



CMS5000TM

Monitoring System

PN 074-508-P1F



Trademarks

The trademarks of the products mentioned in this manual are held by the companies that produce them.

Teflon[®] and Tedlar[®] are registered trademarks of Dupont.

Swagelok[®] is a registered trademark of Swagelok Co.

PEEK[™] is a trademark of Victrex plc.

Fischer[®] Connectors is a registered trademark of Fischer Connectors SA.

Intel[®] and Pentium[®] are registered trademarks of Intel.

All other brand and product names are trademarks or registered trademarks of their respective companies.

Disclaimer

The information contained in this manual is believed to be accurate and reliable. However, INFICON assumes no responsibility for its use and shall not be liable for any special, incidental, or consequential damages related to the use of this product.

Due to our continuing program of product improvements, specifications are subject to change without notice.

Copyright

©2022 All rights reserved.

Reproduction or adaptation of any part of this document without permission is unlawful.



**EU 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: CMS5000 Air and Water Monitoring Equipment.

Applicable Directives: 2014/35/EU (LVD)
1999/5/EC (R&TTE / EMC)
(The required compliance statement concerning this directive can be found in Chapter 4 of this manual.)
2014/30/EU (General EMC)
2011/65/EU (RoHS2)

Applicable Standards:

Safety: EN 61010-1:2010 3rd Edition

Emissions: ETSI EN 300 328 v1.8.1 (2.4 Ghz)
(ERM for equipment operating in the 2.4 GHz ISM band)
ETSI EN 301 893 v1.7.1 (5 Ghz)
EN 61326-1: 2013 (Radiated & Conducted Emissions)
(EMC – Measurement, Control & Laboratory Equipment)

CISPR 11/EN 55011 Edition 2009-12 Emission standard for industrial, Scientific and medical (ISM) radio RF equipment

FCC Title 47 Part 15 Class A emission requirements (USA)

Immunity: EN 61326:2013 (Industrial EMC Environments)
(EMC – Measurement, Control & Laboratory Equipment)
Immunity per Table 2

ETSI EN 301 489-17 V2.2.1: 2012 (General EMI)
(ERM - EMC - Specific conditions for 2.4 GHz)

RoHS: Fully compliant with Exemptions

Wireless Restrictions:

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

CE Implementation Date: March 10, 2022

UKCA Implementation Date: March 10, 2022

Authorized Representative:

Andrew Klamm Digitally signed by Andrew Klamm
Date: 2022.04.12 16:13:48 -04'00'

Andrew Klamm
Quality Manager
INFICON Inc.

Samuel Carroll Digitally signed by Samuel Carroll
Date: 2022.04.12 16:28:58 -04'00'

Sam Carroll
Vice President of Engineering, ISS
INFICON Inc.

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.

Warranty

INFICON warrants that the products sold by it are delivered free from any defect in materials, workmanship and construction, and meet the products' specifications set forth by INFICON.

INFICON warrants the products for two (2) years from the date of shipping invoice of the products to the customer. The warranty excludes carrier gas, GC columns, concentrator tubes, and all other items deemed by INFICON as consumables. In the event the customer finds any defective products which do not meet the aforesaid warranty, it shall give notice to that effect to INFICON. The customer will return defective systems, accessories and parts to be repaired to INFICON or INFICON contracted suppliers after obtaining a Return Material Authorization (RMA) from INFICON Service Department.

INFICON liability under this warranty is limited to such products as are returned, transportation prepaid, to INFICON plant no later than thirty (30) days after the expiration of the warranty coverage and are found by INFICON examination to have failed because of defective workmanship. At INFICON election, it may either repair and return the product, or furnish a replacement product, with transportation paid by INFICON in either case.

This warranty is made and accepted in lieu of all other warranties, express or implied, whether of merchantability or of fitness for a particular purpose or otherwise, as buyer's exclusive remedy for any defects in the product sold hereunder. All other obligations and liabilities of INFICON, whether in contract or tort (including negligence) or otherwise, are expressly excluded. In no event shall INFICON be liable for any costs, expenses or damages, whether direct or indirect, on any claim of defective product, in excess of the price paid by the buyer for the products plus return transportation charges prepaid.

No warranty is made by INFICON for any INFICON product which has been installed, used or operated contrary to INFICON written instruction manual or which has been subject to misuse, negligence or accident, or has been repaired or altered by anyone other than INFICON or which has been used in a manner or for a purpose for which the product was not designed.



Table Of Contents

| |
|------------|
| Cover Page |
| Trademarks |
| Disclaimer |
| Copyright |
| Warranty |

Chapter 1

Introduction

| | | |
|-------|---|-----|
| 1.1 | Introduction | 1-1 |
| 1.2 | Theory of Operation | 1-2 |
| 1.2.1 | Purge and Trap Sampling System | 1-2 |
| 1.2.2 | Gas Chromatograph | 1-3 |
| 1.2.3 | Micro Argon Ionization Detector (MAID). | 1-4 |
| 1.3 | Radioactive Source | 1-5 |
| 1.4 | Definition of Note, Hint, Danger, Warning, and Caution Paragraphs | 1-6 |
| 1.5 | How To Contact Customer Support | 1-7 |
| 1.5.1 | Returning CMS5000 | 1-7 |

Chapter 2

Specifications

| | | |
|-------|---|-----|
| 2.1 | Gas Chromatograph Specifications | 2-1 |
| 2.2 | Micro Argon Ionization Detector (MAID) Specifications | 2-1 |
| 2.3 | Communication | 2-2 |
| 2.4 | Physical Operating Requirements | 2-2 |
| 2.4.1 | Operating Environment | 2-2 |
| 2.5 | Analysis and Protocols | 2-3 |

Chapter 3

System Setup

| | | |
|-------|---|-----|
| 3.1 | CMS5000 Feature Options. | 3-1 |
| 3.1.1 | Analytical Unit. | 3-1 |
| 3.1.2 | Sampling Source | 3-1 |
| 3.1.3 | Integration | 3-1 |
| 3.1.4 | Ship Kits | 3-1 |
| 3.1.5 | Laptop Installed with CMS IQ Software | 3-1 |
| 3.2 | CMS5000 Ship Kit Contents. | 3-2 |

| | | |
|---------|--|------|
| 3.3 | CMS5000 Diagram | 3-2 |
| 3.4 | Mounting Instructions | 3-3 |
| 3.5 | Water Monitoring Assembly Instructions | 3-4 |
| 3.6 | Attaching the Water Sampling Vessel | 3-7 |
| 3.7 | Connecting the Water Supply | 3-9 |
| 3.8 | Air Monitoring Assembly Instructions | 3-10 |
| 3.8.1 | Ambient Air Sampling | 3-10 |
| 3.8.2 | In-line Air Sampling | 3-12 |
| 3.8.2.1 | In-Line Sampling | 3-13 |
| 3.9 | Connecting the Argon Supply | 3-14 |
| 3.10 | Connecting the Power Supply | 3-15 |
| 3.11 | Instrument Equilibration | 3-15 |
| 3.11.1 | Calibration | 3-15 |
| 3.12 | Communication Options | 3-16 |
| 3.12.1 | Connecting the Ethernet Cable | 3-16 |
| 3.12.2 | Attaching the Wireless Antenna | 3-16 |
| 3.12.3 | Connecting the I/O Cable | 3-16 |

Chapter 4

Setting Up Computer Communication

| | | |
|---------|---|------|
| 4.1 | Introduction | 4-1 |
| 4.2 | Configuring the Computer for CMS5000 Communication | 4-1 |
| 4.3 | Setting Up Computer Communications | 4-8 |
| 4.4 | Wireless Regulatory Compliance Information | 4-12 |
| 4.4.1 | Regulatory Compliance Information for UNITED STATES Users | 4-12 |
| 4.4.1.1 | FCC Statement | 4-12 |
| 4.4.1.2 | FCC RF Exposure Statement | 4-13 |
| 4.4.2 | Regulatory Compliance Information for CANADIAN Users | 4-13 |
| 4.4.2.1 | Industry Canada (IC) Notices | 4-14 |

Chapter 5

Input/Output Configuration

| | | |
|-----|--|-----|
| 5.1 | Introduction | 5-1 |
| 5.2 | Input Method Triggering | 5-2 |
| 5.3 | Replace Argon Cylinder Alarm | 5-2 |
| 5.4 | Out of Specification Alarm | 5-3 |

Chapter 6

Software Setup

| | | |
|-----|------------------------------------|------|
| 6.1 | Introduction | 6-1 |
| 6.2 | FTP Connection | 6-1 |
| 6.3 | System Integration | 6-12 |
| 6.4 | Defining Startup Methods | 6-12 |
| 6.5 | Input Methods | 6-15 |
| 6.6 | Method Sequence | 6-17 |

Chapter 7

System Status

| | | |
|-----|-------------------------|-----|
| 7.1 | Introduction | 7-1 |
| 7.2 | SYS Function | 7-1 |
| 7.3 | TIME Function | 7-2 |
| 7.4 | NET Function | 7-3 |
| 7.5 | STAT Function | 7-3 |
| 7.6 | FIRM Function | 7-5 |

Chapter 8

Basic Operation

| | | |
|-----|---|-----|
| 8.1 | Introduction | 8-1 |
| 8.2 | Default Methods | 8-1 |
| 8.3 | System Check Standard | 8-1 |
| 8.4 | Operating CMS5000 using the Front Panel | 8-2 |

Chapter 9

Review Data Function

| | | |
|-----|--------------------------------|-----|
| 9.1 | Review Data Function | 9-1 |
|-----|--------------------------------|-----|

Chapter 10

System Function

| | | |
|--------|--|------|
| 10.1 | Introduction | 10-1 |
| 10.2 | System Function | 10-1 |
| 10.3 | Set Date, Time and Time Zone | 10-3 |
| 10.3.1 | Set Network Info | 10-5 |
| 10.3.2 | Set Language | 10-9 |

Chapter 11

Exit Function

| | | |
|------|----------------------------------|------|
| 11.1 | Exit Function | 11-1 |
| 11.2 | Accessing Exit Options | 11-1 |
| 11.3 | Restart System | 11-3 |

| | | |
|------|---------------------------------------|------|
| 11.4 | Reboot System | 11-4 |
| 11.5 | Return to CMS5000 Main Menu | 11-4 |

Chapter 12

CMS IQ System Setup

| | | |
|------------|---|-------|
| 12.1 | Introduction | 12-1 |
| 12.2 | System Setup | 12-1 |
| 12.2.1 | Connecting to CMS5000 | 12-2 |
| 12.2.2 | System Setup Menu | 12-2 |
| 12.2.3 | File Menu | 12-3 |
| 12.2.3.1 | Generate Trend Report | 12-5 |
| 12.2.4 | Functions Menu | 12-12 |
| 12.2.5 | System | 12-12 |
| 12.2.5.1 | Port Settings | 12-13 |
| 12.2.5.2 | Display | 12-16 |
| 12.2.5.2.1 | Screen Layout | 12-16 |
| 12.2.5.2.2 | Colors | 12-17 |
| 12.2.5.2.3 | Selecting Colors | 12-18 |
| 12.2.5.2.4 | Fonts | 12-19 |
| 12.2.5.2.5 | Restore Colors and Fonts Defaults | 12-19 |
| 12.2.5.2.6 | Plot | 12-19 |
| 12.2.5.3 | Miscellaneous | 12-20 |
| 12.2.5.3.1 | Data File Increment Digits | 12-21 |
| 12.2.5.3.2 | Default Pathways | 12-22 |
| 12.2.5.3.3 | Changing Default CMS Folder | 12-23 |
| 12.2.5.3.4 | Changing Default NIOSH Database Folder | 12-25 |
| 12.2.5.3.5 | Method Editor in Wizard Mode | 12-27 |
| 12.2.5.3.6 | Allow Multiple Connections | 12-28 |
| 12.2.6 | Tools Menu | 12-28 |
| 12.2.6.1 | System Setup | 12-28 |
| 12.2.6.2 | System Properties | 12-28 |
| 12.2.6.3 | Sensor Properties | 12-29 |
| 12.2.6.4 | Set Access Level | 12-29 |
| 12.2.6.4.1 | Changing Access Levels | 12-29 |
| 12.2.6.4.2 | Setting or Changing the Access Level Password | 12-31 |
| 12.2.7 | View Menu | 12-32 |
| 12.2.7.1 | Main Toolbar | 12-32 |
| 12.2.7.2 | Sensor Toolbar | 12-32 |
| 12.2.7.3 | Function Toolbar | 12-32 |

| | | |
|------------|---|-------|
| 12.2.7.4 | Toolbars Use Large Icons | 12-32 |
| 12.2.7.5 | Sensor Status Grid | 12-33 |
| 12.2.8 | Window Menu | 12-33 |
| 12.2.9 | Help Menu | 12-34 |
| 12.3 | System Setup Icons | 12-34 |
| 12.4 | Safety DB | 12-36 |
| 12.5 | Manage Files | 12-39 |
| 12.5.1 | Copy Function | 12-40 |
| 12.5.2 | Backup Function | 12-41 |
| 12.5.3 | Rename Function | 12-42 |
| 12.5.4 | Delete Function | 12-43 |
| 12.6 | Status Icon | 12-46 |
| 12.6.1 | Status | 12-46 |
| 12.6.2 | CMS5000 Time Zone | 12-47 |
| 12.6.2.1 | Setting the Time Zone | 12-48 |
| 12.6.2.2 | Setting Date and Time | 12-49 |
| 12.6.2.2.1 | Sync Date and Time to Computer | 12-49 |
| 12.6.2.2.2 | Enter Date and Time Manually | 12-50 |
| 12.6.3 | CMS5000 Information | 12-53 |
| 12.6.4 | Pressure Flows and Temperatures | 12-54 |
| 12.6.4.1 | Pressures | 12-55 |
| 12.6.4.2 | Method Start Temperature Tolerances | 12-56 |
| 12.6.4.3 | Carrier Gas Alarm | 12-57 |
| 12.6.5 | Input/Output | 12-58 |
| 12.6.6 | Data Settings | 12-59 |
| 12.6.6.1 | Notification | 12-60 |
| 12.6.6.2 | Logged Items | 12-61 |
| 12.6.6.3 | Log Path and Maintain Logs | 12-61 |
| 12.6.6.4 | Directories | 12-62 |
| 12.6.6.5 | Configure FTP Settings | 12-62 |
| 12.6.7 | Functions | 12-63 |
| 12.6.8 | Parameters | 12-64 |
| 12.6.8.1 | Startup Method | 12-64 |
| 12.6.8.2 | Enable Water Adjustment | 12-65 |
| 12.6.8.3 | Enable CkStd Autocal | 12-65 |
| 12.6.8.4 | Auto Baseline Function | 12-67 |
| 12.6.8.5 | Run Time Prompt Enable | 12-68 |
| 12.6.8.6 | Summary Report Options | 12-69 |
| 12.7 | Front Panel Display Icon | 12-70 |

| | | |
|----------|----------------------------|-------|
| 12.8 | CMS5000 Sensor Status Icon | 12-71 |
| 12.8.1 | Update CMS5000 Software | 12-72 |
| 12.8.2 | Bring Online | 12-72 |
| 12.8.2.1 | Communication Messages | 12-72 |
| 12.8.3 | Disconnect | 12-72 |

Chapter 13

Data Review

| | | |
|------------|-----------------------------------|-------|
| 13.1 | Introduction to Data Review | 13-1 |
| 13.2 | Accessing the Data Review Feature | 13-1 |
| 13.3 | Menu Bar | 13-4 |
| 13.3.1 | Data Review Menu | 13-4 |
| 13.4 | Data Review Toolbar | 13-5 |
| 13.5 | Data File Information Window | 13-6 |
| 13.6 | Reports | 13-7 |
| 13.6.1 | Access Reports | 13-7 |
| 13.6.2 | Summary Reports | 13-8 |
| 13.6.3 | Quantitative Reports | 13-8 |
| 13.7 | Chromatogram Window Options | 13-10 |
| 13.7.1 | Manual Scale | 13-10 |
| 13.7.2 | View All Data | 13-13 |
| 13.7.3 | View Temperature Profile | 13-14 |
| 13.7.4 | Change Plot Color | 13-15 |
| 13.7.5 | Peaks | 13-16 |
| 13.7.5.1 | Search for Peaks | 13-16 |
| 13.7.5.1.1 | Add Peaks | 13-17 |
| 13.7.5.1.2 | Redo Peak Search | 13-18 |
| 13.7.5.1.3 | Peak Search Parameters | 13-18 |
| 13.7.5.1.4 | Report Preview | 13-19 |
| 13.7.5.2 | Show/Update Current Peaks | 13-20 |
| 13.7.5.3 | Edit Base Points | 13-21 |
| 13.7.5.4 | Clear the Peaks | 13-23 |
| 13.7.5.5 | Label the Peaks | 13-23 |
| 13.7.5.6 | Change Search Parameters | 13-24 |
| 13.7.5.7 | Previous Search Results | 13-24 |
| 13.7.6 | Control Panel | 13-26 |
| 13.7.7 | Properties | 13-27 |
| 13.8 | How to Access the Scan Cursor | 13-28 |
| 13.9 | Using the Zoom Function | 13-29 |

| | | |
|---------|----------------------------|-------|
| 13.10 | Range Tool | 13-34 |
| 13.10.1 | Background Tools | 13-37 |

Chapter 14

Run Method

| | | |
|------|--------------------------------|------|
| 14.1 | Run Method Procedure | 14-1 |
|------|--------------------------------|------|

Chapter 15

Chromatogram Overlay

| | | |
|------|---------------------------------|------|
| 15.1 | Introduction | 15-1 |
| 15.2 | Chromatogram Overlay | 15-1 |
| 15.3 | Retention Time Shift | 15-4 |
| 15.4 | Chromatogram Subtract | 15-5 |

Chapter 16

Method Editor

| | | |
|----------|---|-------|
| 16.1 | The Method Editor | 16-1 |
| 16.2 | Wizard Mode | 16-2 |
| 16.3 | Accessing Method Editor | 16-3 |
| 16.4 | Description Screen | 16-4 |
| 16.5 | Startup | 16-5 |
| 16.5.1 | CMS5000 Temperatures (°C) | 16-6 |
| 16.5.2 | Method Type Selection | 16-6 |
| 16.6 | Inlet | 16-6 |
| 16.6.1 | Inlet States | 16-8 |
| 16.6.2 | GC Temperature Profiles | 16-12 |
| 16.6.3 | Scan Events | 16-13 |
| 16.7 | Search | 16-14 |
| 16.7.1 | Setting Up a Quantitative Search | 16-15 |
| 16.7.2 | Compound Specific Search Parameters | 16-17 |
| 16.8 | Data | 16-18 |
| 16.8.1 | Data File Information | 16-19 |
| 16.8.2 | Date and Time Appendix | 16-20 |
| 16.8.2.1 | Date and Time Format | 16-21 |
| 16.8.3 | Use Default Directory | 16-22 |
| 16.8.4 | Data Display | 16-22 |
| 16.9 | Summary Screen | 16-23 |
| 16.10 | Saving a Method | 16-24 |

Chapter 17

Calibration

| | | |
|----------|--|-------|
| 17.1 | Introduction To Calibration | 17-1 |
| 17.2 | Method Development | 17-1 |
| 17.3 | Check Standard | 17-2 |
| 17.4 | Calibrating the Check Standard | 17-2 |
| 17.5 | Calibrating the Analytical Method | 17-10 |
| 17.5.1 | Multiple Standards vs Multiple Calibration Methods | 17-10 |
| 17.5.2 | Water Standards | 17-11 |
| 17.5.3 | Air Standards | 17-14 |
| 17.5.3.1 | Directly Filling Tedlar Bag | 17-15 |
| 17.5.3.2 | Diluting Gas Samples | 17-16 |
| 17.5.4 | Running Standards | 17-19 |
| 17.6 | Using the Calibrate Function | 17-20 |
| 17.7 | Water Beta | 17-36 |
| 17.8 | Glossary of Terms in the Calibrate Window | 17-37 |
| 17.8.1 | Method | 17-37 |
| 17.8.2 | Data Files | 17-38 |
| 17.8.3 | Peak Search Section | 17-39 |
| 17.8.4 | Calibrate Options | 17-39 |
| 17.8.5 | Analytes | 17-39 |
| 17.8.6 | View Reports | 17-40 |
| 17.8.7 | Calibrate Display | 17-41 |

Chapter A

Appendix

| | | |
|-------|--------------------------------|-----|
| A.1 | Modbus Protocol | A-1 |
| A.2 | Ethernet Integration | A-4 |
| A.2.1 | CMS5000API.H | A-5 |

Chapter 1

Introduction

1.1 Introduction

CMS5000 Monitoring System is used to monitor volatile organic compounds (VOCs) in either water or air without requiring sample pre-treatment. Designed as a stationary instrument, CMS5000 is ideal for long-term VOC monitoring with minimal operator intervention required. (See [Figure 1-1](#) and [Figure 1-2](#).)

Air samples are collected directly into the instrument using an internal sample pump. Water samples are collected using a Purge and Trap sampling system. Samples are trapped on a Tri-Bed concentrator and thermally desorbed onto a low thermal mass gas chromatograph (GC) column. VOCs are separated while traveling through the column and are analyzed using a Micro Argon Ionization Detector (MAID).

Figure 1-1 Exterior CMS5000 in air sampling configuration

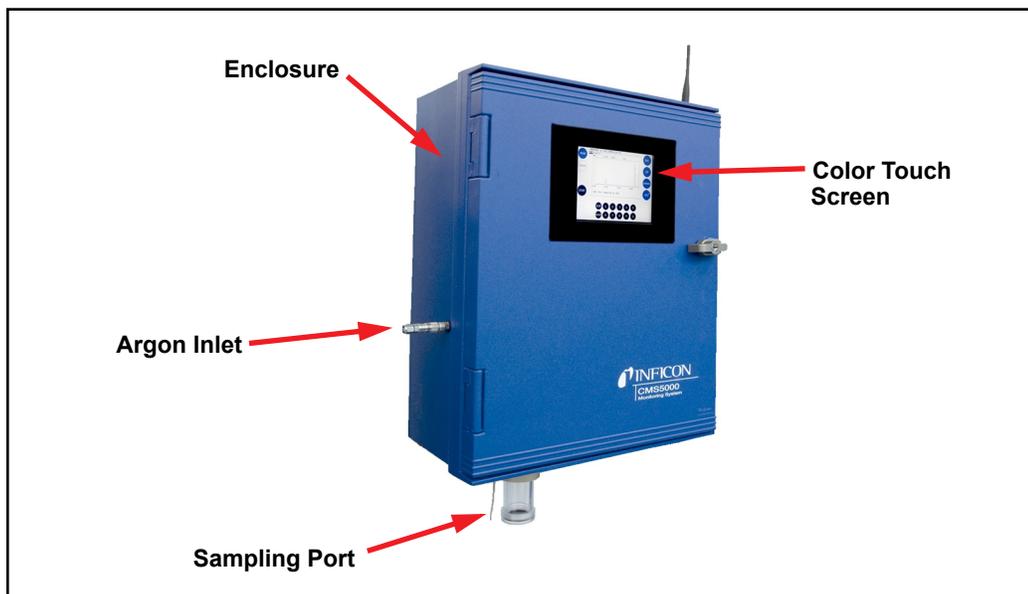
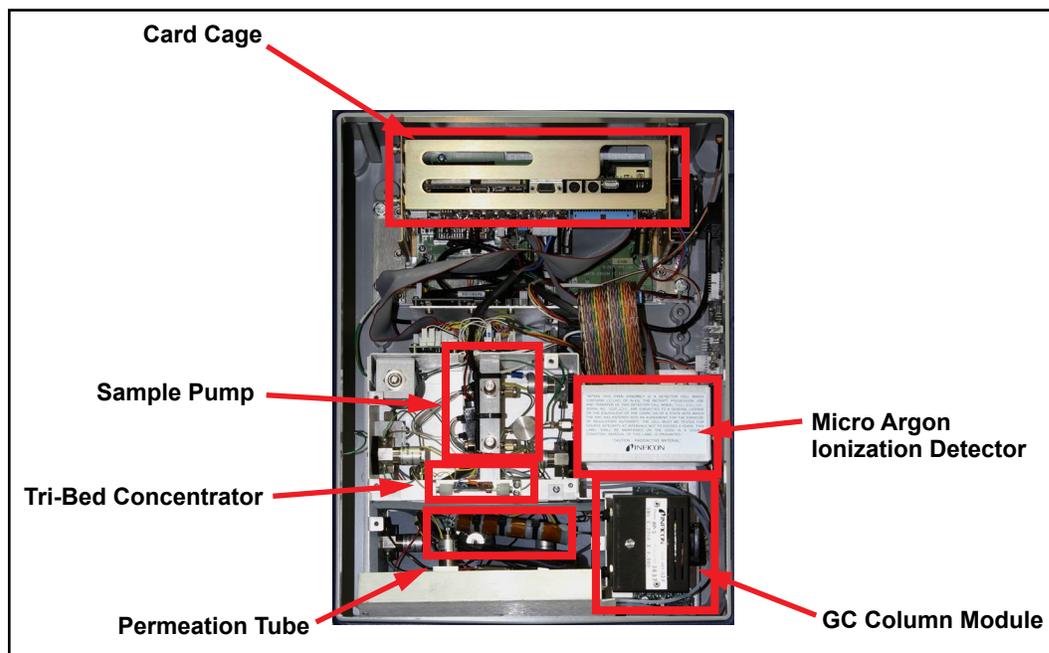


Figure 1-2 Interior CMS5000



1.2 Theory of Operation

1.2.1 Purge and Trap Sampling System

VOCs collected from air or water samples are drawn into CMS5000 by an internal pump and adsorbed onto the Tri-Bed concentrator. For air analysis, air is drawn directly into the instrument.

For water analysis, argon is bubbled into the sample. The bubbles rise and collect at the top, or headspace, of the sample collection tube. As the bubbles rise, a portion of the VOCs pass from the water phase to the gas phase, also known as “partitioning.” The ratio of the VOC concentration in the water phase, VOC_{water} , to the concentration in the gas phase, VOC_{gas} , is the partition coefficient. (See equation [1].)

$$\text{Partition Coefficient} = \frac{VOC_{water}}{VOC_{gas}} \quad [1]$$

Each compound will partition according to its solubility in water, its vapor pressure, the specific water sampling matrix, and water temperature. The quantity of VOCs detected is dependent on the partition coefficient. In general, less polar compounds are more readily detected than more polar compounds.

The VOCs are then desorbed into the GC column by heating the concentrator and reversing the carrier gas flow.

CMS5000 contains an onboard permeation tube containing toluene, which is used as a check standard for internal calibration. The lifetime of the permeation tube is approximately 6 to 8 years.

1.2.2 Gas Chromatograph

The gas chromatograph performs a time separation of the sample compounds.

Argon is used as the carrier gas to transport analytes through a capillary column module. The inside of the column is coated with a thin layer of material known as the stationary phase. The stationary phase selectively attracts components in a sample mixture. The mixture of sample compounds in argon gas, also known as the mobile phase, interact with chemicals of the stationary phase. The chemicals which spend the least time interacting with the stationary phase will elute (exit) from the column first.

The time taken for an individual compound to elute from the column is referred to as the *retention time* (RT). If the GC conditions remain constant, a given compound should elute from the column at the same time for each analysis. Retention time is primarily based on polarity, boiling point, and vapor pressure of a compound.

The retention time of a compound is affected by the column temperature. The column is housed in a temperature controlled oven that can be programmed to increase the temperature over time (ramping). As the temperature increases, compounds move through the column faster.

The signal of a gas chromatograph charted over time is called a chromatogram. The chromatogram depicts the separation of various compounds from one another by the action of the gas chromatograph.

