edition

Emissions: EN 61326-1:2020 (Radiated & Conducted Emissions)

(EMC - Measurement, Control & Laboratory Equipment)

CISPR 11:2015/AMD2:2019

EN 55011:2016/A11:2020 Emission Standard for Industrial, Scientific and

Medical (ISM) radio RF equipment

FCC Title 47 CFR Part 18 Class A emission requirements (USA)

Immunity: EN 61326:2020 (Industrial EMC Environments)

(EMC - Measurement, Control & Laboratory Equipment)

Immunity per Table 2

CE and UKCA Implementation Date: November 11, 2022

Andrew Klamm Digitally signed by Andrew Klamm Date: 2022.11.30 21:22:11:05:00

Samuel Carroll Digitally signed by Samuel Carroll Date: 2022.11.30 10:29:32 -05'00'

Authorized Representatives:

Andrew Klamm Quality Manager, ISS

Samuel Carroll Vice President of Engineering

ANY QUESTIONS RELATIVE TO THIS DECLARATION OR TO THE SAFETY OF INFICON'S PRODUCTS SHOULD BE DIRECTED, IN WRITING, TO THE AUTHORIZED REPRESENTATIVE AT THE ABOVE ADDRESS.



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