1.2.3 Micro Argon Ionization Detector (MAID)



WARNING - Radioactive

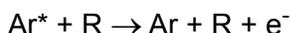
Due to U.S. Nuclear Regulatory Commission regulations, the CMS5000 detector oven, which contains a sealed radioactive source, may not be repaired by unauthorized personnel. INFICON will provide the maintenance, repair, replacement, and disposal of the radioactive source, as well as any part of the detector.

The Micro Argon Ionization Detector (MAID) is sensitive to organic compounds having an ionization potential of 11.7 eV or lower, which includes halomethanes, haloethanes, BTEX, and carbon tetrachloride. CMS5000 can detect these compounds, as well as other hydrocarbons, to parts-per-trillion (ppt) levels.

The MAID contains a nickel-63 (Ni-63) radioactive foil and uses argon as a carrier gas. Ni-63 naturally decays into copper-63, a stable isotope, and releases an energetic electron known as a beta particle (β particle). As argon flows over the Ni-63 foil, β particles collide and excite the argon atoms into a metastable state where an electron moves to a higher energy orbit. The excitation energy of argon is approximately 11.7 eV.

$\text{Ar} \rightarrow \text{Ar}^*$ (Energized to excited state)

When an organic molecule (R) enters the detector, it collides with the metastable argon (Ar^*). During this collision, energy is transferred to the organic molecule. The organic molecule will ionize if its ionization energy is 11.7 eV or less. The reaction is illustrated as follows:



High voltage applied across the detector draws electrons to the anode. As organic molecules are ionized, the ejected electrons produce a change in current, which is measured to produce a chromatogram.

1.3 Radioactive Source

CMS5000 MAID contains a metal foil plated with the radioactive isotope Ni-63, with an activity level of up to 2.4 millicuries. The half-life of Ni-63 is approximately 96 years. The source of the radioactivity is sealed within a stainless steel cylinder, located within the detector cavity. Because the instrument is manufactured at the INFICON facility in East Syracuse, NY, USA, New York State regulations are followed. Per New York State radioactive materials license regulations, a wipe test is required for the Ni-63 source every 36 months. The first test is completed at the factory prior to shipment.



WARNING - Radioactive

Do not attempt to repair the detector cell. If the detector cell does not exhibit an electronic signal, the foil may require replacement. Contact INFICON for repair or replacement of the detector cell.

The State of New York Department of Health, Bureau of Environmental Radiation Protection, and the United States Nuclear Regulatory Commission require either a Specific License or a General License to authorize possession and use of the radioactive source in the instrument. INFICON provides a General License to authorize operation of CMS5000 for all end users. A copy of the terms and requirements of a General Licensee (section 12 NYCRR, part 38:41, table 3, item b) accompany INFICON's transfer of each instrument. The safety requirements of the Specific License or General License are designed to protect the user and the public from unnecessary prolonged exposure to radiation. Following these requirements is imperative.



WARNING

CMS5000 has no user serviceable parts. Only factory trained personnel should perform service or maintenance on CMS5000.

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

NOTE: This Note paragraph provides additional information about the current topic.

HINT: This Hint paragraph provides insight into product usage.



WARNING

Failure to heed these messages could result in personal injury.



WARNING - Radioactive

This Warning paragraph warns against the presence of radioactive emissions which may cause physical injury.



CAUTION

Failure to heed these messages could result in damage to the instrument or lead to the loss of data.

1.5 How To Contact Customer Support

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

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

If experiencing a problem with CMS5000, please have the following information readily available:

- ◆ The Sales Order or Purchase Order number of the instrument purchase.
- ◆ The version of Windows operating system.
- ◆ A description of the problem.
- ◆ An explanation of any corrective action that may have already been attempted.
- ◆ The exact wording of any error messages that may have been received.

1.5.1 Returning CMS5000

Do not return any component of CMS5000 to INFICON before speaking with a Customer Support Representative and obtaining a Return Material Authorization (RMA) number. CMS5000 will not be serviced without an RMA number.

Packages delivered to INFICON without an RMA number will be held until the customer is contacted. This will result in delays in servicing CMS5000.

Chapter 2

Specifications

2.1 Gas Chromatograph Specifications

| | |
|--|---|
| GC Column | Standard: DB-1, 0.32 mm ID, 30 m, 4.0 μ m df or equivalent (Alternately, a custom, application specific module may be installed.) |
| Valves | Stainless Steel body / Teflon [®] diaphragm |
| Temperature Programmable Column Module Range. | 50-200°C |
| Carrier Gas | Argon (99.999%) @ 414-689 kPa (60-100 psi) |
| Variable Column Pressure Control | Regulator pre-set to 620.5 kPa (90 psi) |
| Sample Inlet | Air sampling tube or water vessel with purge-and-trap |
| Concentrator | Tri-Bed |

2.2 Micro Argon Ionization Detector (MAID) Specifications

| | |
|------------------------------------|---|
| Ionization Source | Ni-63 2.4 mCi |
| Repeatability | 5 replicates of 1 ppb benzene: RSD calculated <5% |
| Temperature | 110°C (Maximum) |
| Dynamic Range | 3 decades |
| Detection Limit | ppb to ppt for most analytes |

2.3 Communication

| | |
|--|---|
| Computer / Data | Internal Intel® Pentium® processor |
| Integration | TCP/IP USB for local diagnostics I/O Relay Contacts Modbus |
| FTP | Configurable for automated data upload |
| Storage | 160 GB (minimum) hard drive |
| System Status | Status table for system operating changes |
| Wireless Connectivity | 802.11 B/G |
| Display | 6.5 in. VGA color display with touch screen |

2.4 Physical Operating Requirements

| | |
|------------------------------------|--|
| Size | 43 x 83 x 26 cm (16.9 x 32.7 x 10.2 in.) |
| Weight | 25 kg (55.1 lb.) |
| Power Requirement | 100/120 V(ac) ± 10% nominal, 50/60 Hz, 3.6 A, or 230 V(ac) ± 10% nominal, 50/60 Hz, 2.2A A/C Max Draw 3.6 A at 120 V |

2.4.1 Operating Environment

| | |
|---|---|
| Temperature | 5–45°C (Water and Air) (41–113°F) |
| Relative Humidity | 5 - 95% relative humidity @ 31°C, non-condensing |
| Altitude | Up to 2000 m (6562 ft.) |
| Installation (Overvoltage) | Category II |
| Pollution Degree | Category II |

2.5 Analysis and Protocols

| | |
|--|--|
| Integrated Performance Standard | Toluene permeation tube for check standard calibration |
| Detectable Compounds | Volatile organic compounds with an ionization energy under 11.7 eV (e.g., halomethanes, haloethanes, BTEX, and carbon tetrachloride) |
| Acceptance Protocol | Initial setup with 19 compound standard, BTEX standard, or custom standard |
| Data Analysis | Automatic peak detection and area integration for known compounds |

Chapter 3

System Setup

3.1 CMS5000 Feature Options

3.1.1 Analytical Unit

| | |
|-------------------------------------|------------|
| CMS5000 w/ standard column. | 935-600-G1 |
| CMS5000 w/ custom column. | 935-600-G2 |

3.1.2 Sampling Source

| | |
|----------------------------------|------------|
| Water, No Vessel. | 935-700-G1 |
| Water, Standard Vessel | 935-700-G3 |
| Air, Sampling System. | 935-701-G1 |

3.1.3 Integration

| | |
|--|------------|
| Ethernet, 802.11g, Wireless | 935-710-G1 |
| I/O Relays and 1 m (3 ft.) cable, Ethernet, and 802.11g Wireless | 935-711-G1 |
| Modbus, I/O Relays and 1 m (3 ft.) cable, Ethernet, and 802.11g Wireless. | 935-711-G2 |
| Modbus, Ethernet, 802.11g Wireless | 935-711-G4 |

3.1.4 Ship Kits

| | |
|----------------------------------|------------|
| CMS5000 120 V (USA). | 935-721-G1 |
| CMS5000 230 V (Europe) | 935-721-G2 |
| CMS5000 230 V (UK) | 935-721-G3 |
| CMS5000 230 V (China). | 935-721-G4 |

3.1.5 Laptop Installed with CMS IQ Software

| | |
|---|------------|
| CMS IQ Software, No Laptop. | 935-030-G1 |
| Laptop w/CMS IQ Software (USA). | 935-731-G1 |
| Laptop w/CMS IQ Software (Europe) | 935-731-G2 |
| Laptop w/CMS IQ Software (UK). | 935-731-G3 |
| Laptop w/CMS IQ Software (China) | 935-731-G4 |

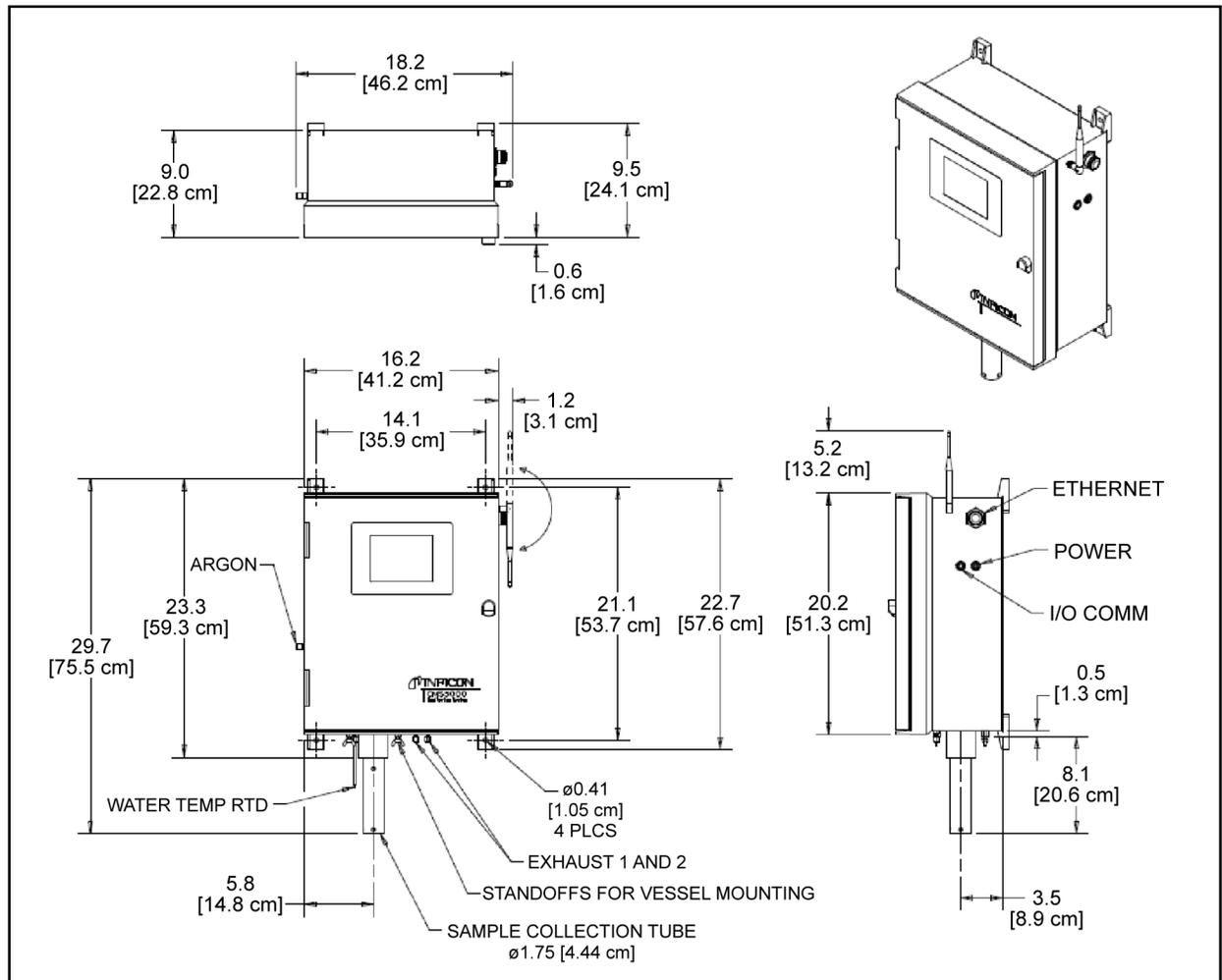
3.2 CMS5000 Ship Kit Contents

The ship kit contains the following items:

| | |
|--------------------------------------|---------------------------|
| Power Supply | 930-469-P1 (110 V USA) |
| | 930-469-P2 (230 V Europe) |
| | 930-469-G3 (230 V UK) |
| | 930-469-G4 (230 V China) |
| Ethernet Cable | 600-1319-P2 |
| CMS5000 Operator Manual | 074-508-P1 |
| Argon Tank Regulator | 935-412-P1 |
| Argon Fill Line | 935-212-G1 |
| Quick Disconnect Stem | 059-0329 |
| CMS5000 Training CD | 074-5020-G1 |

3.3 CMS5000 Diagram

Figure 3-1 CMS5000 dimensional diagram



3.4 Mounting Instructions



WARNING

CMS5000 Monitoring System weighs over 25 kg (55 lb.). Use proper safety procedures and PPE when mounting CMS5000.

CMS5000 Monitoring System requires mounting as well as some minor assembly. The four mounting brackets included in the ship kit need to be attached to the four corners on the back of the CMS5000. Position the bracket on the analytical module by lining up the openings in the bracket to the holes on the CMS5000. Place the washer over the hex bolt, and using a socket wrench, screw in the hex bolt until tight. (See Figure 3-2.) Refer to the instructions included with the bracket hardware.

NOTE: The nuts included with the hex bolts are not needed to mount the brackets to the CMS5000.

Figure 3-2 Attaching the mounting brackets



Structural mounting hardware is not included. Select the proper mounting hardware. CMS5000 is shipped with four (4) mounting brackets to support the instrument. The mounting surface must be able to support 25 kg (55.1 lbs), plus the weight of the water vessel or air sampling vessel.

CMS5000 weighs 25 kg (55.1 lbs). All plumbing to and from the sampling vessel must be supported independent of the analytical module, as the system design will not support any additional weight.

For air monitoring, CMS5000 should be mounted in an optimal location for collecting air samples of interest. Avoid locations affected by air currents from heating or cooling systems, doors, windows, or structural openings.

To ensure proper operation when utilizing CMS5000 for continuous water monitoring, it is necessary to determine optimal mounting height and CMS5000 placement. This is to accommodate both the water intake, as well as allow for clearance of the sample collection tube when attaching and removing the sampling vessel. Allow a minimum of a 38.1 cm (15 in.) clearance below the mounted sampling vessel for vessel removal. Verify that CMS5000 is level when mounted or that any slope is less than 5%. (Refer to Figure 3-1 for unit dimensions.)



WARNING

If CMS5000 is used in a manner not specified by INFICON, the protection of interior components provided by the casing may be impaired.

3.5 Water Monitoring Assembly Instructions

NOTE: If using CMS5000 for air monitoring, skip to section 3.8, Air Monitoring Assembly Instructions, on page 3-10.

- 1 The temperature sensor, or RTD, is unattached and taped to the bottom of CMS5000 for shipment. Remove the tape, guide the excess wire back into the port nearest to the beige sample collection tube mounting bracket located on the bottom of CMS5000.
- 2 Tighten the stainless steel Swagelok® fitting 1/4 turn past finger-tight, using a 7/16 in. open-ended wrench. (See Figure 3-3.)

Figure 3-3 Attaching the temperature sensor



- 3 Install the PEEK™ purge tube (found in the ship kit) to the left port, inside the beige sample collection tube mounting bracket. (See Figure 3-4.)

**CAUTION**

Ensure the sample inlet and purge tube are installed in the proper port.

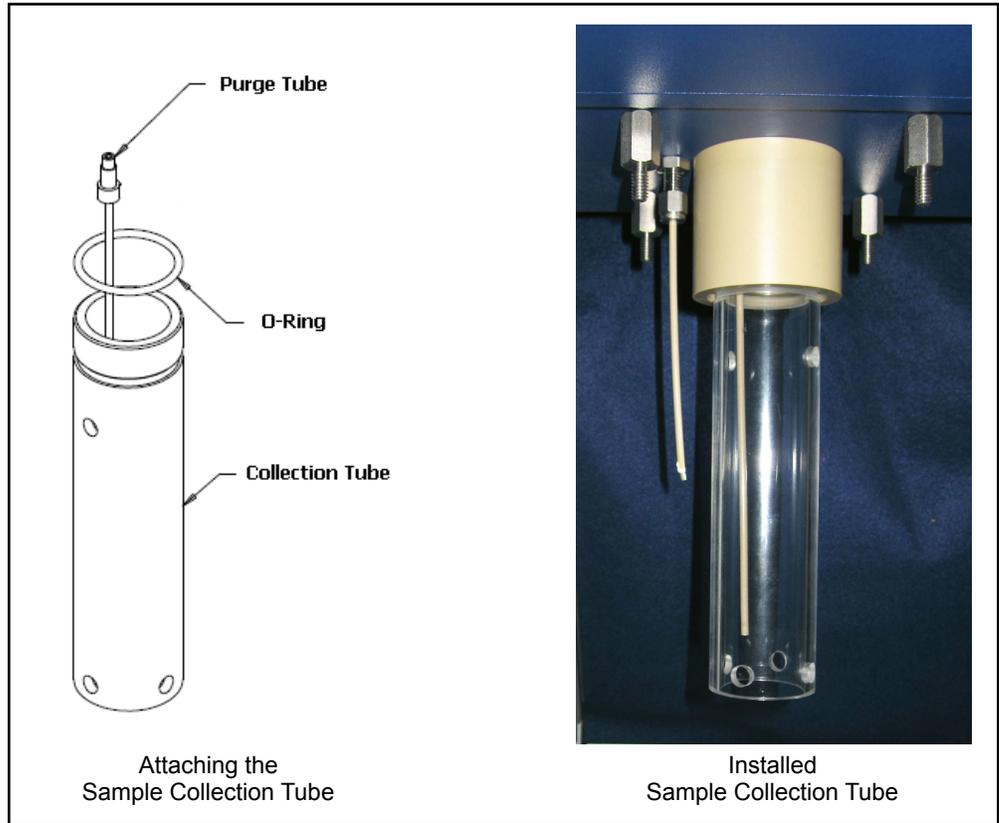
Placing the sample inlet line in the center port during water sampling will allow water to be drawn into CMS5000 causing severe damage.

Figure 3-4 Attaching the PEEK purge tube for water monitoring



- 4** Install the collection tube o-ring into the beige sample collection tube mounting bracket. (Refer to Figure 3-4.)
- 5** Screw the clear acrylic sample collection tube from the ship kit into the beige sample collection tube mounting bracket located on the bottom of CMS5000 until finger-tight. Do not overtighten. (See Figure 3-5.)

Figure 3-5 Attaching the sample collection tube

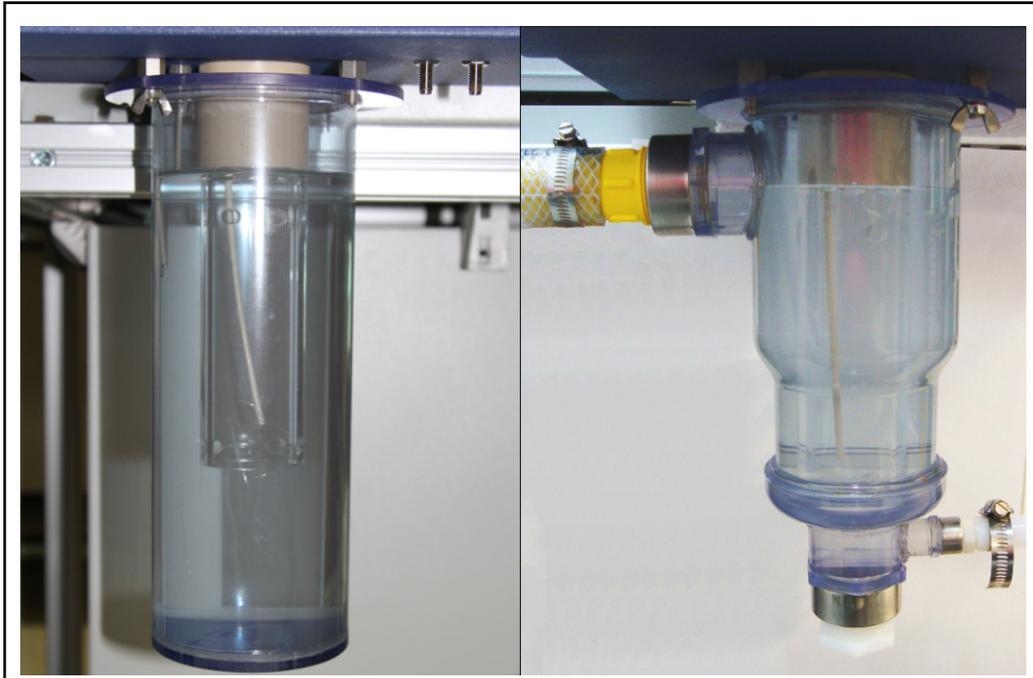


3.6 Attaching the Water Sampling Vessel

NOTE: If using CMS5000 for air monitoring, skip to section 3.8, Air Monitoring Assembly Instructions, on page 3-10.

The optional calibration and sampling vessels mount to the bottom of CMS5000 using the wing nuts supplied with the vessel. (See Figure 3-6.)

Figure 3-6 Optional calibration and sampling vessels (shown left to right)



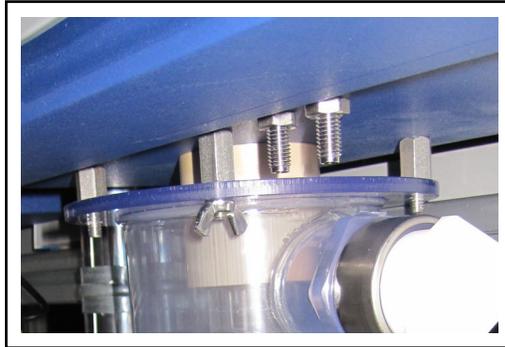
NOTE: Calibration and sampling vessel designs may vary.

To attach the sampling vessel to CMS5000:

- 1 Align the four openings on the flange of the sampling vessel with the mounting screw standoffs attached to CMS5000.
- 2 Hold the vessel against the mounting screw standoffs.

- 3 Secure the sampling vessel in place by threading on the wing nuts until finger-tight. (See Figure 3-7.)

Figure 3-7 Attaching the sampling vessel



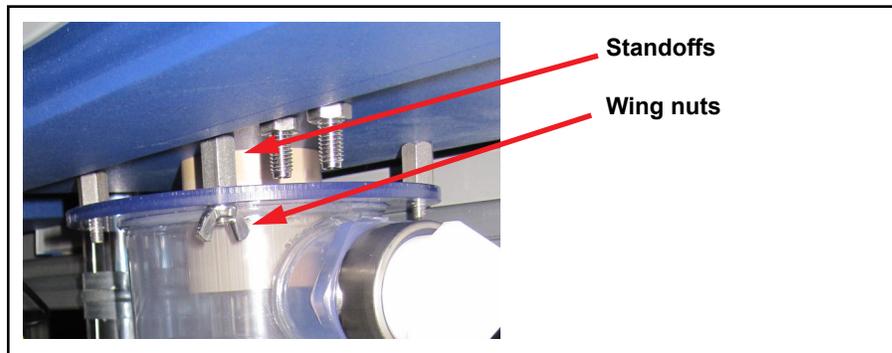
The standoffs provide space between CMS5000 and the vessel to prevent water from entering CMS5000 in the event of water overflow. (See Figure 3-8.)



CAUTION

Do not allow water to enter the sampling inlet. Severe damage to CMS5000 will occur.

Figure 3-8 Standoffs to prevent overflow



3.7 Connecting the Water Supply

NOTE: If using CMS5000 for air monitoring, skip to section 3.8, Air Monitoring Assembly Instructions, on page 3-10.

It is the responsibility of the integrator to configure all plumbing. Support the weight of all plumbing lines and associated hardware independently of CMS5000.



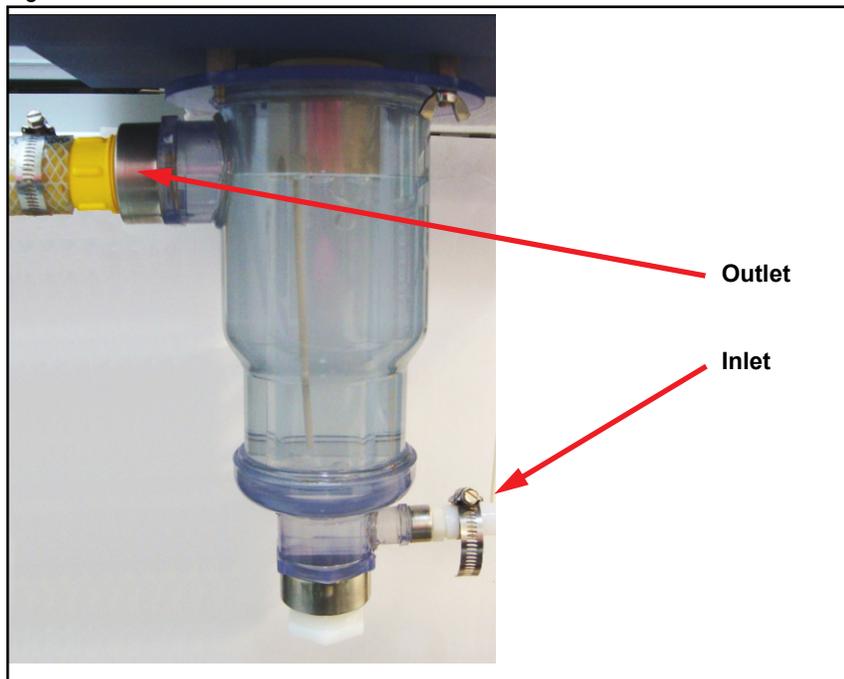
WARNING

INFICON is not responsible for personal injury or damage to CMS5000 that is a result of improper plumbing connections.

Attach the water inlet line to the 1/4 in. threaded side port, at the bottom of the sampling vessel. Attach the outlet line to the 1-1/4 in. threaded side port, at the top of the sampling vessel. The outlet line must be larger than the water inlet line. Flow rate should not exceed 1 L/min. (See Figure 3-9.)

NOTE: The 1-1/4 in. connection at the bottom of the sampling vessel is an optional connection for fast sample turnover or particulate removal.

Figure 3-9 Water flow



3.8 Air Monitoring Assembly Instructions

CMS5000 monitors air via two possible configurations:

- ◆ Ambient air sampling, uses an air collection tube with integrated filter to prevent large particulates from entering CMS5000
- ◆ In-line air sampling

3.8.1 Ambient Air Sampling

Ambient air sampling requires the air sampling tube. (See Figure 3-10.)

Figure 3-10 CMS5000 air sampling tube



NOTE: The temperature sensor, or RTD, is unattached and taped to the bottom of CMS5000 for shipment. The RTD is designed for water monitoring only. Attaching the RTD is optional for air monitoring and will not affect analysis. Refer to [section 3.5, Water Monitoring Assembly Instructions](#), on page 3-4 for instructions on attaching the RTD.

- 1 Install the collection tube o-ring into the beige sample collection tube mounting bracket. (Refer to Figure 3-11.)

Figure 3-11 Connect o-ring to top of sample collection tube



- 2 Attach the air sampling tube by threading it into the beige sample collection tube mounting bracket, located on the bottom of CMS5000, until finger-tight. Do not overtighten. (See Figure 3-12.)

Figure 3-12 CMS5000 with air sampling tube attached

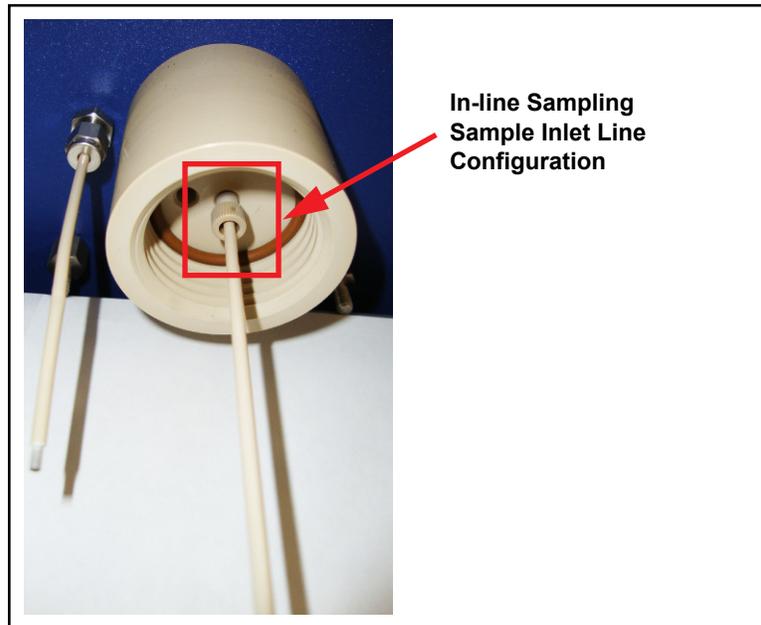


3.8.2 In-line Air Sampling

In-line air sampling can be used when calibrating air standards, or when sampling directly from a closed system.

To prepare CMS5000 for in-line air sampling, attach the sample inlet line to the center port. (See Figure 3-13.)

Figure 3-13 Sample inlet line in position for in-line air sampling



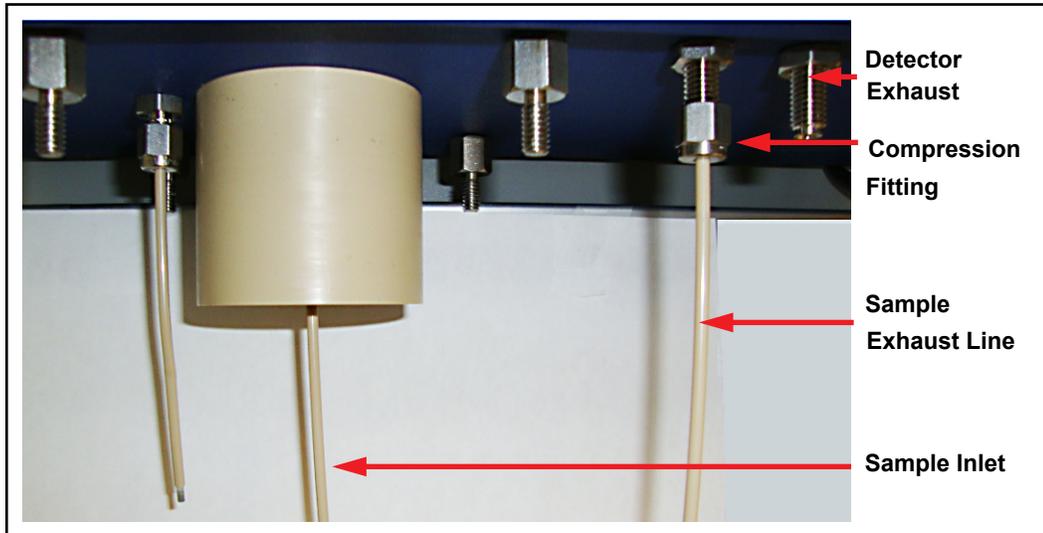
CAUTION

Do not allow water to enter the sampling inlet. Severe damage to CMS5000 will occur if water enters the sampling inlet.

3.8.2.1 In-Line Sampling

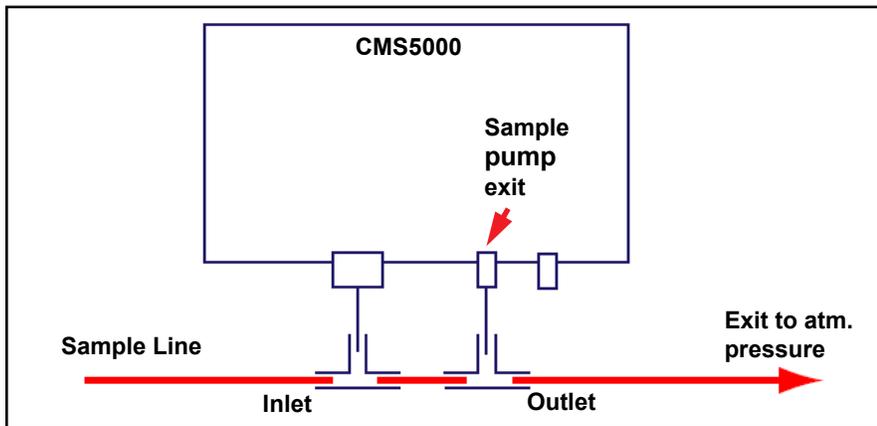
The pressure of the sample in the air line must be greater than the pressure of the CMS5000 exhaust, and should not exceed 1 atmosphere (atm). Maintaining the pressure differential will prevent any sample from re-entering the sample path and collecting on the concentrator. The exhaust line is attached to the sample exhaust port via a compression fitting. (See Figure 3-14.) The exhaust line diameter must be greater than or equal to the diameter of the sample inlet line.

Figure 3-14 Exhaust line attached



An example of in-line sampling setup is shown in Figure 3-15.

Figure 3-15 Example in-line air sampling setup



3.9 Connecting the Argon Supply

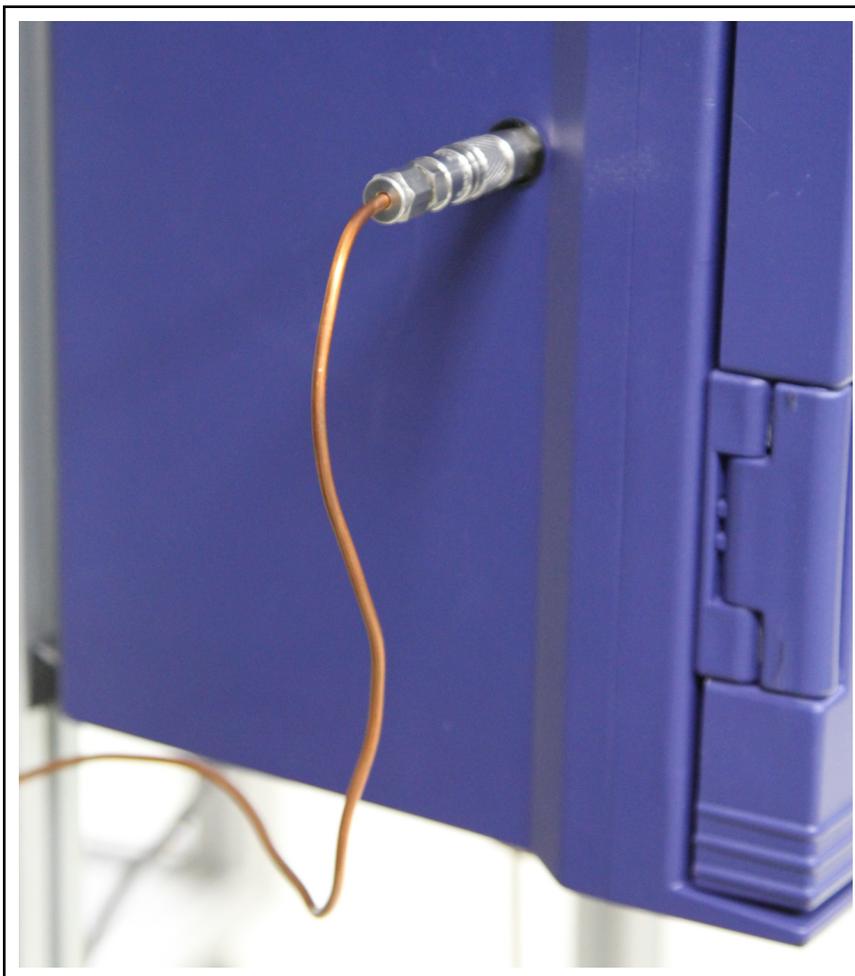
User supplied ultra-high purity grade argon (99.999%) is required for optimal operation of the MAID. The included regulator is preset at the factory to 6.2 kPa (90 psi). Connect the argon supply to CMS5000 using the included copper argon supply line and quick connect valve. The fitting for the quick connect valve is located on the left side of the analytical module. (See Figure 3-16.)



CAUTION

Failure to use the recommended argon purity, substituting the copper argon supply line with a permeable material (e.g. Teflon) or adding a join in the line will result in poor instrument performance and possible instrument damage.

Figure 3-16 Connecting the argon supply to CMS5000



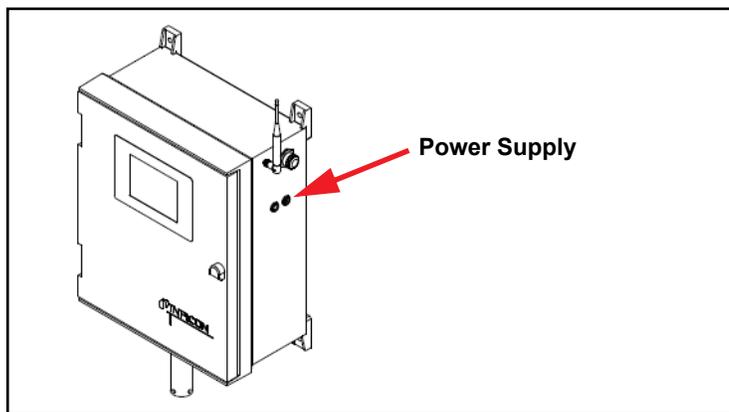
3.10 Connecting the Power Supply

- 1 Connect the 4-pin Fischer® connector from the power supply to the 4 pin receptacle near the rear of the upper right side of CMS5000.
- 2 Connect the plug end of the power supply to a reliable earthed socket outlet. CMS5000 will power on automatically. CMS5000 does not have an “on/off” switch. (See Figure 3-17.)

HINT: Position the power cord for easy access, since it is used for shutting off and restarting the instrument.

NOTE: CMS5000 should be operated with the front panel door closed and fastened in order to ensure the stability of the heated internal components.

Figure 3-17 Connecting the power supply



3.11 Instrument Equilibration

When CMS5000 is initially set up, or after prolonged periods of time when CMS5000 is powered off or is not being purged with argon, the MAID detector will require equilibration. Power on the unit and purge with argon for 24 - 28 hours.

CMS5000 contains an onboard permeation tube containing toluene, which is used for internal calibration. The permeation tube is designed to continually emit toluene at a consistent rate when heated to 55°C.

The detector is considered to be equilibrated when a stable response for toluene is observed from consecutive runs of the check standard method. When the instrument is initially set up, or after prolonged periods of time when CMS5000 is powered off, small amounts of toluene may build up and need to be purged before stable operation can be attained. (See section 17.4, Calibration.)

3.11.1 Calibration

Once CMS5000 is equilibrated, the check standard method and analytical method must be calibrated. (See Chapter 17, Calibration.)

3.12 Communication Options

3.12.1 Connecting the Ethernet Cable

The Ethernet port, used to connect CMS5000 to a computer or network, is located on the upper right side of CMS5000 next to the wireless antenna.

- 1 Unscrew and remove the water tight shipping cap.
- 2 Plug the end of the Ethernet cable with the water tight cap into CMS5000. Screw on the water tight cap until finger-tight. (See Figure 3-18.)
- 3 Plug the other end of the Ethernet cable into a computer or network.

NOTE: See Chapter 4, [Setting Up Computer Communication](#) for additional information.

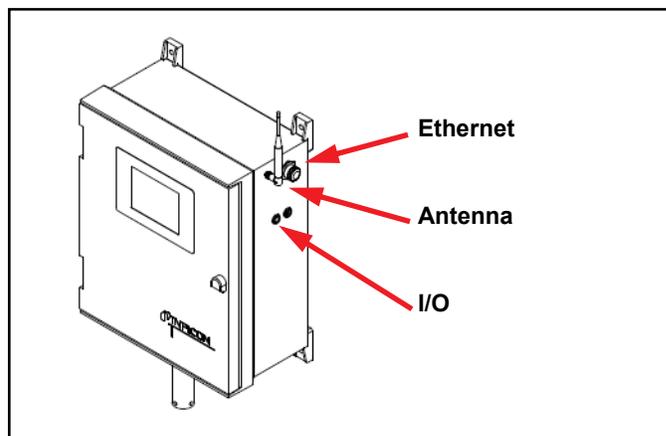
3.12.2 Attaching the Wireless Antenna

For wireless communication with CMS5000, the antenna must be attached to the port in front of the Ethernet port. Screw the antenna into the port until finger-tight. (See Figure 3-18.)

3.12.3 Connecting the I/O Cable

The multi-pin I/O receptacle is located on the right side of CMS5000, next to the power supply receptacle. (See Figure 3-18.) Plug the 19-pin Fischer Connector from the I/O cable into CMS5000 and configure the other end of the cable as desired. (See Chapter 5, [Input/Output Configuration](#) for more information.)

Figure 3-18 Connecting the Ethernet and I/O



Chapter 4

Setting Up Computer Communication

4.1 Introduction

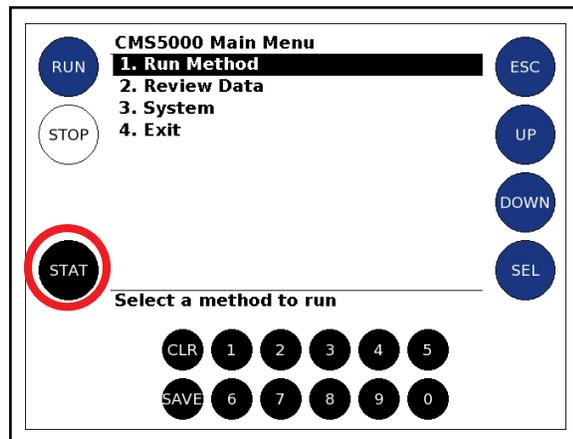
Communication can be established between CMS5000 and the computer to run analyses and review data from the computer. It is necessary to establish this communication to calibrate CMS5000 methods and setup software parameters. Communication can be established using an Ethernet cable or the CMS5000 wireless connection.

4.2 Configuring the Computer for CMS5000 Communication

In order to communicate with CMS5000, the computer must be assigned a manual IP Address, based on the IP Address of CMS5000.

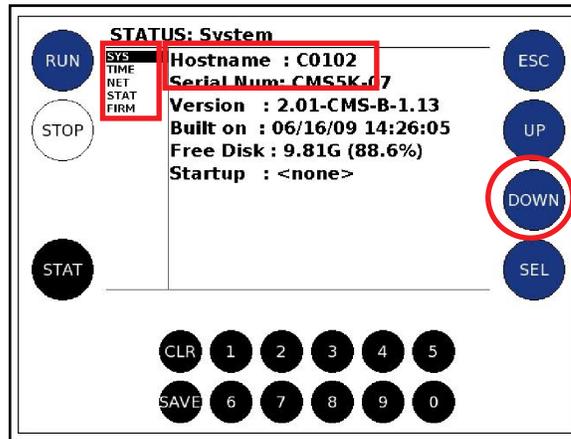
- 1 Tap **STAT** on the front panel of CMS5000 to display the **STATUS** screen. (See Figure 4-1.)

Figure 4-1 STAT button



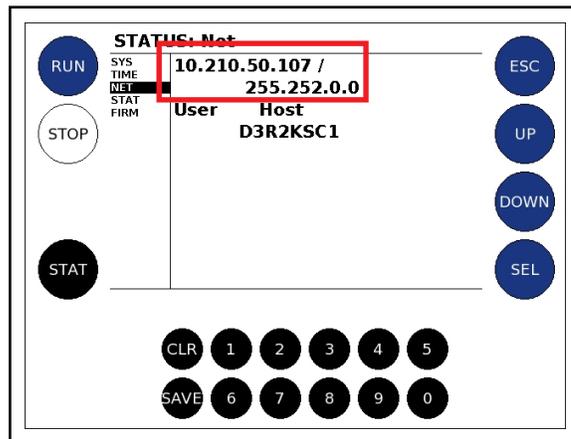
- The C# (format Cxxxx) of CMS5000 is listed under **Hostname** in the **SYS** tab. Tap **DOWN** to highlight **NET**. (See Figure 4-2.)

Figure 4-2 Accessing NET screen



- Each CMS5000 will have a unique IP address, for example: 10.210.50.107. The subnet mask is also displayed on the **NET** screen, for example: 255.252.0.0. (See Figure 4-3.)

Figure 4-3 NET screen



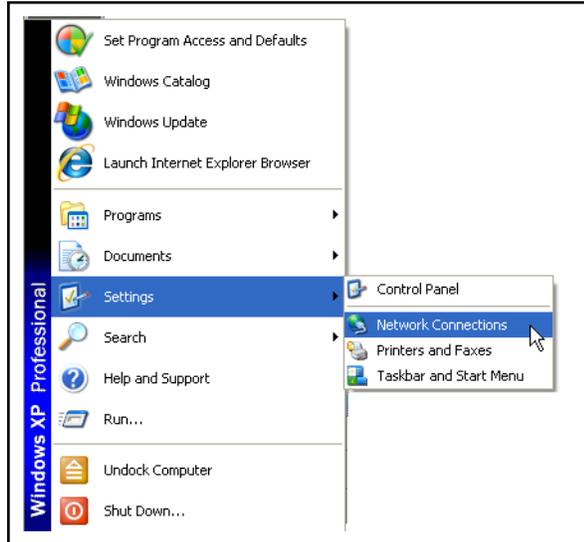
- On the computer, click **Start**. (See Figure 4-4.)

Figure 4-4 Start button



4a Hover over **Settings** and click **Network Connections**. (See Figure 4-5.)

Figure 4-5 Network Connections

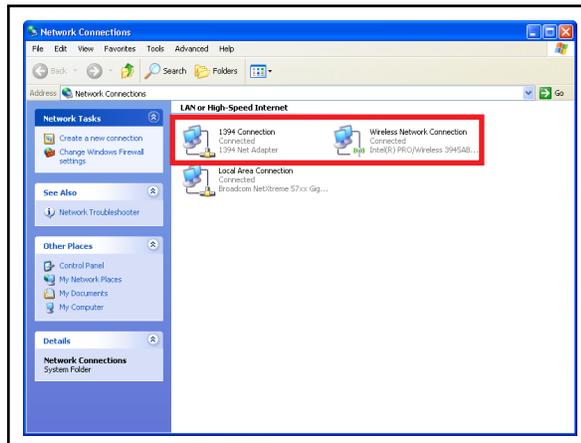


NOTE: Appearance of windows may vary depending on the operating system in use.

5 Double-click the desired connection type. (See Figure 4-6.)

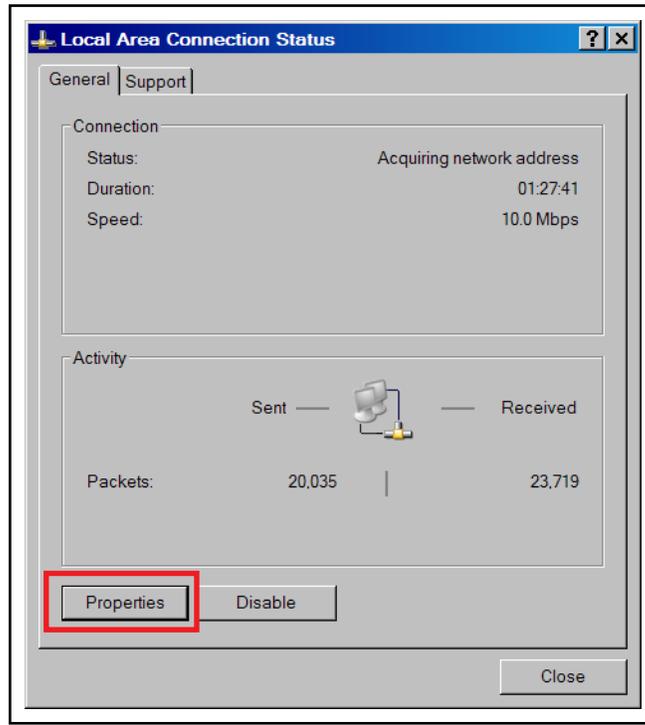
- ◆ **Local Area Connection** to connect with an Ethernet cable
- ◆ **Wireless Connection** to connect wirelessly

Figure 4-6 Select connection



- 6 The **Connection Status** window will display. Click **Properties**.
(See Figure 4-7.)

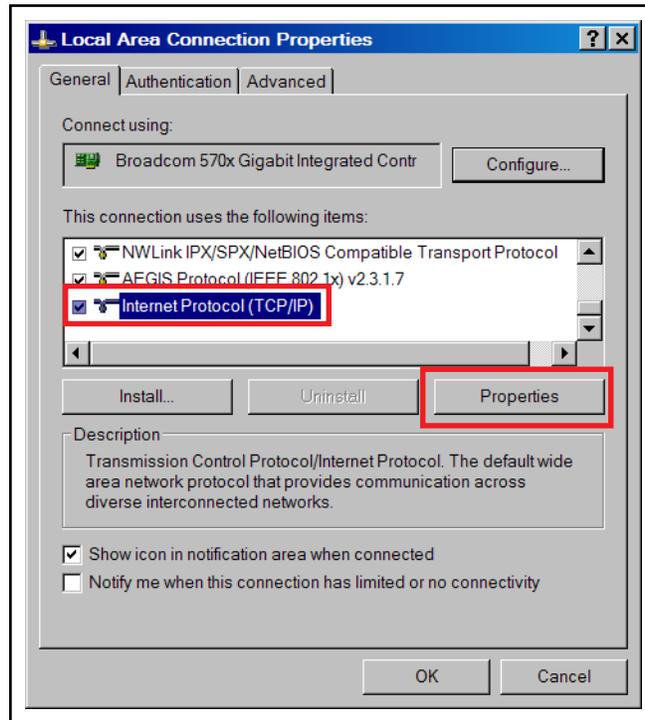
Figure 4-7 Local Area Connection Status window



NOTE: The same process is followed when entering an IP address for a wired or wireless connection; however, the IP addresses entered for each differ as described in the following sections.

- 7 On the **General** tab, scroll down and highlight **Internet Protocol (TCP/IP)**, click **Properties**. (See Figure 4-8.)

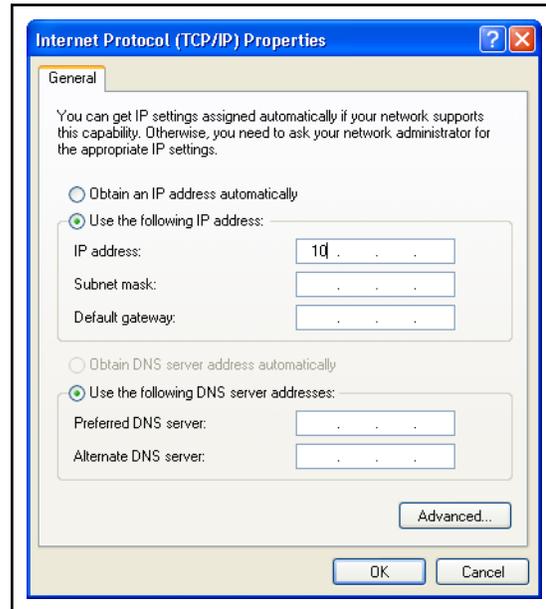
Figure 4-8 Selecting Internet Protocol (TCP/IP) and Properties button



NOTE: If there is more than one Internet Protocol to choose from, select **Internet Protocol Version 4 TCP/IPv4**.

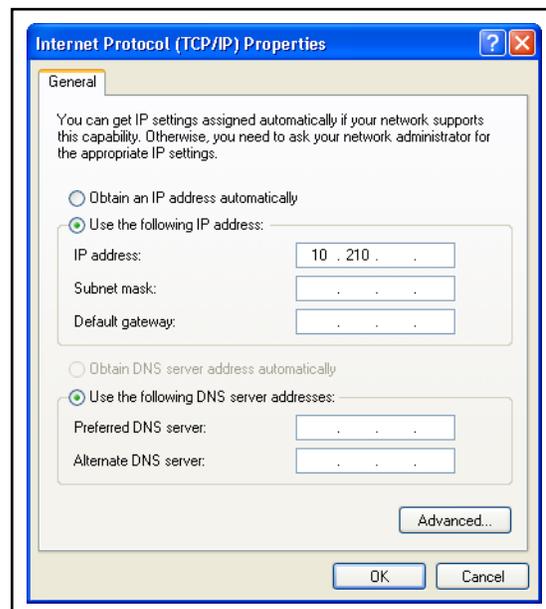
- 8 Select **Use the following IP address**. (See Figure 4-9.)
- 9 For the first segment, enter the first number of the IP address, displayed on CMS5000. For example, if the IP address is **10.210.50.107**, enter **10** into the first slot. Refer to **Step 1**, **Step 2** and **Step 4** of this section to find the IP address for CMS5000.

Figure 4-9 Entering first segment of IP address



- 10 For the second segment of the IP address, enter **210** if connecting with an Ethernet cable or **209** if connecting via wireless. (See Figure 4-10.)

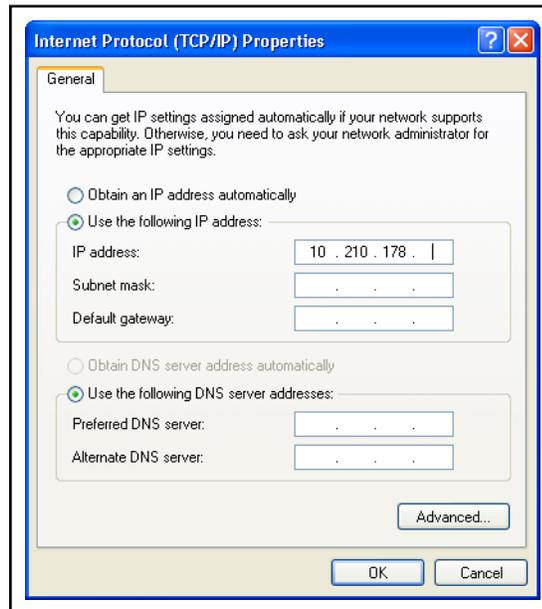
Figure 4-10 Entering second segment of IP address



- 11** For the third segment of the IP address, add 128 to the number displayed on CMS5000. In this example, adding 128 to 50 equals 178, so **178** would be entered into the third slot. (See Figure 4-11.)

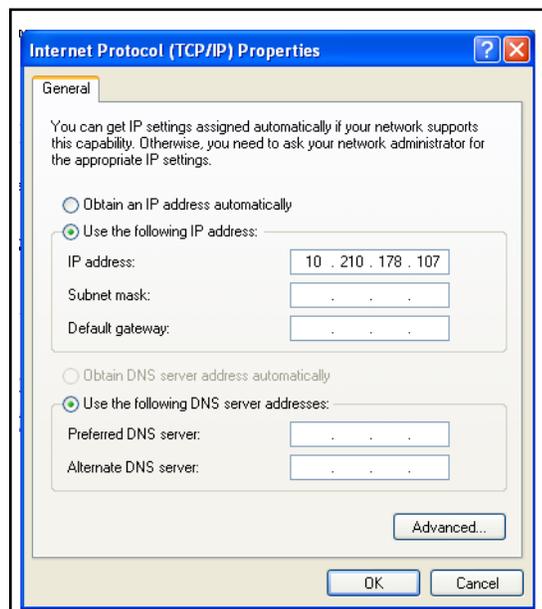
NOTE: The maximum total number cannot exceed 255. If the total of the third number is greater than 255, add 5 to the original third number.

Figure 4-11 Entering third segment of IP address



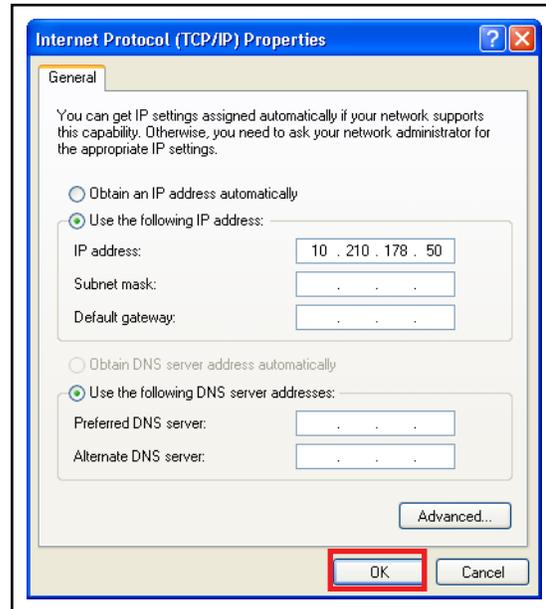
- 12** For the fourth segment, enter the last number of the IP address displayed on CMS5000. In this example, **107** would be entered into the fourth slot. (See Figure 4-12.)

Figure 4-12 Entering fourth segment of IP address



- 13 Repeat steps Step 9 through Step 12 to enter the Subnet mask: **255.252.0.0**
- 14 Click **OK** to close the **Internet Protocol (TCP/IP) Properties** window. (See Figure 4-13.)

Figure 4-13 Closing the Internet Protocol Properties window



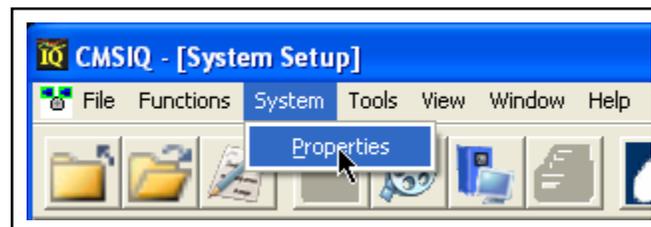
4.3 Setting Up Computer Communications

NOTE: Setting up communication is an Advanced User function. To change the access level, see section 12.2.6.4, Set Access Level, on page 12-29.

NOTE: CMS IQ must be installed on the computer. Instructions for installation are included with the installation CD.

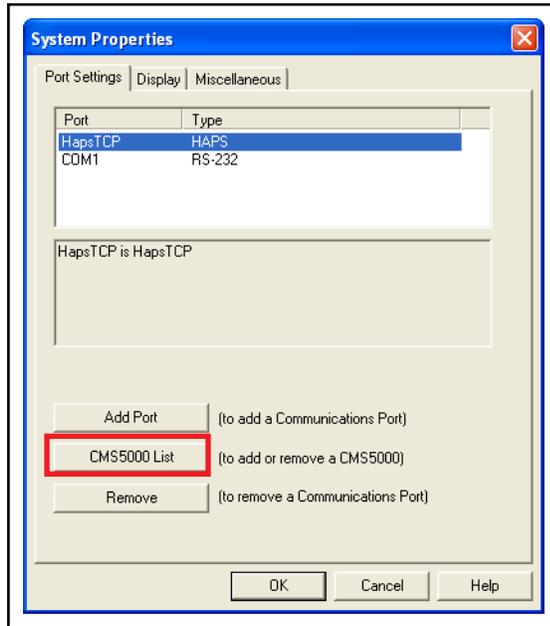
- 1 Open CMS IQ Software.
- 2 From the **System** menu, select **Properties**. The system properties window will open. (See Figure 4-14.)

Figure 4-14 Selecting Properties from the System menu



- 3 Click **CMS5000 List**. (See Figure 4-15.)

Figure 4-15 CMS5000 List button

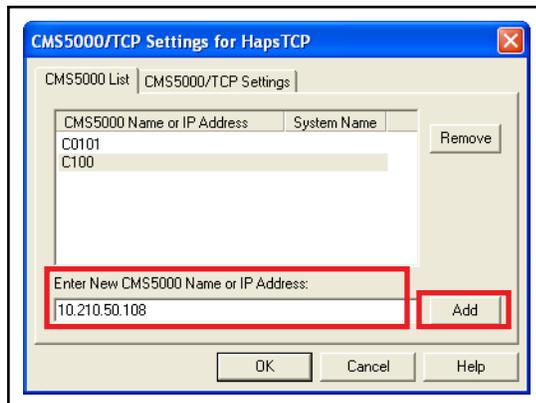


- 4 Enter the CMS5000 C# or IP address into the **Enter New CMS5000 Name or IP Address** box. (See Figure 4-16.)

NOTE: The C# (format: Cxxxx) and IP address can be found on the front panel of CMS5000 by tapping **STAT** from the Main Menu. Refer to section 4.2, Configuring the Computer for CMS5000 Communication, on page 4-1.

- 5 Click **Add**. (See Figure 4-16.)

Figure 4-16 Add CMS5000

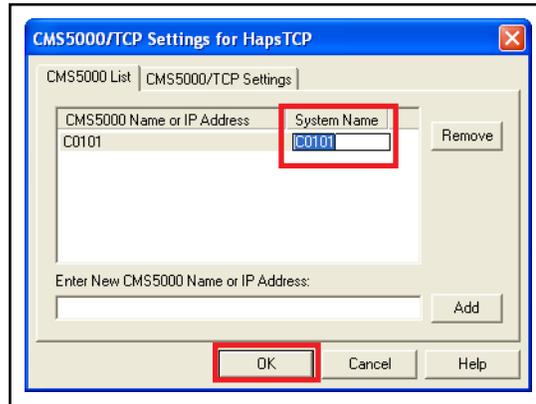


- 6 The newly added CMS5000 will be displayed in the **CMS5000 List**. (See Figure 4-17.)

NOTE: To make a custom name for the instrument, highlight the System Name box and type in the desired name.

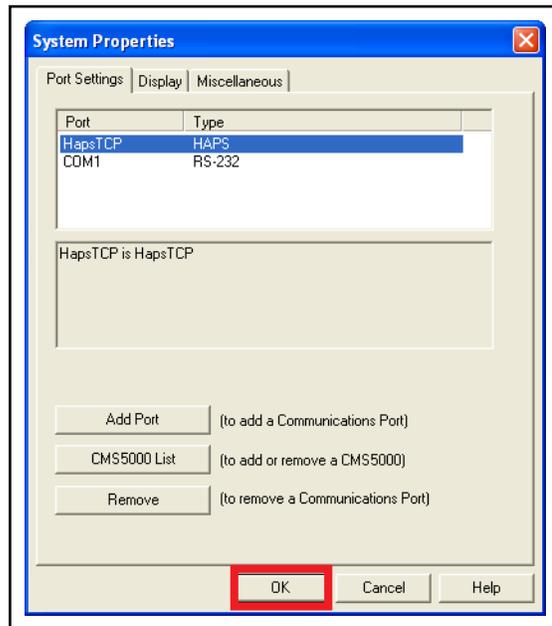
7 Click **OK**.

Figure 4-17 Closing the CMS5000/TCP window



8 Click **OK** to close the System Properties window. (See Figure 4-18.)

Figure 4-18 Closing the System Properties window



- 9 The newly added **CMS5000** icon will now be displayed at the bottom of the System Setup window. (See Figure 4-19.) When the CMS5000 icon is overlaid with a gray “X,” the CMS5000 is not trying to communicate with the computer.

Figure 4-19 Newly added CMS5000



- 10 Clicking the **CMS5000** icon will begin communication between CMS5000 and the computer, indicated by the absence of the “X” over the CMS5000 Sensor in the System Setup window. (See Figure 4-20.)

Figure 4-20 Active CMS5000 sensor icon



NOTE: If CMS IQ is configured for multiple connections, right click on the desired CMS icon and select **Bring Online**. (See section 12.2.5.3, Miscellaneous, on page 12-20.)

If the CMS5000 icon is overlaid with a blue “X,” communication was established and then lost. (See Figure 4-21.) If the CMS5000 icon is overlaid with a red “X,” communication cannot be established. (See Figure 4-21.) If either “X” is overlaid on the CMS5000 icon, confirm the computer is connected through either an Ethernet or wireless connection, and the IP address is properly configured. (Refer to section 4.2, Configuring the Computer for CMS5000 Communication, on page 4-1.) If CMS5000 still does not connect to the computer, restart CMS5000. (See Chapter 11, Exit Function.)

Figure 4-21 Communication between CMS5000 and computer has been lost



Figure 4-22 Communication cannot be established between CMS5000 and computer



4.4 Wireless Regulatory Compliance Information

4.4.1 Regulatory Compliance Information for UNITED STATES Users

This section of the Operating Manual lists FCC compliance information for CMS5000 wireless communication.

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

FCC ID: F4AWLNN551

This device complies with Part 15 of the FCC rules and is subject to the following two conditions:

- 1 This device may not cause harmful interference.
- 2 This device must accept any interference received, including interference that may cause undesired operation.



CAUTION

To maintain compliance with FCC standards and regulations and to ensure the proper operation of the wireless communication system used within CMS5000, ONLY use the antenna that was originally supplied with the instrument. If original antenna is lost or damaged, please contact the INFICON service department for a replacement antenna (IPN 035-0050).

4.4.1.1 FCC Statement

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

- ◆ Reorient or relocate the receiving antenna
- ◆ Increase the separation between the equipment and receiver

- ◆ Connect the equipment into an outlet on a circuit different from that to which the receiver is connected
- ◆ Consult the dealer or an experienced radio/TV technician for assistance

4.4.1.2 FCC RF Exposure Statement



WARNING

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

4.4.2 Regulatory Compliance Information for CANADIAN Users

This section of the Operating Manual lists Industry Canada (IC) compliance information for CMS5000.

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

IC: 3913A-WLNN551

This device complies with RSS-210 of Industry Canada (IC) and is subject to the following two conditions:

- 1** This device may not cause harmful interference.
- 2** This device must accept any interference received, including interference that may cause undesired operation.

4.4.2.1 Industry Canada (IC) Notices

This equipment complies with Canadian RSS-210.



CAUTION

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

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

Chapter 5

Input/Output Configuration

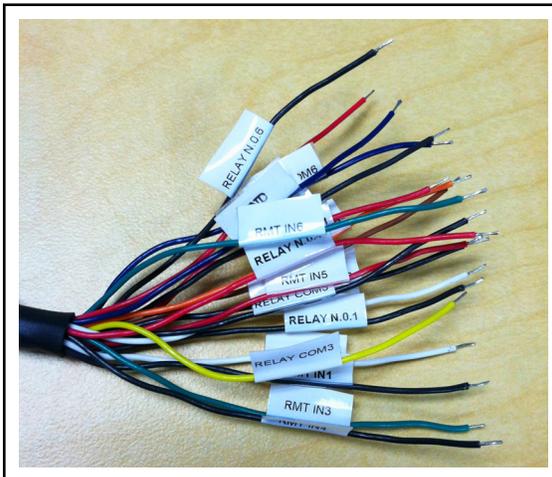
5.1 Introduction

CMS5000 is equipped with a 19-pin input/output (I/O) port. The optional I/O cable (PN 600-1388-P1) can be configured to allow remote triggering of methods. The I/O cable also allows for the external transmission of alarms indicating that argon cylinder replacement is required, and a component being measured has exceeded a set level. (See Figure 5-1.) The leads of the I/O cable are individually tagged. (See Figure 5-2.)

Figure 5-1 19-Pin I/O port and associated cable



Figure 5-2 Labeling of 19-pin I/O cable leads



5.2 Input Method Triggering

CMS IQ software allows the assignment of up to four input methods. The associated leads on the I/O cable can be configured to trigger the start of the defined methods.

- 1 Define the desired input methods in CMS IQ software. See [section 6.5, Input Methods](#), on page 6-15 for information on defining input methods.
- 2 To trigger the start of a method remotely, the appropriate lead of the I/O cable needs to contact either of the ground leads as follows:

Input method 1 **RMT IN1**

Input method 2 **RMT IN2 (White)**

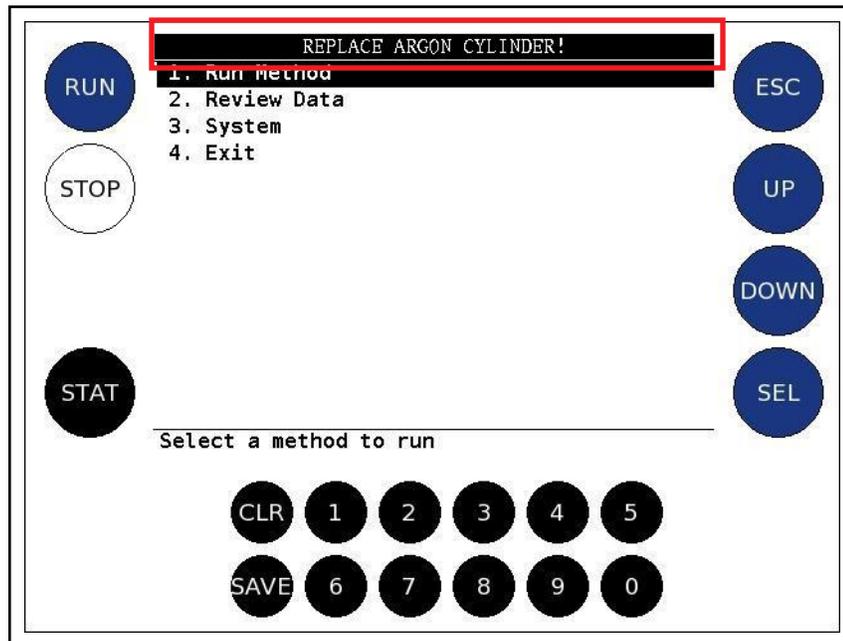
Input method 3 **RMT IN3**

Input method 4 **RMT IN4**

5.3 Replace Argon Cylinder Alarm

When the supply of argon has decreased to a point where CMS5000 can no longer operate, CMS5000 will actuate an internal relay establishing continuity between the **RELAY NO 3** and **RELAY COM3** leads of the I/O cable. The user is responsible for determining how the output signal is integrated into their system. A **REPLACE ARGON CYLINDER!** message will also appear on the CMS5000 front panel, as shown in [Figure 5-3](#).

Figure 5-3 REPLACE ARGON CYLINDER! warning message

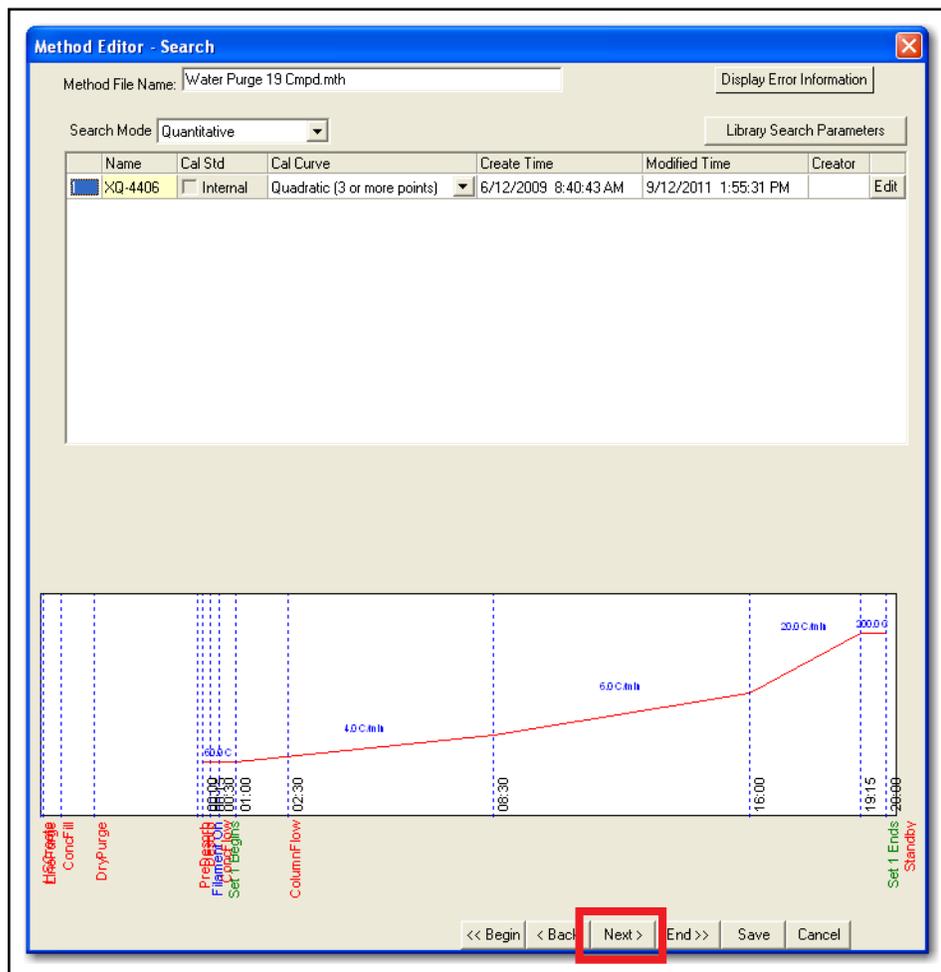


5.4 Out of Specification Alarm

Actionable alarms can be defined in a method, for individual analytes, that will trigger an output through the I/O cable when an out of specification result is obtained.

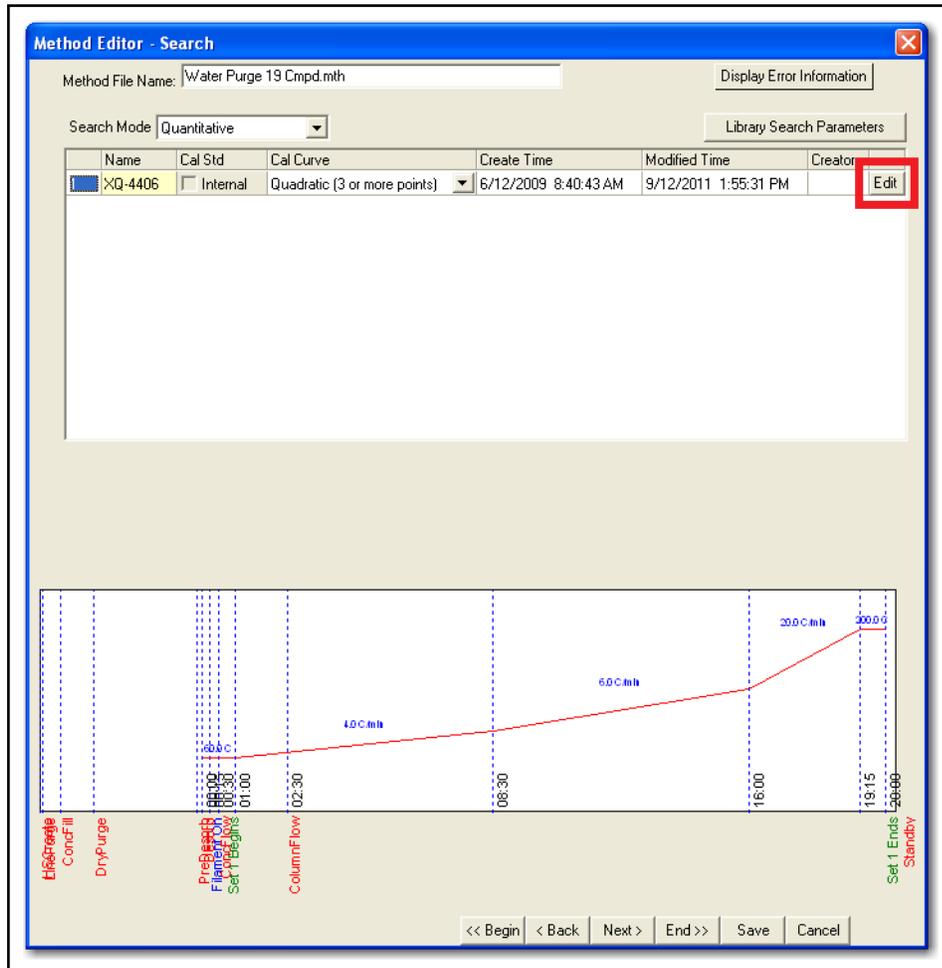
- 1 Open the desired method file in **Method Editor**. (See Chapter 16, Method Editor for more information.)
- 2 Click **Next** in **Method Editor** until the **Search** screen is displayed. (See Figure 5-4.)

Figure 5-4 Method Editor - Search window



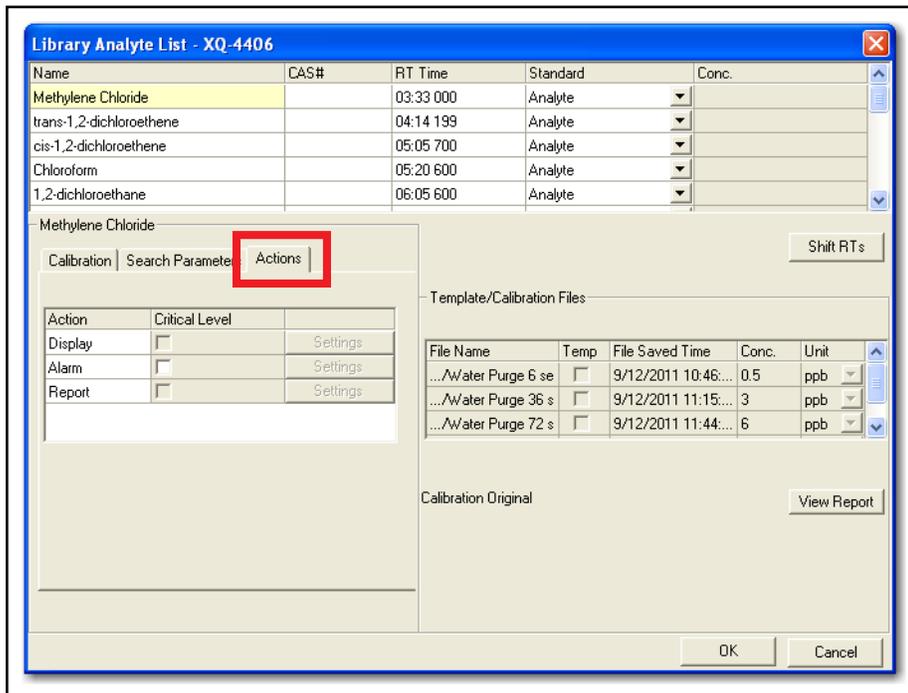
- 3 Click **Edit** for the library containing the analyte(s) for which an alarm point is being set. (See Figure 5-5.)

Figure 5-5 Edit library button



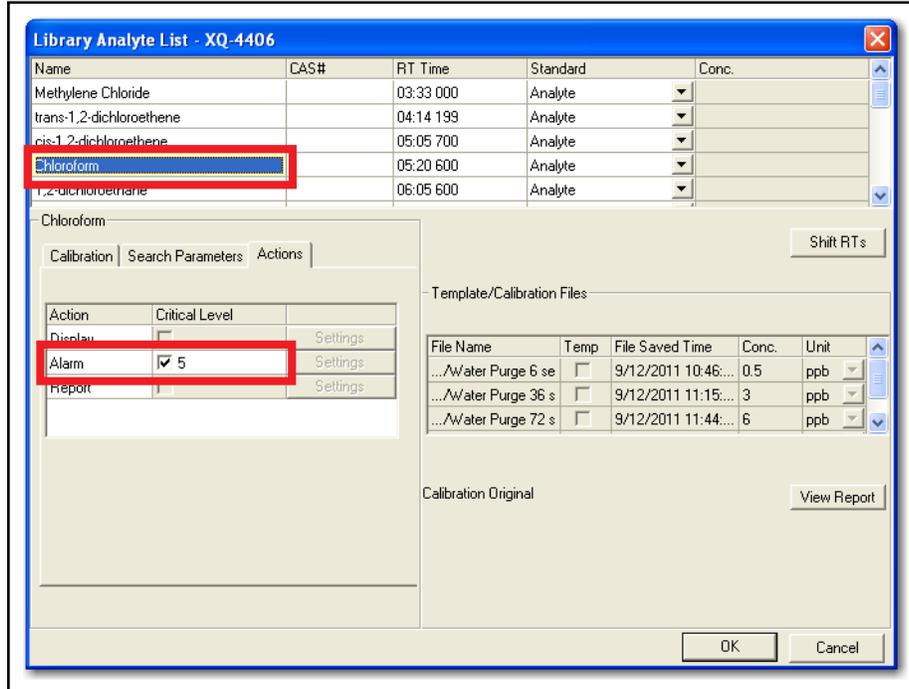
- 4 The **Library Analyte List** window will be displayed. Select the **Actions** tab. (See Figure 5-6.)

Figure 5-6 Library Analyte List - Actions tab



- 5 Click the analyte name for which an alarm is being set. In this example, **Chloroform** is selected. (See Figure 5-7.)
- 6 Select the checkbox next to **Alarm** and enter the desired alarm set point in the box that is enabled.

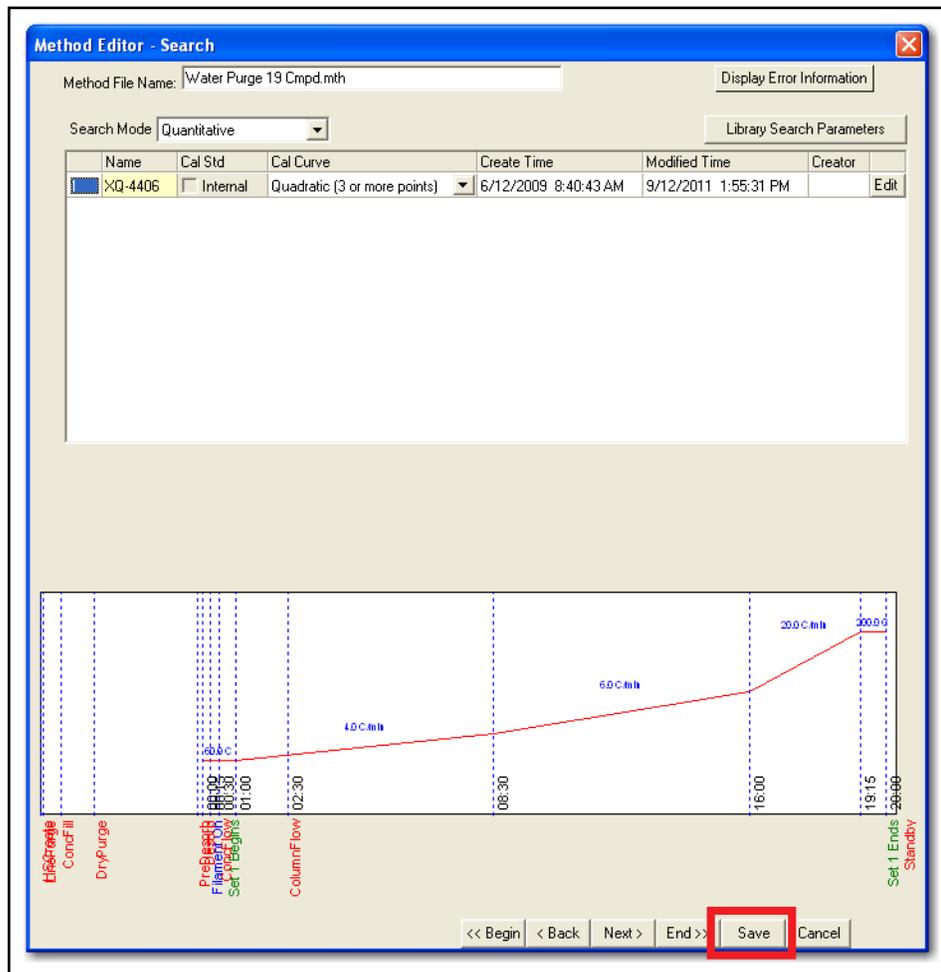
Figure 5-7 Setting Alarm set point



NOTE: Alarm set points will correspond to the concentration unit (eg. ppb, ppm) used when calibrating the method. (See section 17.6, Using the Calibrate Function, on page 17-20.)

- 7 Click **OK** to close the **Library Analyte List** window.
- 8 Click **Save** to save the method with the desired name. (See Figure 5-8.)

Figure 5-8 Saving the method



- 9 Once the alarm set point has been defined, when an out of specification result is obtained, an alarm output signal will be sent through the I/O cable. CMS5000 will actuate an internal relay establishing continuity between the **RELAY NO 1** and **RELAY COM1** leads of the I/O cable. The user is responsible for determining how the output signal is integrated into their system.

NOTE: When running a method sequence and an out of specification alarm is triggered, the alarm will be cleared as soon as the next method in the sequence starts. No user intervention is required to acknowledge or clear an alarm in the software.

Chapter 6

Software Setup

6.1 Introduction

Various software parameters in CMS IQ need to be established for optional CMS5000 operation and communication methods. This includes defining startup methods, method sequences, I/O input methods, and FTP server(s) information.

6.2 FTP Connection

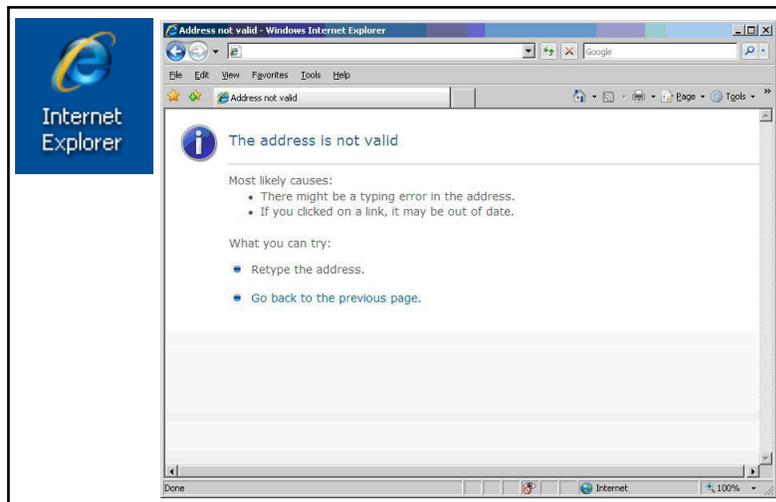
Up to three FTP servers, each with its own unique IP address, user name, and password, can be configured to upload data files and can be enabled or disabled independently.

If an FTP server is enabled, CMS5000 will maintain a queue for uploading data files. After each run, CMS5000 will upload the files onto the queues. If CMS5000 cannot connect or login to an FTP server, the data file will be stored in the queue until another data file is ready to be uploaded. CMS5000 will attempt to upload both the new and the previous data file.

If there is a loss of power to the server, the data files will continue to be stored in the queues. CMS5000 also provides an option to clear the files in the queue if the data is no longer desired.

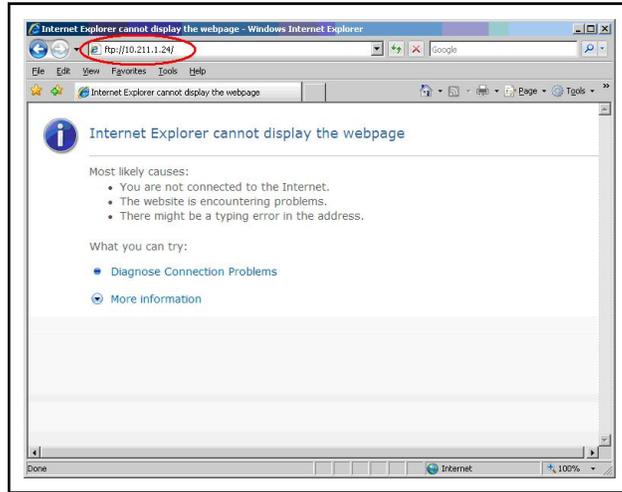
- 1 Verify that the computer will connect to the FTP server. If the computer can connect to both the FTP server and CMS5000, it can be configured to upload data files.
- 2 To verify the connection, first open Internet Explorer. (See Figure 6-1.)

Figure 6-1 FTP server



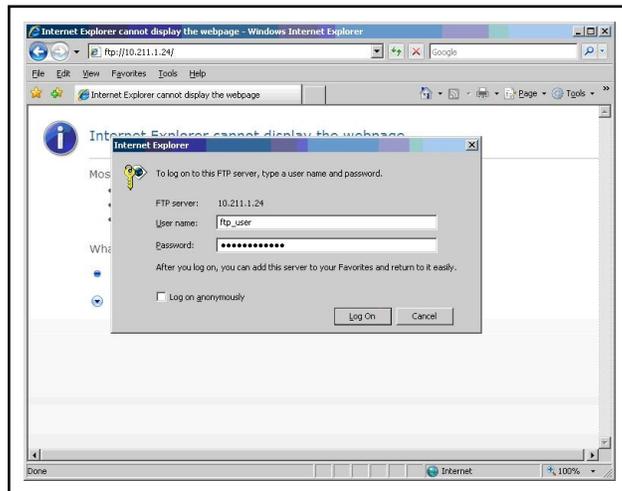
- 3 Enter the FTP address of the server into the address bar using the following format: **FTP://<IP address>**. (See Figure 6-2.)

Figure 6-2 FTP server



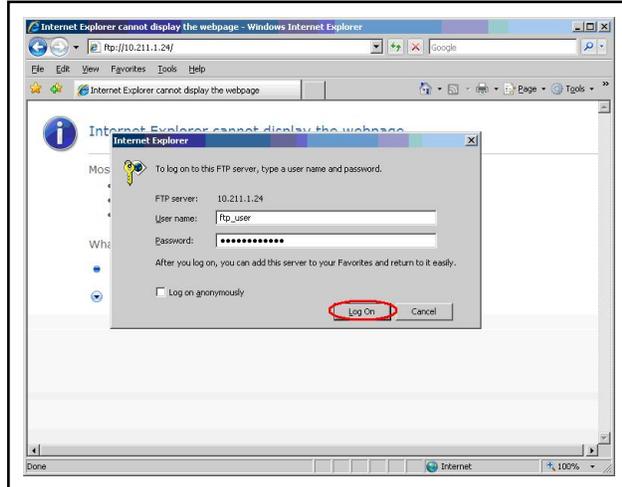
- 4 Press **Enter** on the keyboard. The login window is displayed. (See Figure 6-3.)

Figure 6-3 Pop-Up window



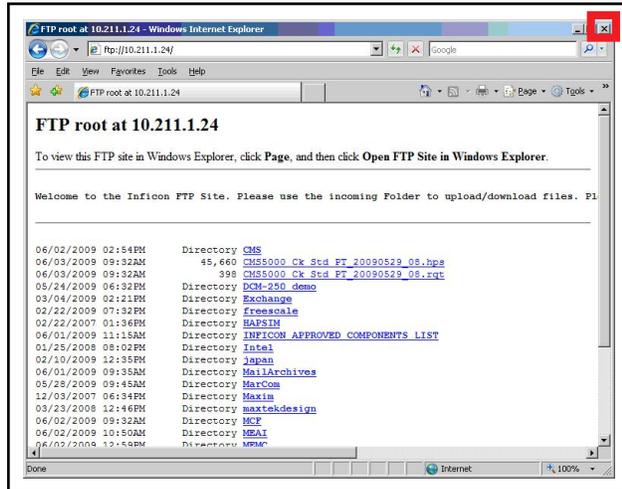
- 5 Type the **User name** and **Password** of the FTP server.
- 6 Click **Log On**. (See Figure 6-4.)

Figure 6-4 Entering User name and Password



- 7 Once the computer connects to the FTP site, a window similar to Figure 6-5 is displayed. Once the connection is verified, click "X" to close the window.

Figure 6-5 FTP site



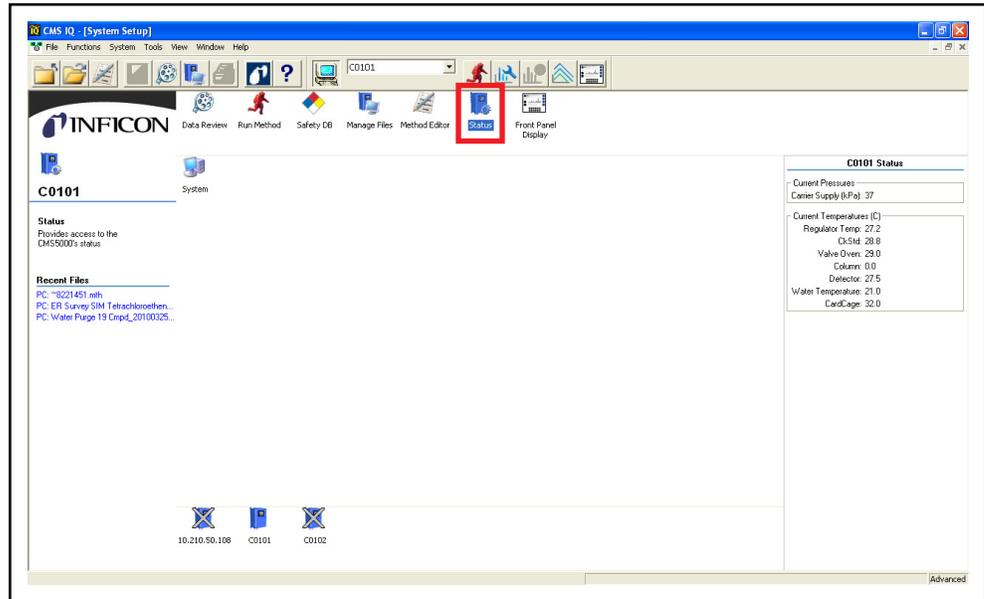
- 8 Double-click the **CMS IQ** icon to open the software. (See Figure 6-6.)

Figure 6-6 CMS IQ icon



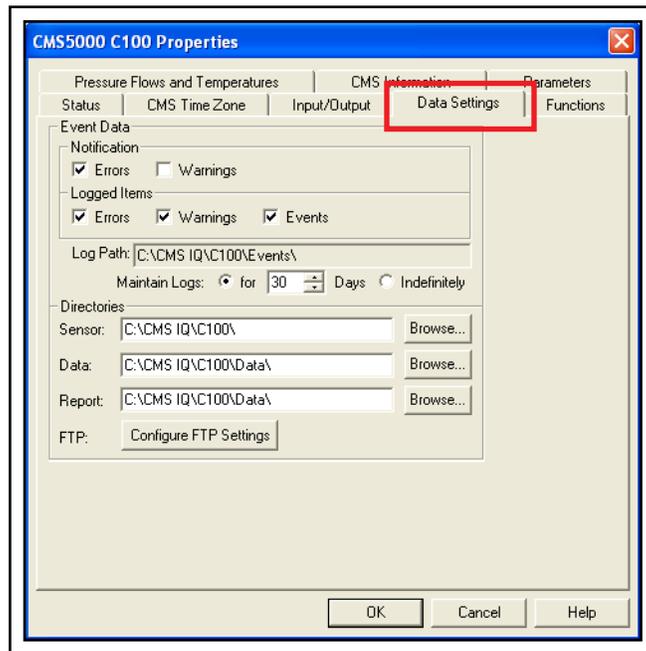
9 Double-click the **Status** icon. (See Figure 6-7.)

Figure 6-7 Status icon



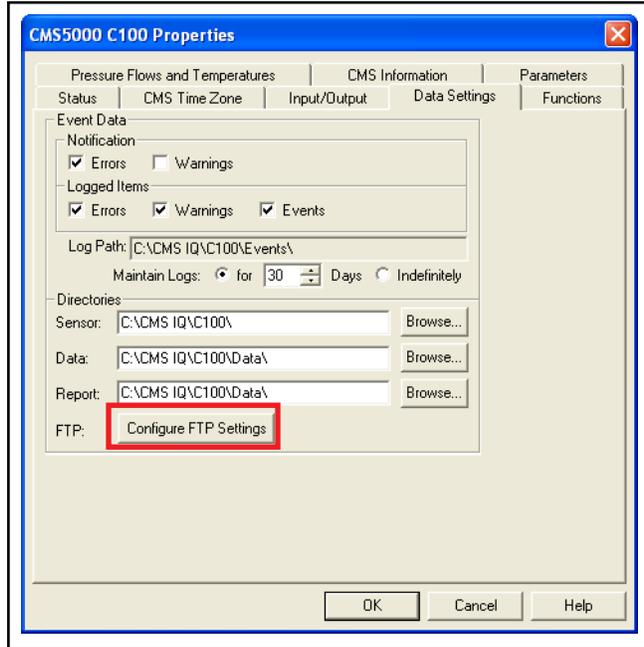
10 Click the **Data Settings** tab. (See Figure 6-8.)

Figure 6-8 Data Settings tab



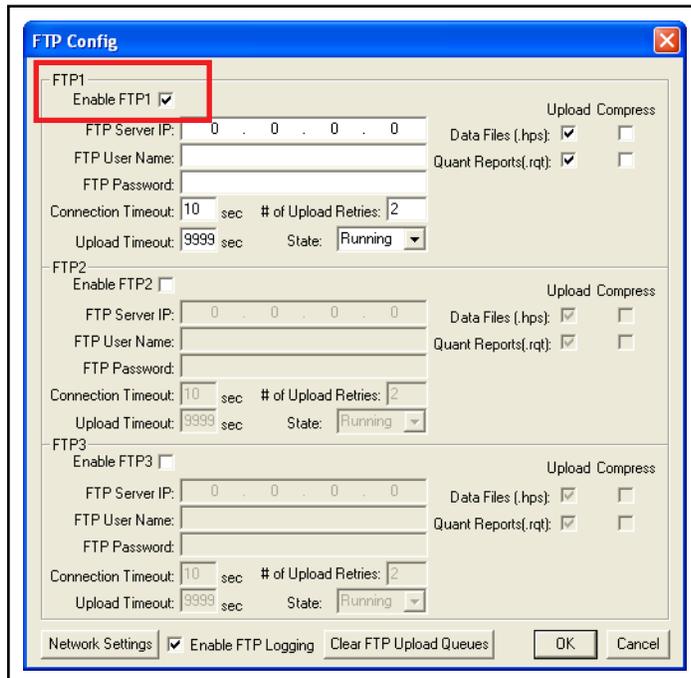
11 Click **Configure FTP Settings**. (See Figure 6-9.)

Figure 6-9 Configure FTP Settings button



12 The **FTP Config** window is displayed. Enable the number of FTP servers to upload by selecting the **Enable FTP** checkboxes. **Enable FTP1** is selected by default. Up to three FTP servers can be enabled. (See Figure 6-10.)

Figure 6-10 FTP Config window

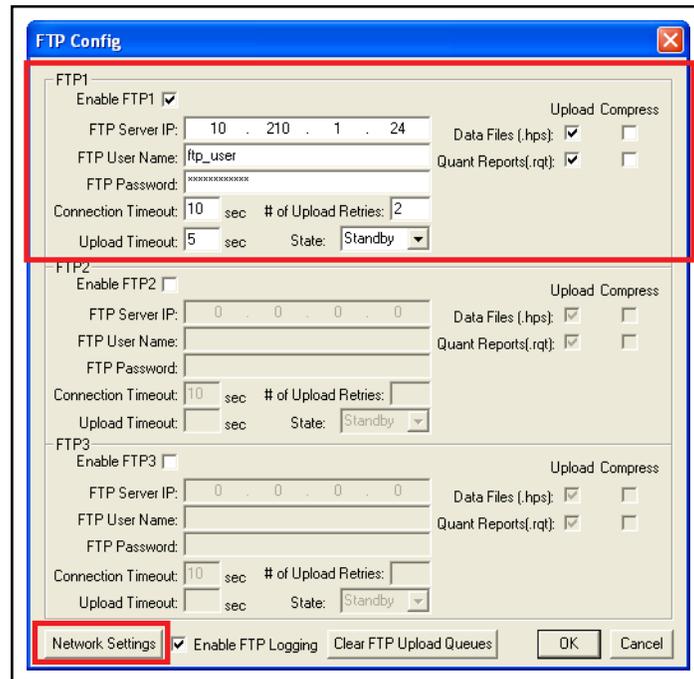


13 Enter:

- ◆ **FTP Server IP address**
- ◆ **FTP User Name**
- ◆ **FTP Password**
- ◆ **Connection Timeout** (the amount of time CMS5000 will wait for a response from the FTP site)
- ◆ **Upload Timeout** (the allotted time for a single file to upload)
- ◆ **# of Upload Retries** (the number of times CMS5000 will attempt to communicate with the FTP server if the **Upload Timeout** is reached)

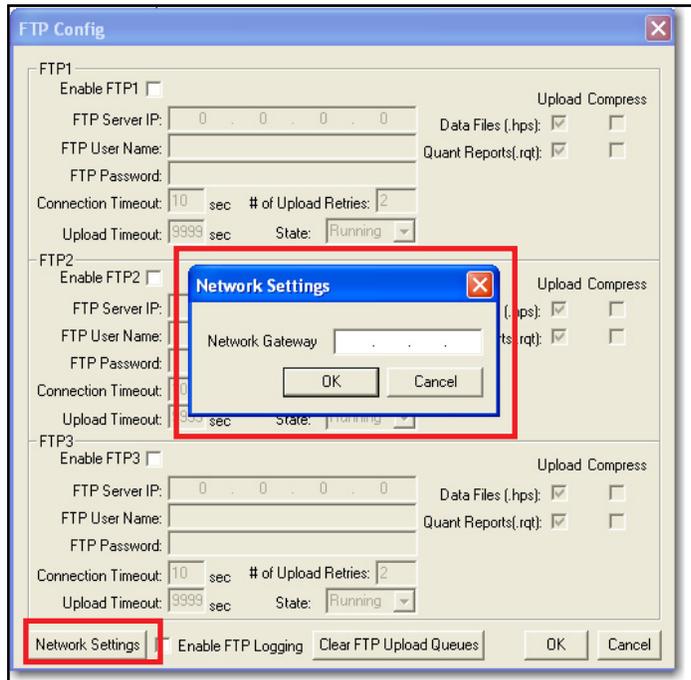
NOTE: State will display **Standby** mode. When CMS5000 is actively transmitting data to the FTP server, **State** will display **Running**. (See Figure 6-11.)

Figure 6-11 Entering FTP server information



- Click **Network Settings**. The **Network Settings** window is displayed. (See Figure 6-12.)

Figure 6-12 Network Settings button and Network Settings window



- To locate the Network Gateway, click **Start**. (See Figure 6-13.)

Figure 6-13 Start button



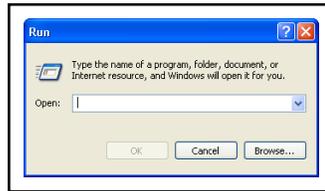
- Click **Run...** (See Figure 6-14.)

Figure 6-14 Selecting Run...



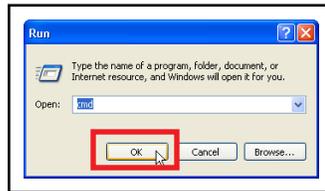
- 17 The **Run** window is displayed. (See Figure 6-15.)

Figure 6-15 Run window



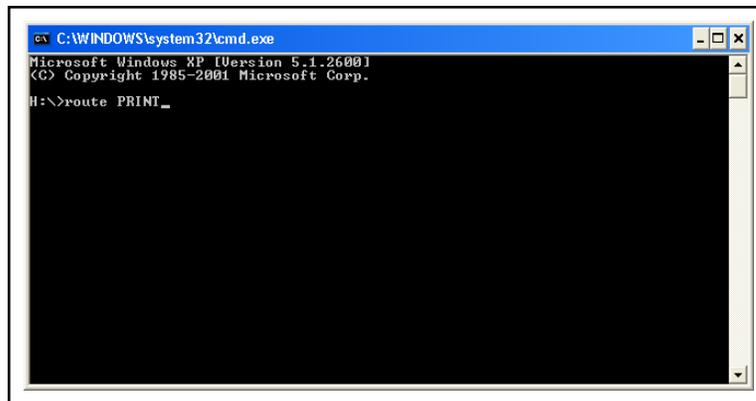
- 18 Enter **cmd** and click **OK**. (See Figure 6-16.)

Figure 6-16 Entering cmd and OK button



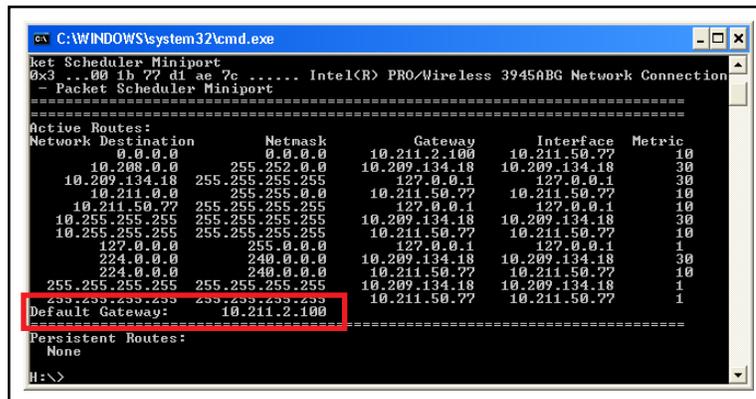
- 19 At the command prompt, type **route PRINT**. (See Figure 6-17.)

Figure 6-17 Entering route PRINT



- 20 The **Default Gateway**: setting is displayed. (See Figure 6-18.)

Figure 6-18 Default Gateway displayed



- 21 Type the **Default Gateway**: setting in the **Network Gateway** box. (See Figure 6-19 and Figure 6-20.)

Figure 6-19 Network Settings window

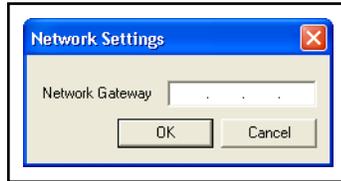
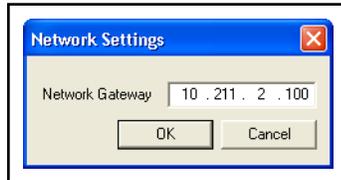
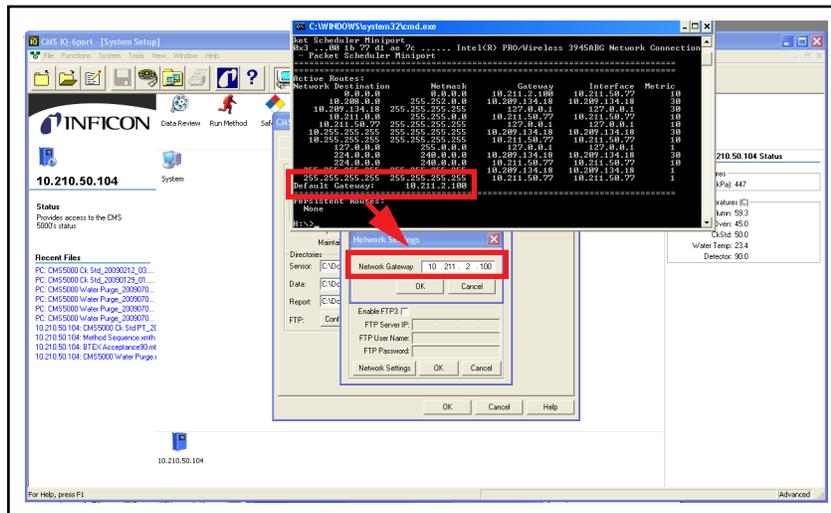


Figure 6-20 Entering Network Gateway



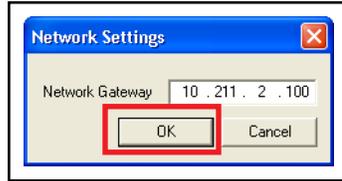
- 22 Confirm the default gateway at the bottom of the window matches the Network Gateway setting in CMS IQ. If not, re-enter the default gateway setting displayed on the computer into CMS IQ. (See Figure 6-21.)

Figure 6-21 Matching gateway settings



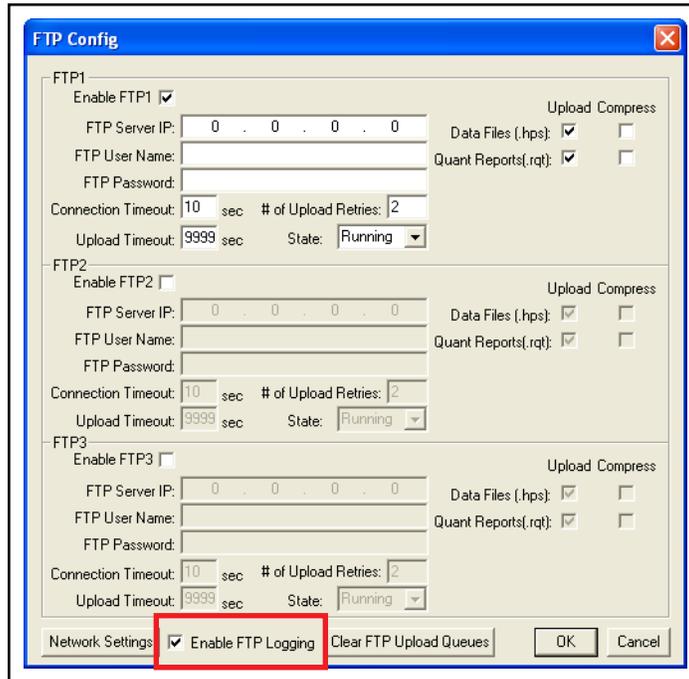
23 Click **OK** to accept the Network Gateway settings. (See Figure 6-22.)

Figure 6-22 Accepting Network Gateway settings



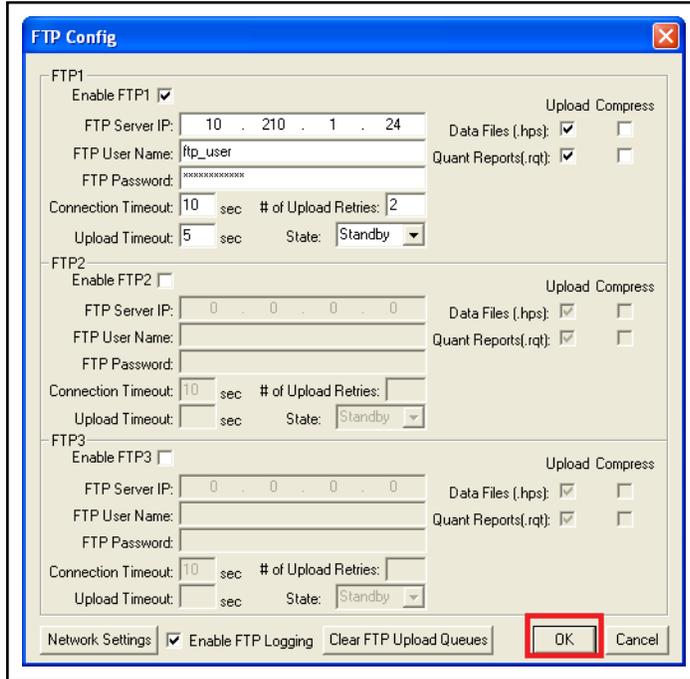
NOTE: Select **Enable FTP Logging** to send reports from CMS5000 to the desired FTP site. (See Figure 6-23.)

Figure 6-23 Enable FTP Logging checkbox option



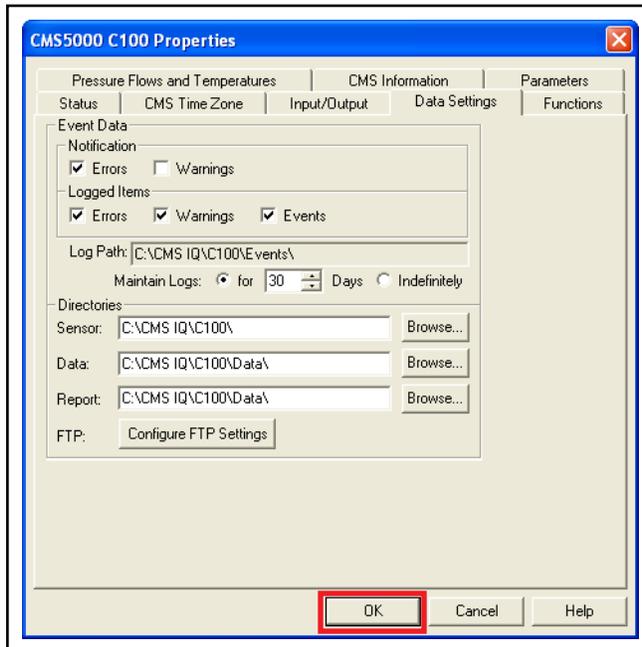
24 Click **OK** to accept the FTP Server settings. (See Figure 6-24.)

Figure 6-24 Accepting FTP Config settings



25 Click **OK** to close the **Properties** window. (See Figure 6-25.)

Figure 6-25 Closing the CMS5000 C100 Properties window



26 The FTP site(s) should now be defined and communicating.

6.3 System Integration

System I/O integration allows only input commands. This includes the selection and start of a method created in the CMS IQ software. See section 6.4, Defining Startup Methods below, for details on how to input methods. See section 6.5, Input Methods, on page 6-15 for details on triggering methods with the I/O port. For more advanced integration details, please contact INFICON.

6.4 Defining Startup Methods

CMS5000 can be operated automatically. In the **Parameters** tab, a **Startup Method** that will automatically run when powering on the system can be defined. Additionally, a method sequence can be selected as a startup method. See section 6.6, Method Sequence, on page 6-17 for information on creating a method sequence.

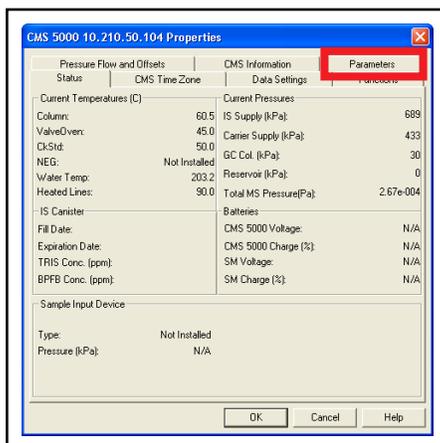
- 1 On the **System Setup** window of CMS IQ software, double-click the **Status** icon. (See Figure 6-26.)

Figure 6-26 Status icon



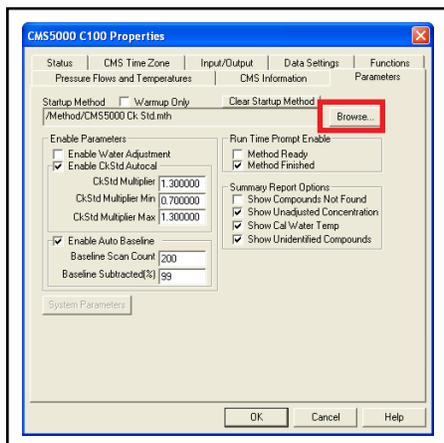
- 2 Select the **Parameters** tab. (See Figure 6-27.)

Figure 6-27 Parameters tab



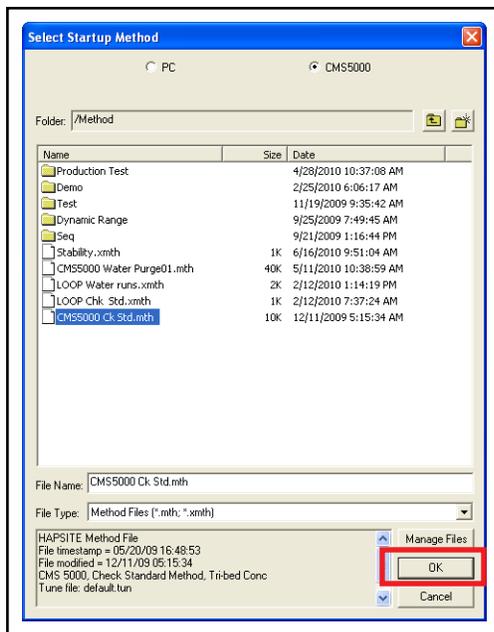
- 3 Click **Browse** to select a startup method. (See Figure 6-28.)

Figure 6-28 Browse... button



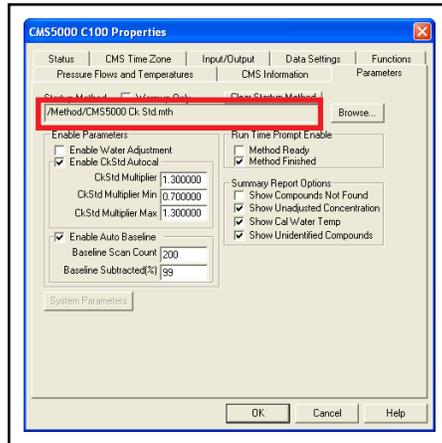
- 4 Double-click the desired method from the method folder, or select the method and click **OK**. (See Figure 6-29.)

Figure 6-29 Choosing a startup method



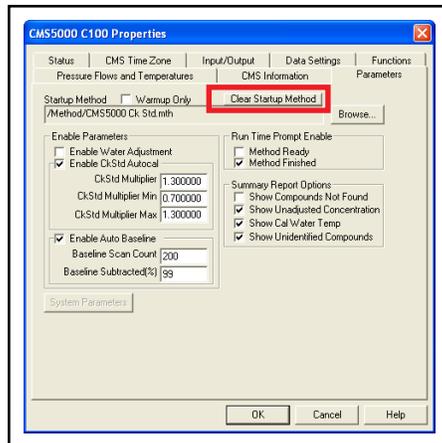
5 The selected method is displayed. (See Figure 6-30.)

Figure 6-30 Startup method



NOTE: Click **Clear Startup Method** to clear the startup method. (See Figure 6-31.)

Figure 6-31 Clear startup method button

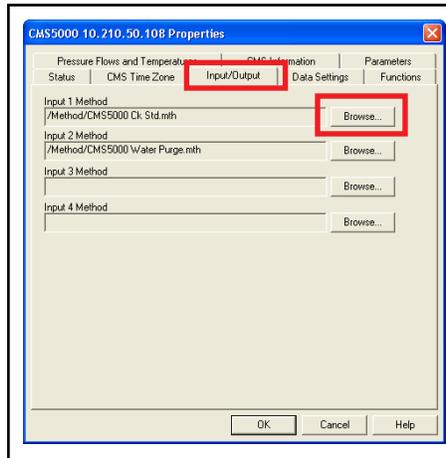


6.5 Input Methods

In the **Input/Output** tab, up to four input methods can be selected. An input method will begin when a relay contact, which has been integrated into the water/air control system, triggers it to start. A method sequence can be defined as an input method, if desired. See section 6.6, *Method Sequence*, on page 6-17 for information on creating a method sequence.

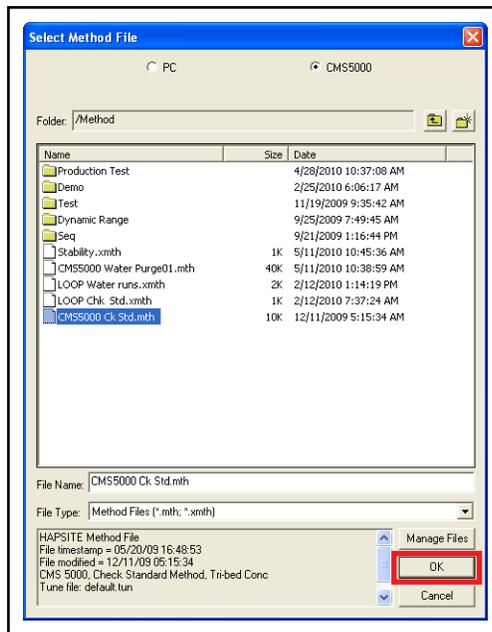
- 1 To enter input methods, click **Browse** for the desired input method. (See Figure 6-32.)

Figure 6-32 Input browse buttons



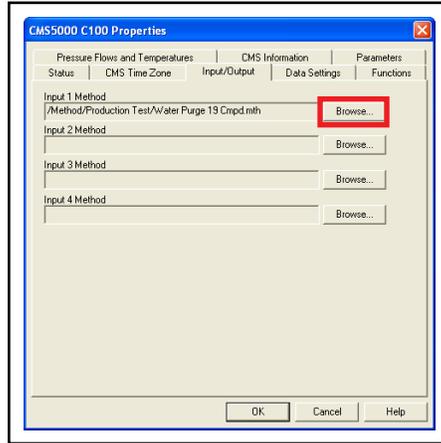
- 2 Double-click the desired method from the method folder or select the method and click **OK**. (See Figure 6-33.)

Figure 6-33 Choosing input method



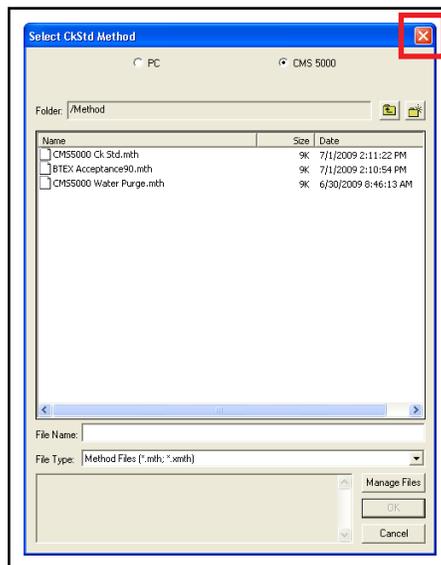
- The selected input method will display in the corresponding **Input Method** box. To clear the input method, click **Browse** for the desired method. (See Figure 6-34.)

Figure 6-34 Clearing input method



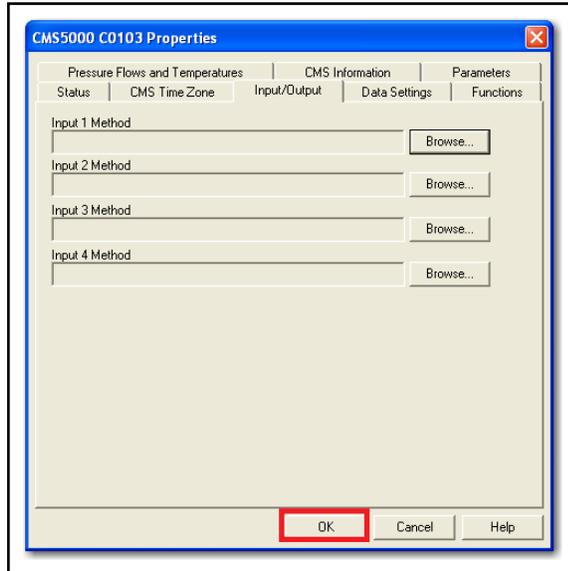
- Click "X" without selecting a method. (See Figure 6-35.)

Figure 6-35 Clicking "X" button



- The method will be cleared from the selected input method line or select the method and click **OK**. (See Figure 6-36.)

Figure 6-36 Input method cleared



6.6 Method Sequence

A sequence of methods, including consecutive runs, can be selected to run at timed intervals. Once a sequence has been started, it can run unattended and unprompted until the sequence has finished, or it can be set to run continuously. Follow the instructions below to create a method sequence.

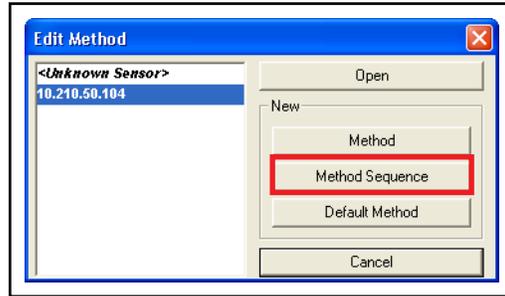
- From the CMS IQ Setup window, double-click the **Method Editor** icon. (See Figure 6-37.)

Figure 6-37 Method Editor icon



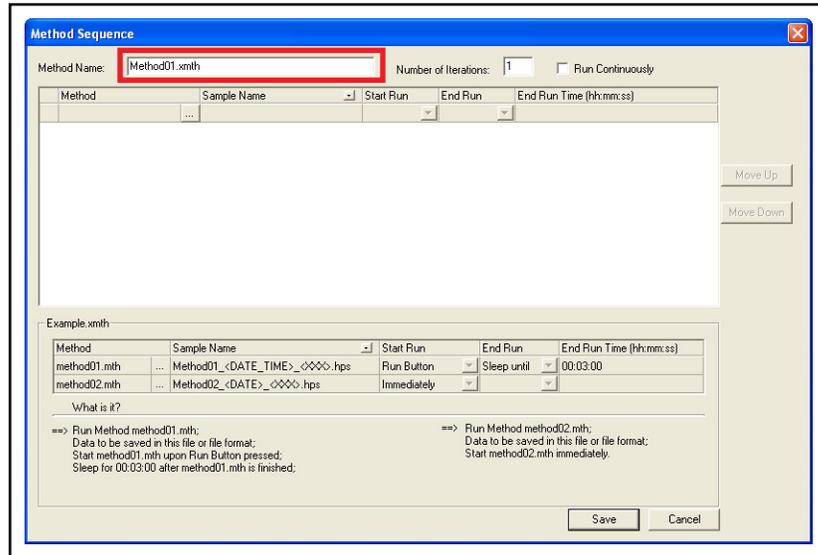
- The **Edit Method** window is displayed. Click **Method Sequence**. (See Figure 6-38.)

Figure 6-38 Edit Method window and Method Sequence button



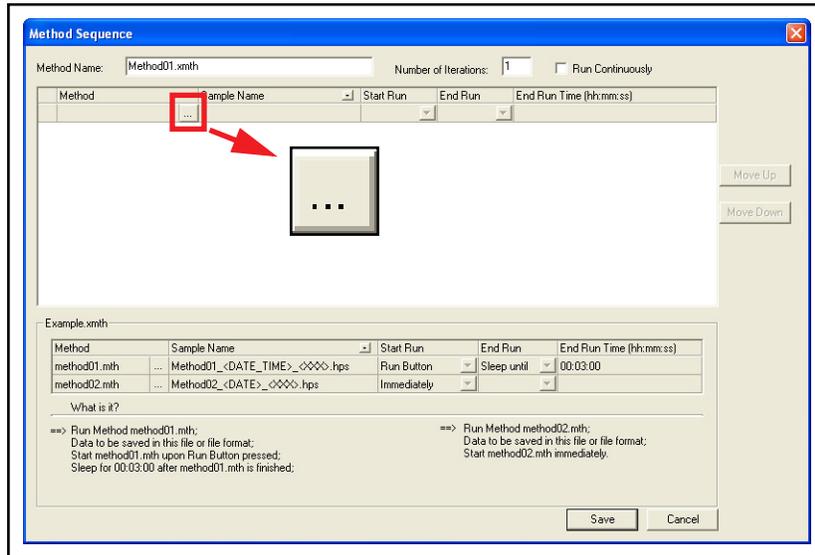
- In the **Method Name** box, type a name for the method sequence or use the name provided. Verify that the file extension for the method name is *.xmth. (See Figure 6-39.)

Figure 6-39 Method Name box



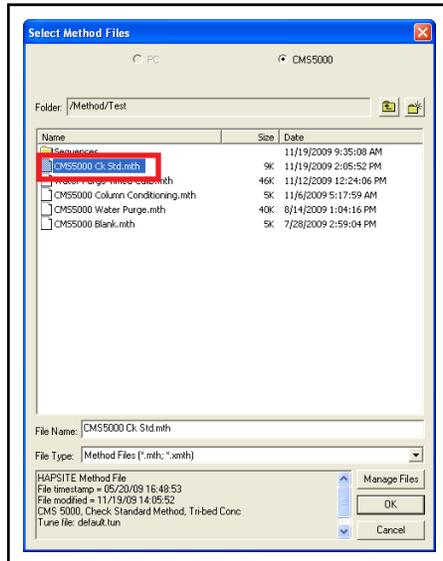
4 Click **Browse (...)** to add a method. (See Figure 6-40.)

Figure 6-40 Browsing for method file



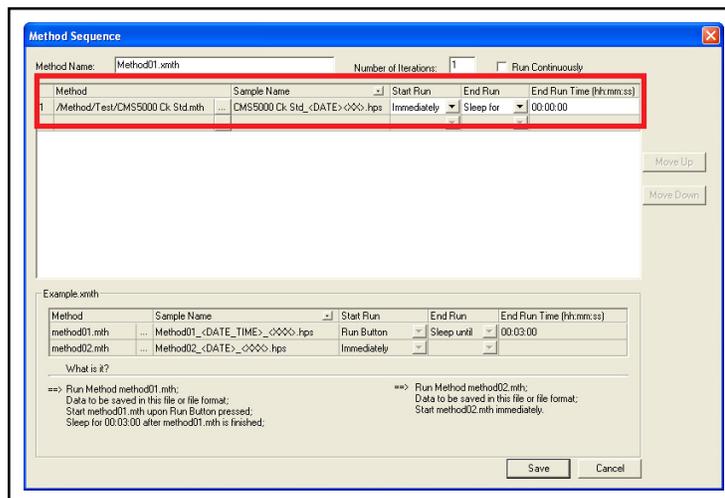
5 A list of methods is displayed. Double-click the desired method for sequencing. (See Figure 6-41.)

Figure 6-41 Selecting method for a sequence



6 The selected method is displayed in the **Method** column. (See Figure 6-42.)

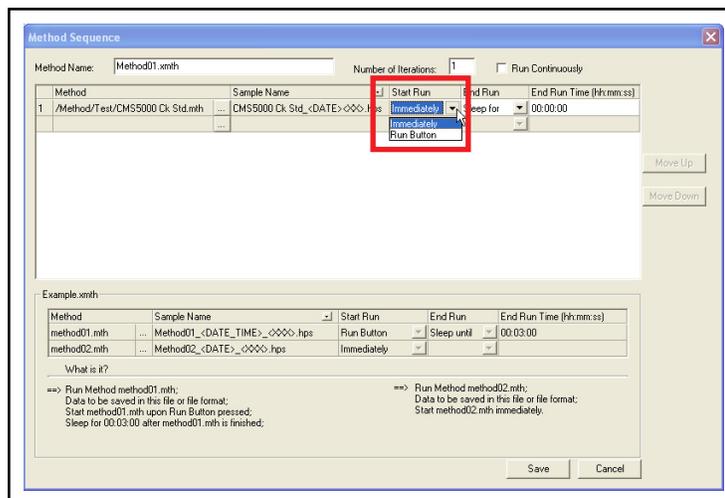
Figure 6-42 Selected method



7 In the **Start Run** column, select either **Immediately** or **Run Button** for each method. This selection determines how each method in the sequence is started. (See Figure 6-43.)

NOTE: If **Run Button** is selected, the Run button on the front panel of the computer must be pressed to start the method. If **Immediately** is selected, the method will automatically commence.

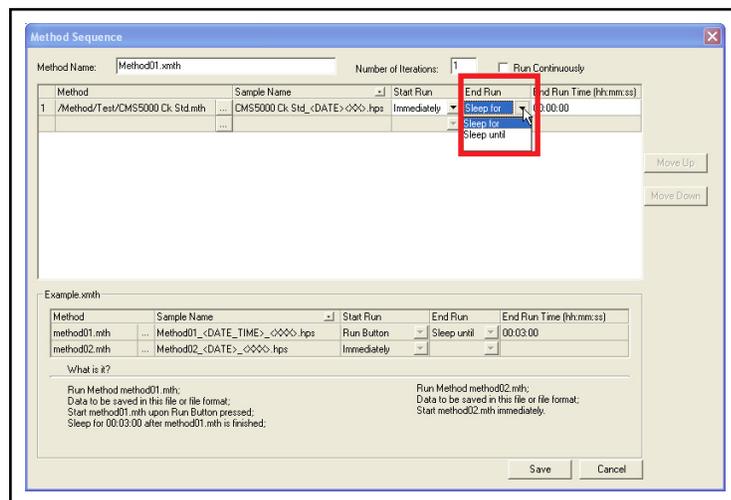
Figure 6-43 Start Run option selection



- 8 In the **End Run** column, select **Sleep for** or **Sleep until** for each method. (See Figure 6-44.)

NOTE: The **Sleep for** option is used to enter a time period between method runs, such as one hour. The **Sleep until** option is used to start a method at a specific time, such as one o'clock. Time is shown in military notation (e.g. 3 p.m. is shown as 15:00:00.)

Figure 6-44 End run option selection

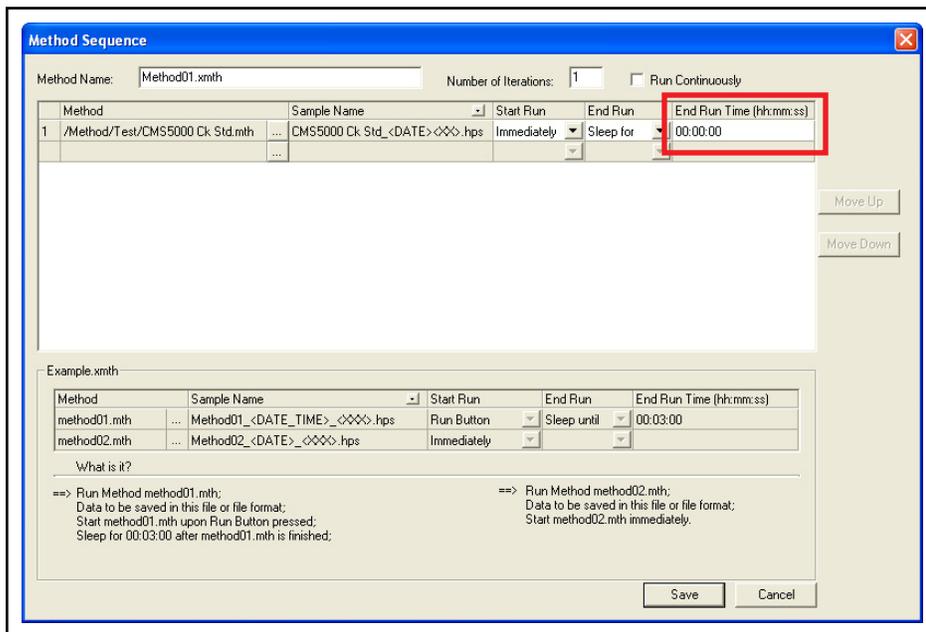


- 9 In the **End Run Time** column, enter the desired time for the next method to start or the length of time to sleep before the next method starts. (See Figure 6-45.)

- ◆ Enter **0:00:00** to run the next method immediately after the previous method has finished
- ◆ **Sleep for** will not account for the run time of methods
- ◆ **Sleep until** does not recognize earlier timestamps. For example, if the sequence was started at 6 AM and the sequence said to **Sleep until 3:00:00**, instead of sleeping until 3 AM the next day, after running the first method the sequence would proceed immediately to the next method

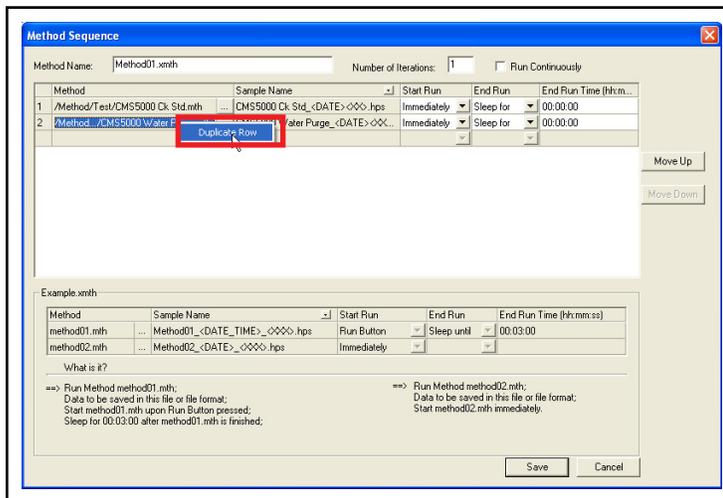
HINT: If using **Sleep until** in a sequence, adding a check standard method to run at **11:59:00** ensures methods always start at the desired times.

Figure 6-45 End Run Time column



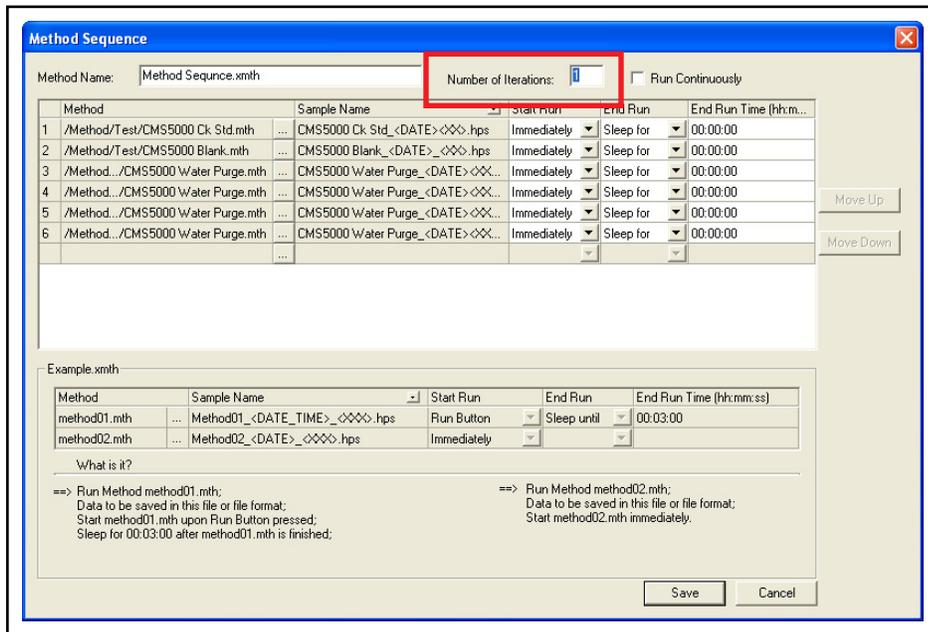
- Repeat Step 4 through Step 9 to add additional methods for sequencing. Alternately, right-click on the added method and select **Duplicate Row**. (See Figure 6-46.)

Figure 6-46 Duplicate Row option



- When the desired sequence has been entered, type a number in the **Number of Iterations** box to repeat the sequence a set number of times. (See Figure 6-47.)

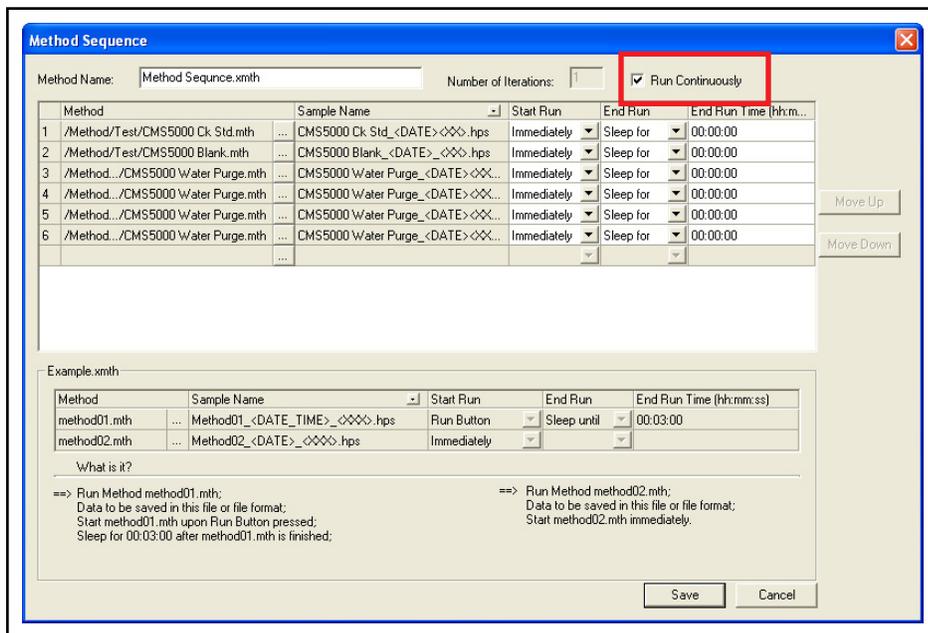
Figure 6-47 Number of Iterations option



- Select the **Run Continuously** checkbox to run a continuous loop of the sequence without stopping. (See Figure 6-48.)

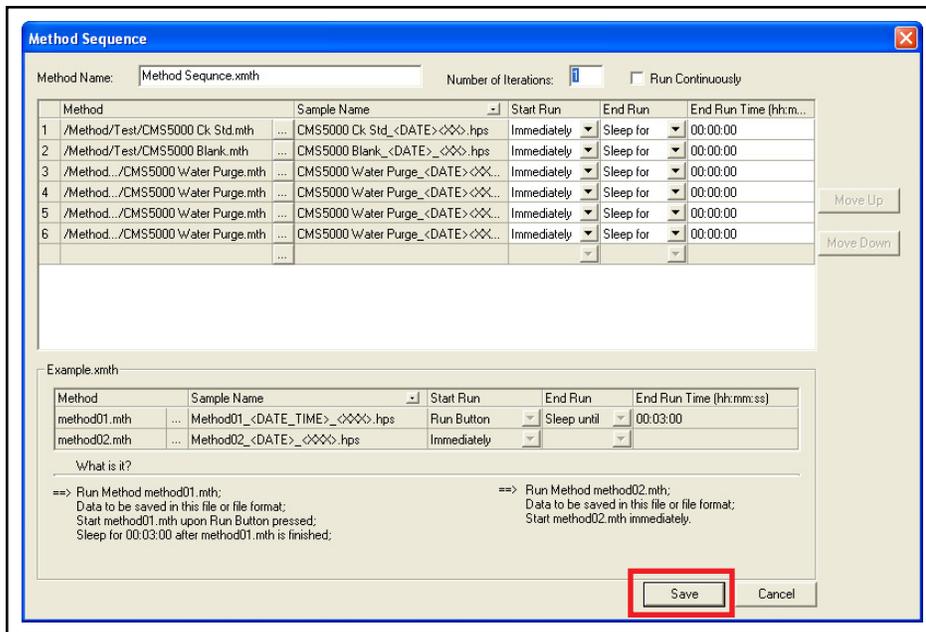
NOTE: When using **Run Continuously**, the **Number of Iterations** box is unavailable.

Figure 6-48 Run Continuously checkbox



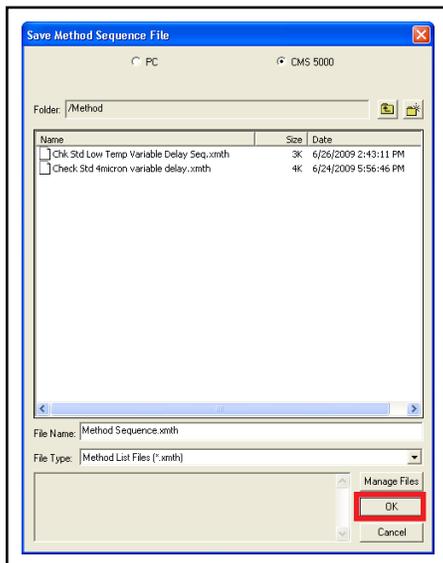
- 13 Click **Save** when the method sequence is complete. (See Figure 6-49.)

Figure 6-49 Saving Method Sequence



- 14 Save the method sequence to the desired location. Click **OK**. (See Figure 6-50.)

Figure 6-50 Saving Method Sequence



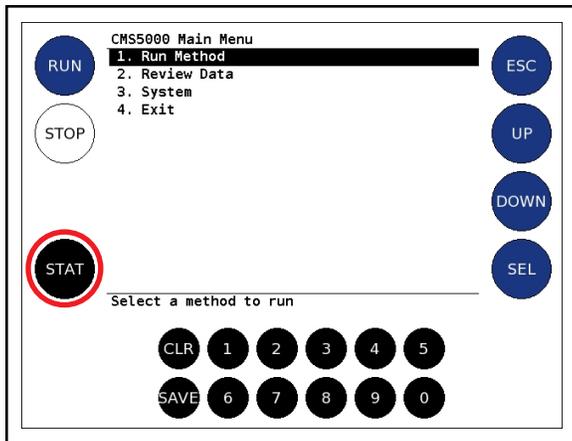
Chapter 7

System Status

7.1 Introduction

The **STAT** button on the CMS5000 front panel provides real time data regarding system parameters **SYS** (system), **TIME**, **NET** (network), **STAT** (status), and **FIRM** (firmware). Tap **STAT** on the Main Menu to access these parameters. (See Figure 7-1.)

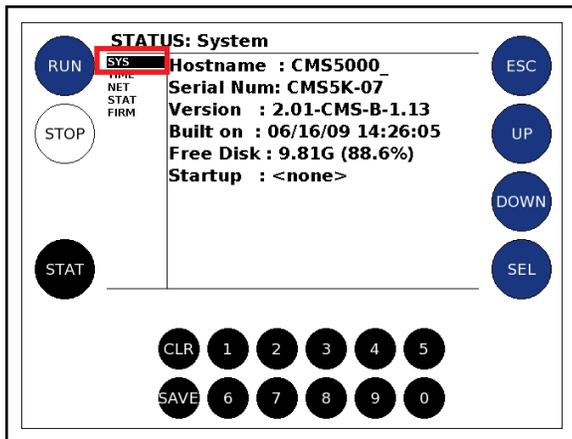
Figure 7-1 STAT button



7.2 SYS Function

The first function, **SYS**, provides basic system information. (See Figure 7-2.)

Figure 7-2 SYS function



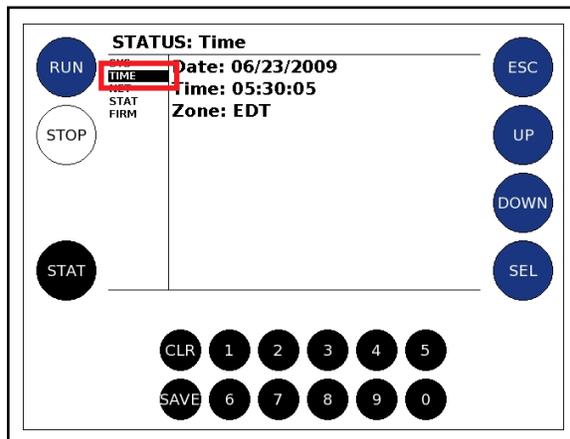
Navigate through the **SYS** options by tapping **UP** or **DOWN**. Information on the System page includes:

- Hostname** Used for computer communication
- Serial Num** (Number). Serial number of the CMS5000 (Used for identification)
- Version**. Version of CMS5000 software that is running the system
- Built on** Date and time that the software was released
- Free Disk** Amount of free disk space available for data storage
- Startup**. Method that will automatically run when CMS5000 is turned on

7.3 TIME Function

The **TIME** function gives **Date**, **Time** (in a 24 hour format), and **Time Zone** information. **TIME** is used to timestamp the data files. (See Figure 7-3.) See section 10.3, Set Date, Time and Time Zone, on page 10-3 for instructions to set the **TIME** function.

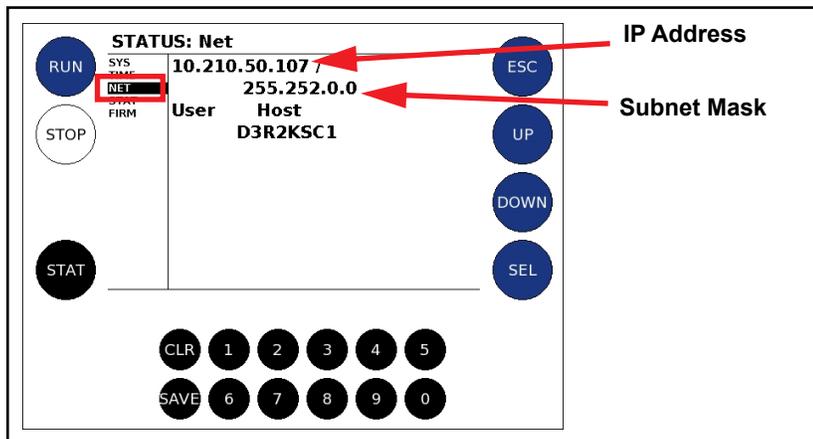
Figure 7-3 TIME function



7.4 NET Function

The **NET** function displays the **IP Address**, **Subnet Mask**, and **User Host**. The IP address and subnet mask are used to set up communication between CMS5000 and a computer. This communication will allow data transfer from CMS5000 to a remote computer for analysis and storage. **User Host** displays the computer communicating with CMS5000. (See Figure 7-4.)

Figure 7-4 NET function

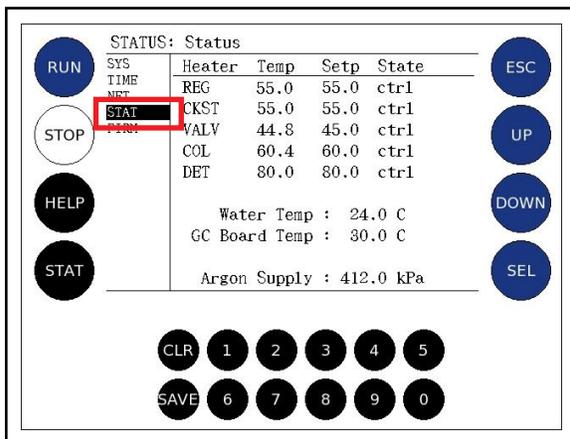


7.5 STAT Function

The **STAT** (status) function displays temperature information and carrier gas pressure. (See Figure 7-5.) This includes:

- ◆ Current temperature and set point temperature of the following heated components: **Regulator**, **Check Standard**, **Valve Oven**, **Column**, and **Detector**
- ◆ State of the heaters (**on**, **off**, or **ctrl**), with **ctrl** indicating that the heaters are within range of their set point
- ◆ Temperature of the water sample and the temperature of the card cage, which contains the CMS5000 circuit boards
- ◆ **Argon Supply** pressure

Figure 7-5 STAT function



NOTE: If the argon pressure is 550 kPa or less, an **Argon Pressure Low!** message will appear. (See Figure 7-6.) If the argon pressure is 345 kPa or less, a **REPLACE ARGON CYLINDER!** message will be displayed. (See Figure 7-7.)

Figure 7-6 Argon Pressure Low! message

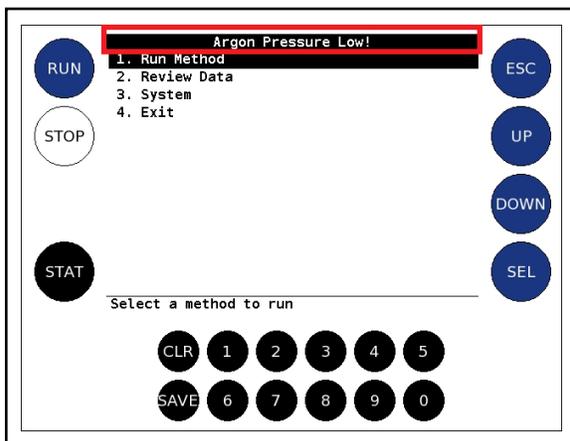
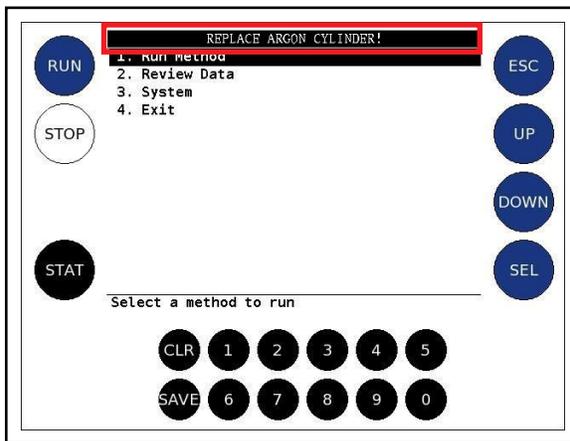


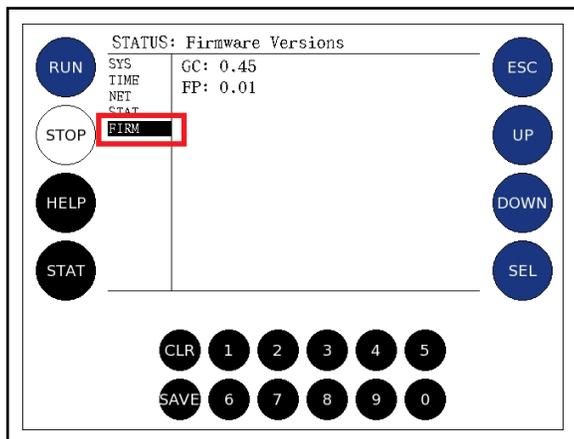
Figure 7-7 REPLACE ARGON CYLINDER! message



7.6 FIRM Function

The **FIRM** (firmware) function displays the firmware version for the **GC** (gas chromatograph) and **FP** (front panel). (See Figure 7-8.)

Figure 7-8 FIRM function



Chapter 8

Basic Operation

8.1 Introduction

CMS5000 can be programmed remotely or from the front panel to operate continually or at timed intervals. Following a method run, analysis results can be uploaded to an FTP server allowing for data review at an off-site location. The results are also stored directly on the CMS5000 storage drive.

CMS5000 will commence sampling the air sample or the headspace above the water sample at the beginning of the method run. During the run, results will be displayed on the front panel.

NOTE: When accessing data from a remote computer, results will be available immediately following the method run.

8.2 Default Methods

Default methods included with CMS5000:

- ♦ **Ck Std** verifies that the retention time and response of the internal check standard is within range and is used for both air and water analysis
- ♦ **Water Purge 19 Cmpd** method detects specifically selected VOCs during water monitoring
- ♦ **BTEX in Air** method detects benzene, toluene, ethylbenzene, and xylenes during air monitoring

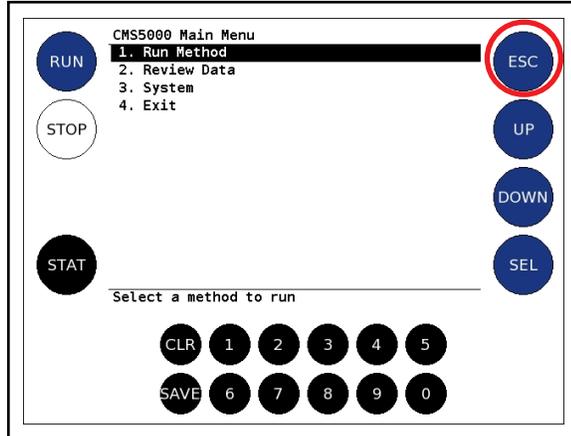
8.3 System Check Standard

A toluene permeation tube is used to check the CMS5000 detector and has a life span of approximately 6 to 8 years. CMS5000 software will use this check to automatically compensate for normal fluctuations in the instrument.

8.4 Operating CMS5000 Using the Front Panel

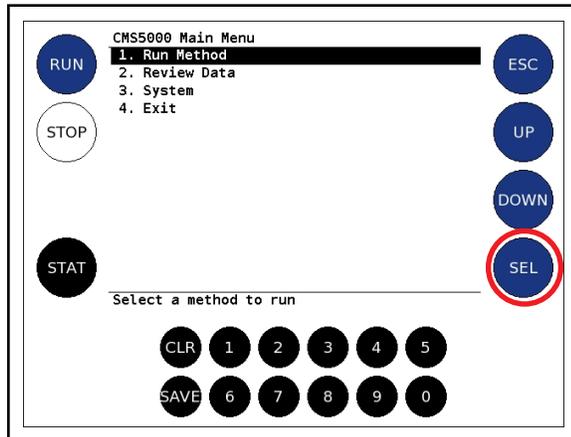
- 1 Tap **ESC** until the **CMS5000 Main Menu** is displayed. (See Figure 8-1.)

Figure 8-1 CMS5000 Main Menu



- 2 **Run Method** will be highlighted. Tap **SEL**. (See Figure 8-2.)

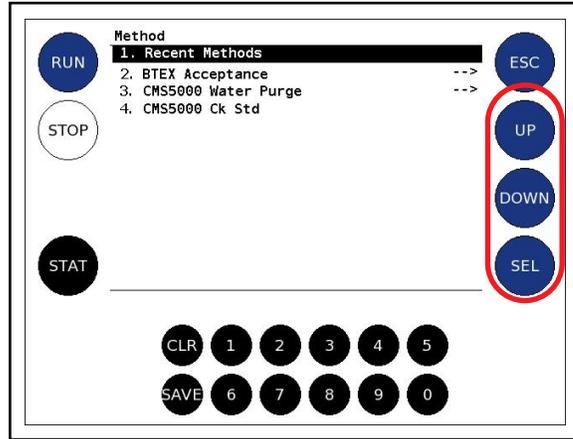
Figure 8-2 Selecting Run Method



- 3 Tap **UP** or **DOWN** to highlight the desired method. Tap **SEL** to run the method. (See Figure 8-3.)

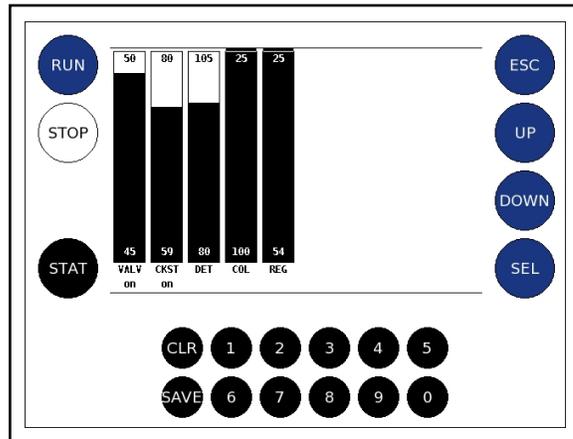
NOTE: Recent Methods will display the 10 most recently run methods.

Figure 8-3 Highlighting method



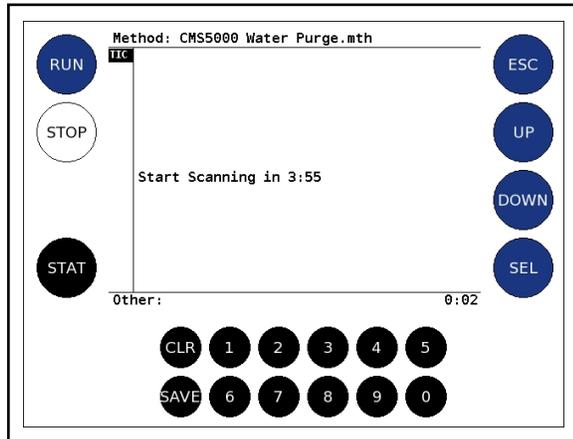
- 4 Prior to the method starting, the system will prepare by heating the components to the required set points. (See Figure 8-4.)

Figure 8-4 Heaters status grid



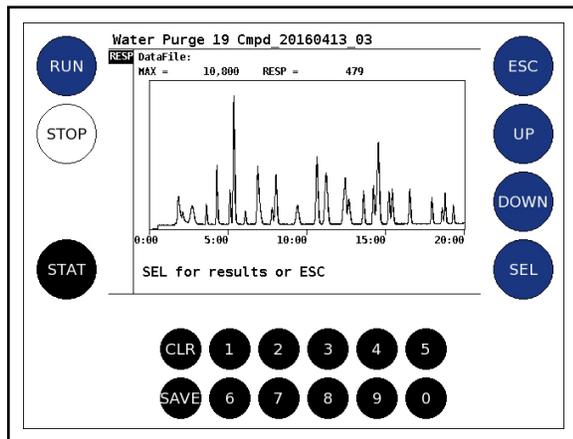
- Once all the components are at the correct temperature, CMS5000 will begin sample collection. “**Start Scanning in...**” will display to show the time remaining before the detector begins to record data. (See Figure 8-5.)

Figure 8-5 Start Scanning message



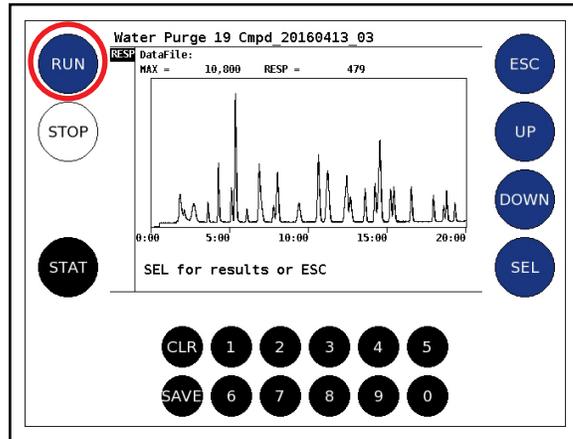
- A chromatogram will display while the method is running. Figure 8-6 depicts a finished chromatogram.

Figure 8-6 Finished chromatogram



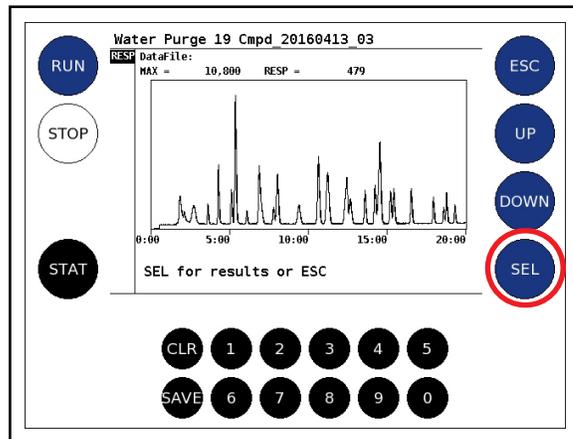
- If desired, tap **RUN** to repeat the same method. (See Figure 8-7.)

Figure 8-7 Run button



- Tap **SEL** to view the results of the run. (See Figure 8-8.)

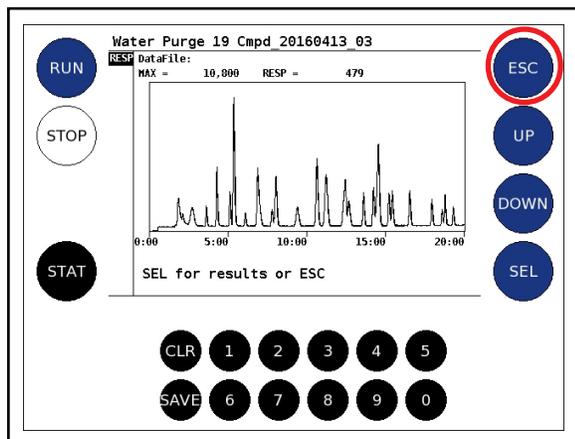
Figure 8-8 Select to view run results



NOTE: For information on viewing reports, see Chapter 9, Review Data Function.

9 Tap **ESC** to return to CMS5000 Main Menu. (See Figure 8-9.)

Figure 8-9 Returning to CMS5000 Main Menu



NOTE: To move data files to the computer, see section 12.5, Manage Files, on page 12-39.

Chapter 9

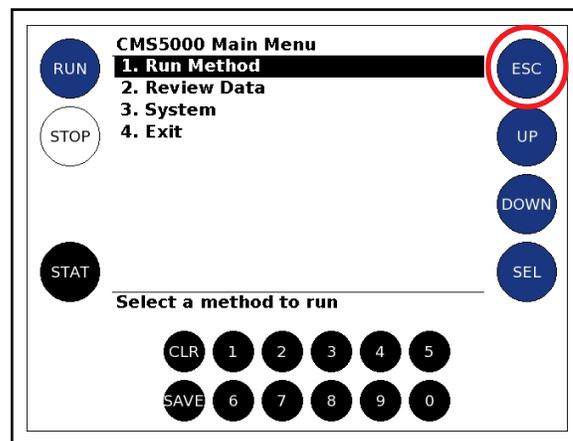
Review Data Function

9.1 Review Data Function

This function recalls data files for review. To access data files, follow the instructions below.

- 1 Tap **ESC** on the front panel until the **CMS5000 Main Menu** is displayed. (See Figure 9-1.)

Figure 9-1 CMS5000 Main Menu



- 2 Tap **DOWN** to highlight the second function, **Review Data**, and tap **SEL**. (See Figure 9-2.) Alternately, tap **2** followed by **SEL**. (See Figure 9-3.)

Figure 9-2 Selecting Review Data

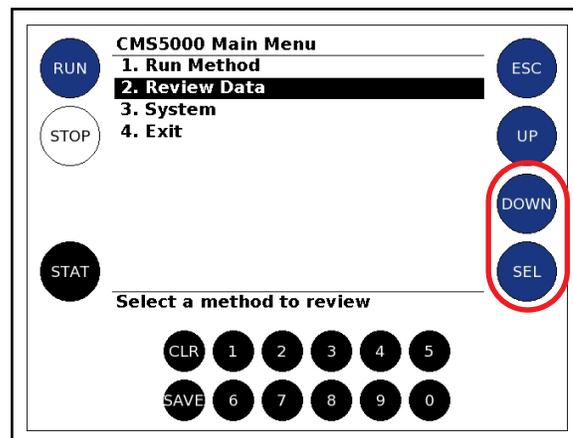
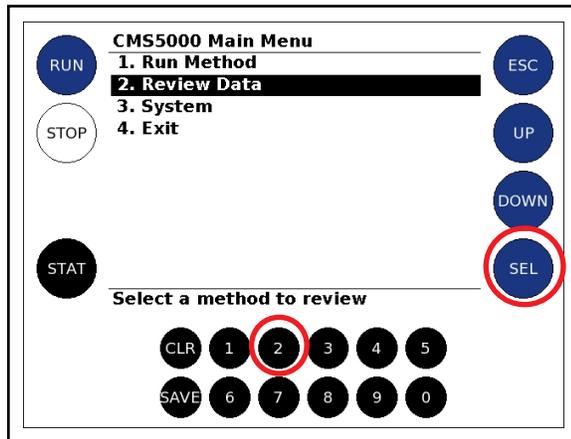
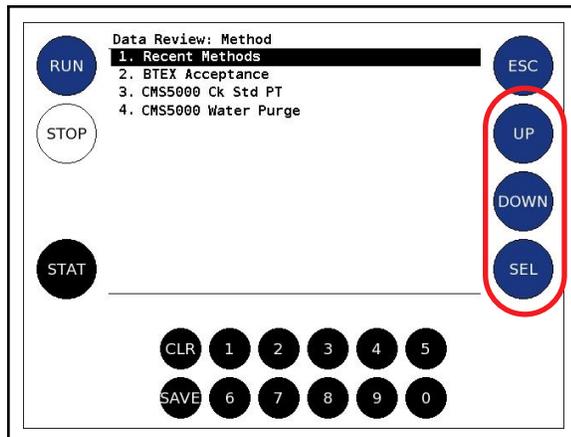


Figure 9-3 Using the number keys to select Review Data



- 3 The data will be arranged in folders by method name. Tap **UP** or **DOWN** to select the desired folder, then tap **SEL**. (See Figure 9-4.)

Figure 9-4 Method folders



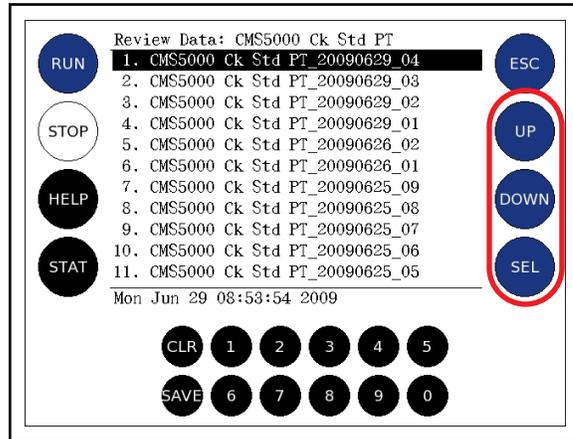
NOTE: **Recent Methods** will display the ten most recently run methods.

NOTE: While method sequences may appear in the list, nothing will occur if they are selected. The individual methods that make up a method sequence must be selected instead.

- 4 Tap **UP** or **DOWN** to highlight the desired data file, then tap **SEL**.
(See Figure 9-5.)

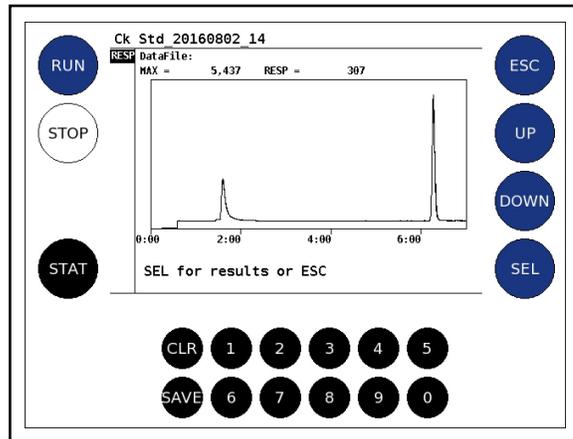
NOTE: Files are named in the following default format: method name_yearmonthday_ sequential number of run for that date. Files will be in chronological order with the most recent data file at the top of the list. To change the file format of new data files, see section 16.8.2, Date and Time Appendix, on page 16-21.

Figure 9-5 Selecting data file



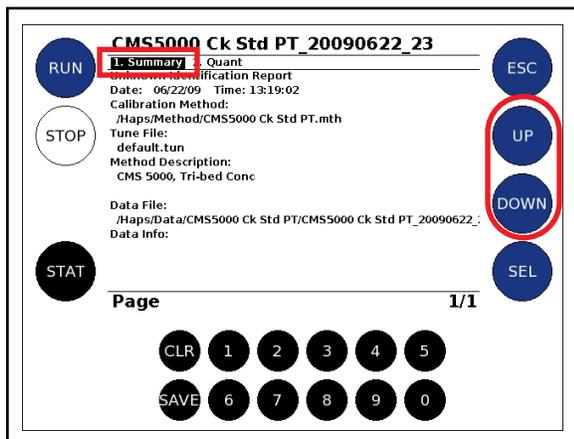
- 5 The selected file is displayed. (See Figure 9-6.)

Figure 9-6 Recalled data file



- 6 Tap **SEL** to retrieve results in a report format.
- 7 A **Summary** report is displayed. This report contains the **Date** and **Time** the sample was run, the **Calibration Method**, **Tune File**, **Method Description**, **Data File** name and **Data Info**. Tap **UP** or **DOWN** to scroll through the full report. (See Figure 9-7.)

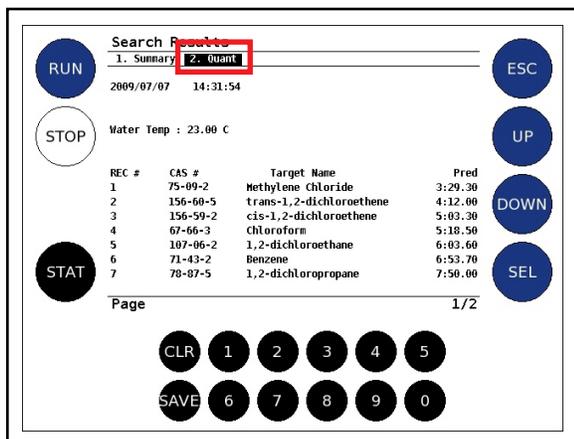
Figure 9-7 Summary report



- 8 To access the **Quant** (Quantitative) Report, tap **Quant**. This report contains the **REC#** (Compound Library Number), **CAS#** (Chemical Abstracts Service Registry Number), **Target Name**, and **PredRT** (predicted retention time). Tap **UP** or **DOWN** to scroll through the report. (See Figure 9-8.)

NOTE: The screen truncates the data file. Accessing the data file through CMS IQ software shows **Actual RT** (actual retention time), **Area**, **Conc** (Concentration adjusted by the check standard and/or water temperature adjustment in units defined by the method), **No Adjust** (Concentration without adjustment), **Limit** (alarm limits established in method), and **Flag** (additional notes when needed). See section 13.6.3, Quantitative Reports, on page 13-8.

Figure 9-8 Quantitative report



- 9 Tap **ESC** to return to the previous screen.

Chapter 10

System Function

10.1 Introduction

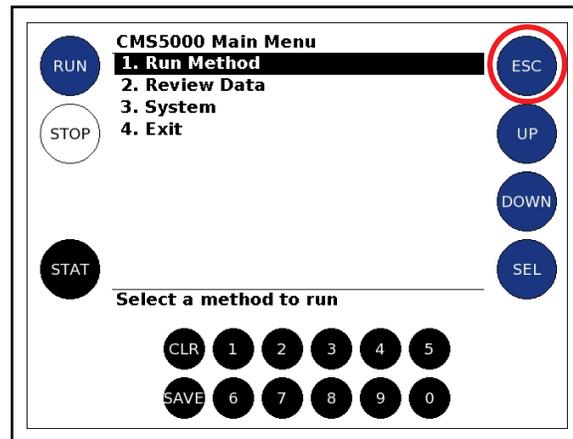
System Function is used to set the date and time, network addresses and language settings.

10.2 System Function

To select the **System** function:

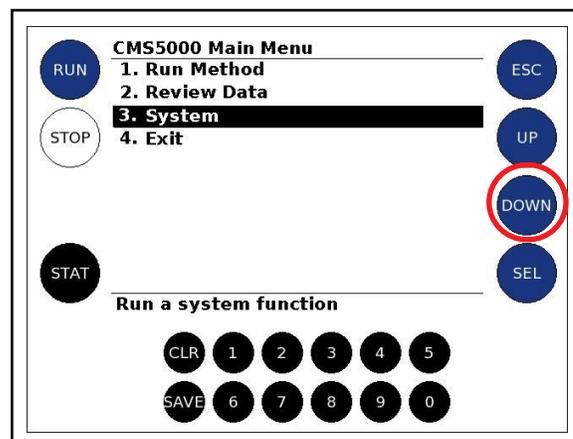
- 1 Tap **ESC** until the **CMS5000 Main Menu** is displayed. (See Figure 10-1.)

Figure 10-1 CMS5000 Main Menu



- 2 Tap **DOWN** until **System** is highlighted. (See Figure 10-2.)

Figure 10-2 System function



3 Tap **SEL**. (See Figure 10-3.)

NOTE: Alternately, tap **3** followed by **SEL**. (See Figure 10-4.)

Figure 10-3 Selecting System

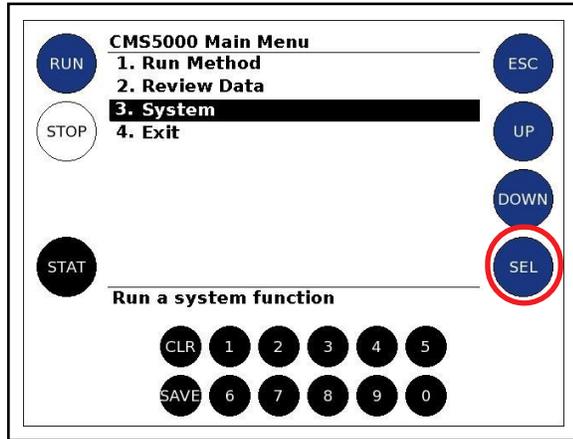
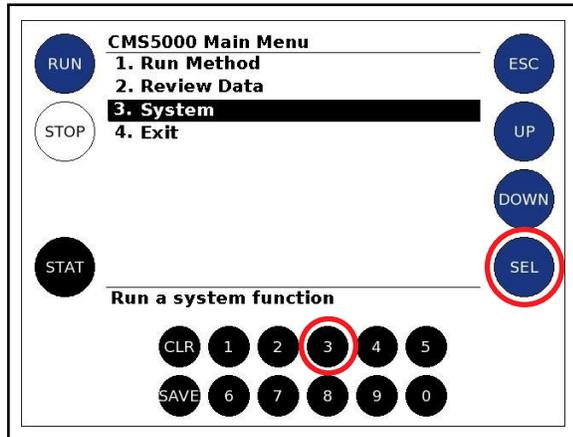


Figure 10-4 Using the number keys to select System

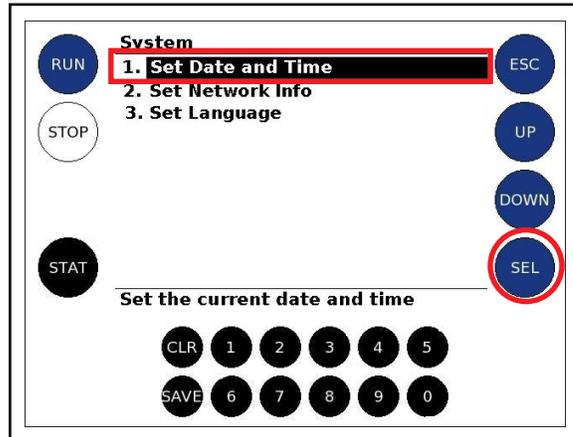


10.3 Set Date, Time and Time Zone

Set Date and Time is used to timestamp the data files.

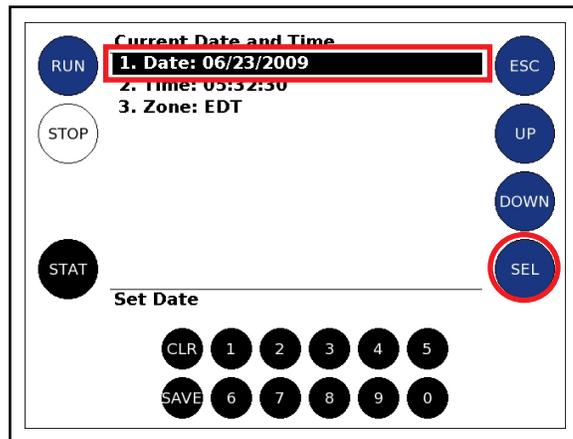
- 1 Tap **SEL** to select **Set Date and Time**. (See Figure 10-5.)

Figure 10-5 Set Date and Time



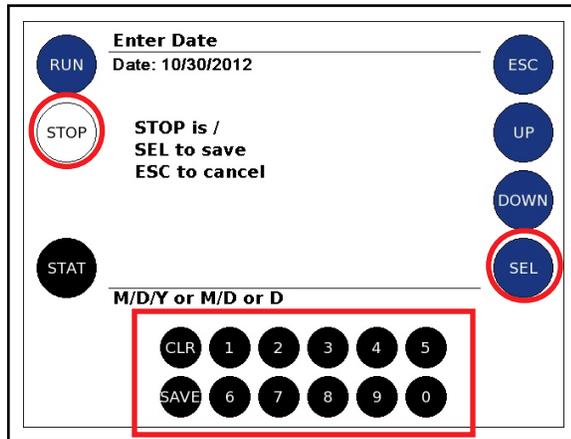
- 2 The **Current Date and Time** screen is displayed. To change the date, tap **SEL** when **Date** is highlighted. (See Figure 10-6.) Alternately, tap **2** followed by **SEL**.

Figure 10-6 Setting the date



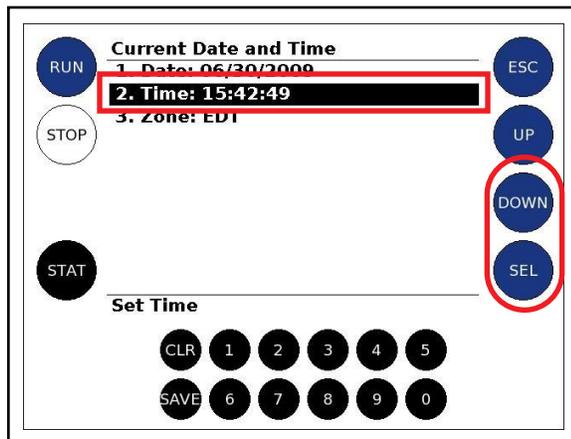
- 3 Tap the **number keys** to enter the date in the format **mm/dd/yyyy**. Tap **STOP** to enter a forward slash. Tap **SEL** to save the date. (See Figure 10-7.)

Figure 10-7 Entering the date



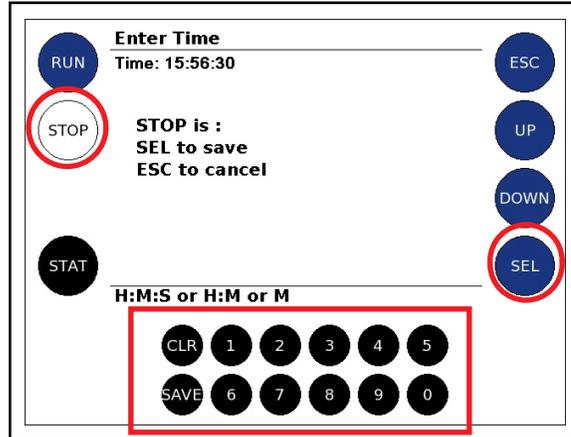
- 4 Upon saving, the **Current Date and Time** screen is displayed.
- 5 To change the time, tap **DOWN** to highlight the **Time** option. Tap **SEL**. (See Figure 10-8.)

Figure 10-8 Time function



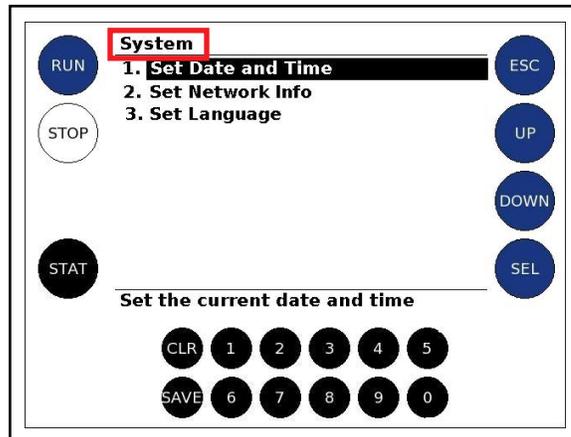
- 6 Enter the time using the **number keys** in the format **HH:MM:SS**. The time is entered in 24-hour notation (e.g. 3 p.m. is entered as 15:00:00.) To enter a colon, tap **STOP**. To save, tap **SEL**. (See Figure 10-9.)

Figure 10-9 Setting the time



- 7 Upon saving, the **System** menu will be displayed. (See Figure 10-10.)

Figure 10-10 System menu



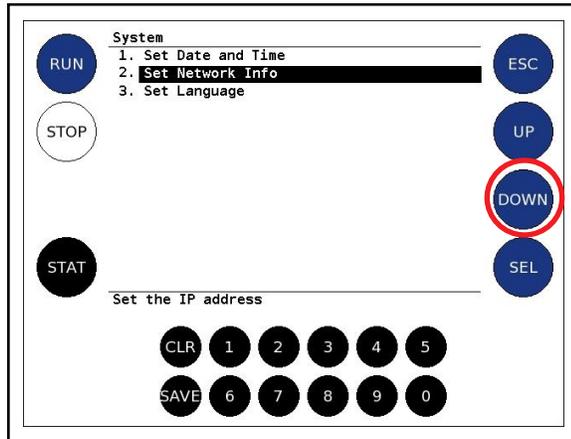
10.3.1 Set Network Info

Set Network Info is used to change the CMS5000 IP address.

NOTE: The CMS5000 IP address should only be changed if it conflicts with an existing network.

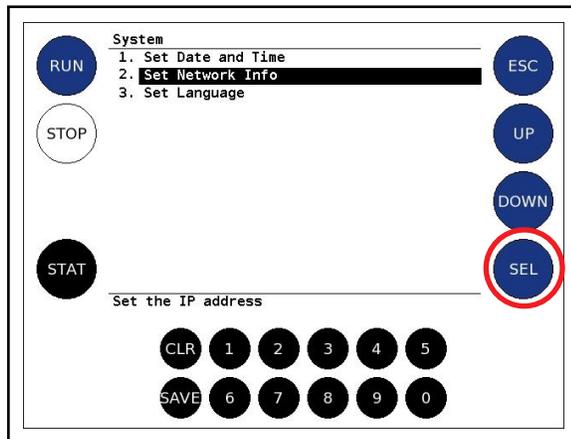
- 1 Tap **DOWN** to highlight **Set Network Info**. (See Figure 10-11.)

Figure 10-11 Set Network Info option



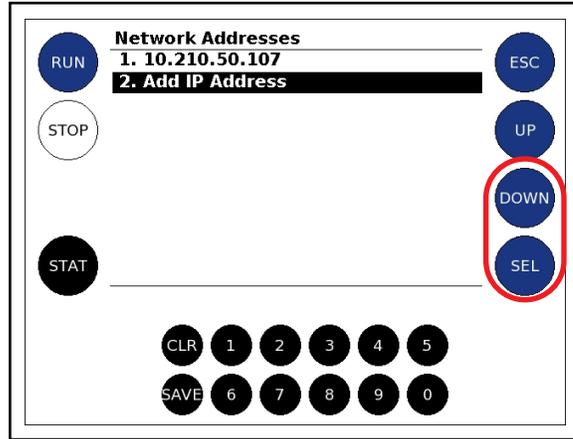
- 2 Tap **SEL**. (See Figure 10-12.)

Figure 10-12 Selecting Set Network Info



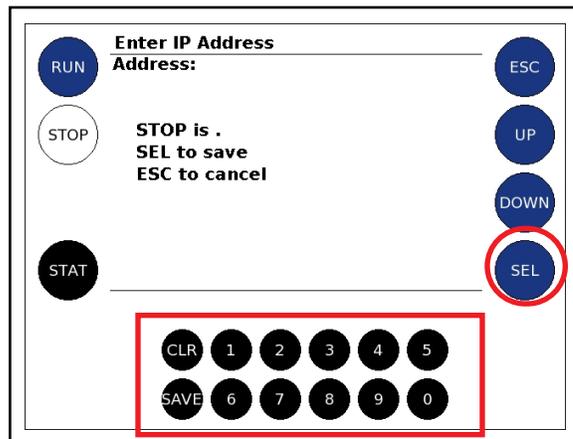
- 3 The CMS5000 IP address is displayed on the **Network Addresses** screen.
- 4 If an additional or alternate IP address is desired, tap **DOWN** to highlight **Add IP Address**. Tap **SEL**. (See Figure 10-13.)

Figure 10-13 Add IP Address function



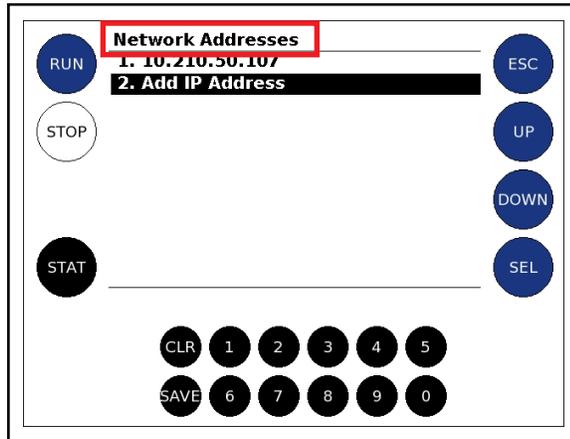
- 5 Tap the **number keys** to enter the new IP address. To enter periods, tap **STOP**. Tap **SEL** to save. (See Figure 10-14.)

Figure 10-14 Enter IP Address screen



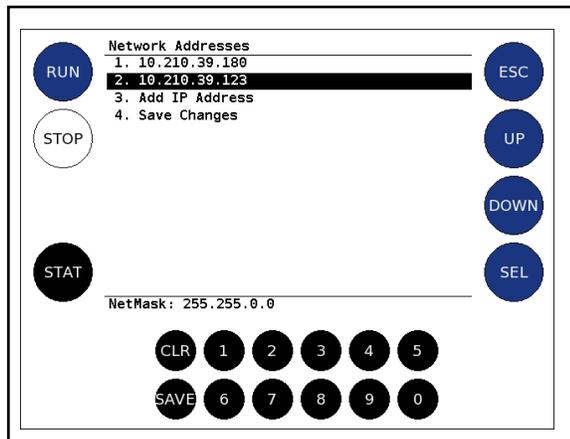
6 The **Network Addresses** screen is displayed. (See Figure 10-15.)

Figure 10-15 Network Addresses screen



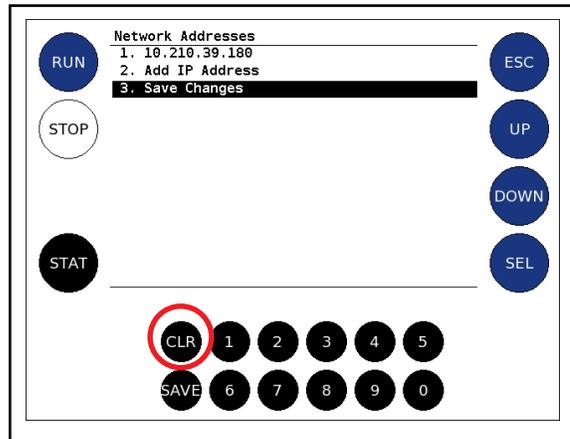
7 To delete an IP address, highlight the IP address to be deleted. (See Figure 10-16.)

Figure 10-16 Select IP Address to be deleted



- 8 Tap the **CLR** button. Tap the button to **Save Changes**. The IP Address is now deleted. (See Figure 10-17.)

Figure 10-17 Save Changes

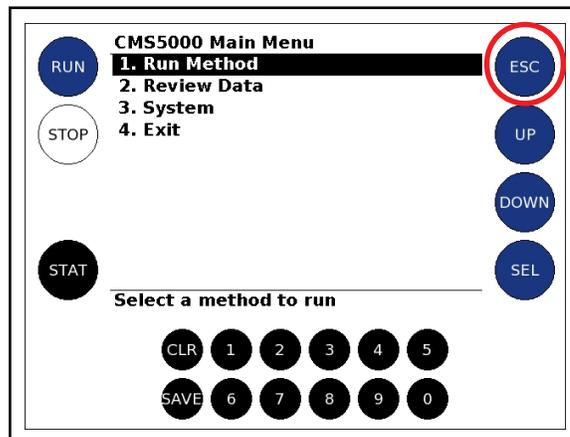


10.3.2 Set Language

Set Language is used to select the desired language displayed on the front panel.

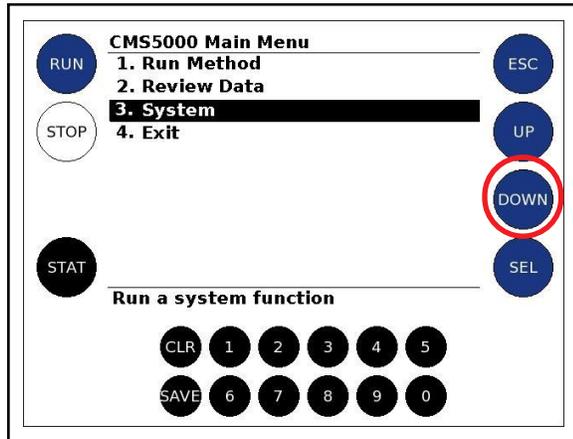
- 1 Tap **ESC** until **CMS5000 Main Menu** is displayed. (See Figure 10-18.)

Figure 10-18 CMS5000 Main Menu



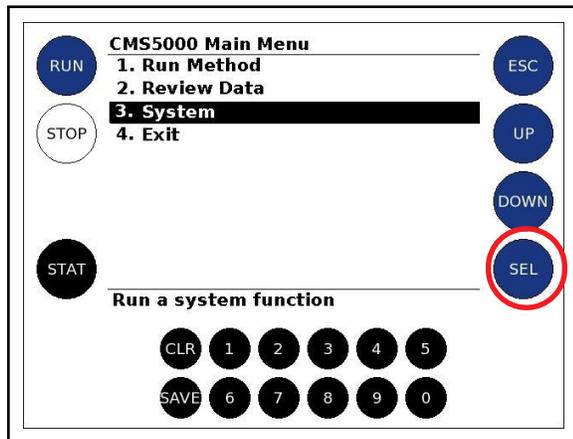
- 2 Tap **DOWN** until **System** is highlighted. (See Figure 10-19.)

Figure 10-19 System function



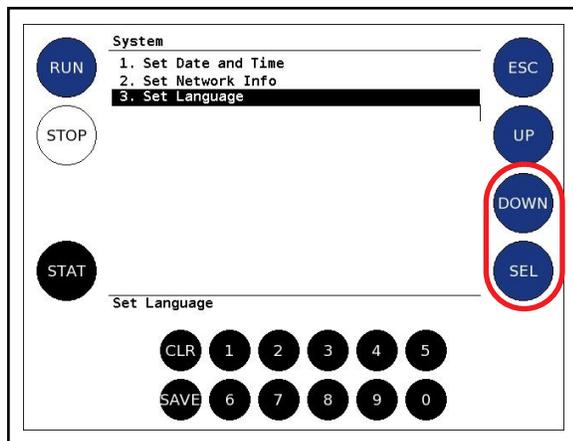
- 3 Tap **SEL**. (See Figure 10-20.)

Figure 10-20 Selecting System



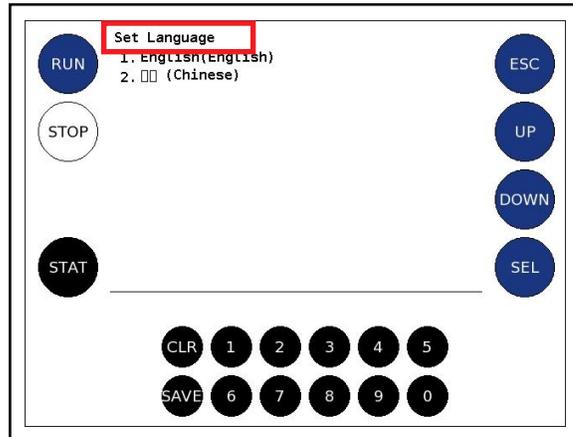
- 4 Tap **DOWN** to highlight **Set Language**. Tap **SEL**. (See Figure 10-21.)

Figure 10-21 Set Language option



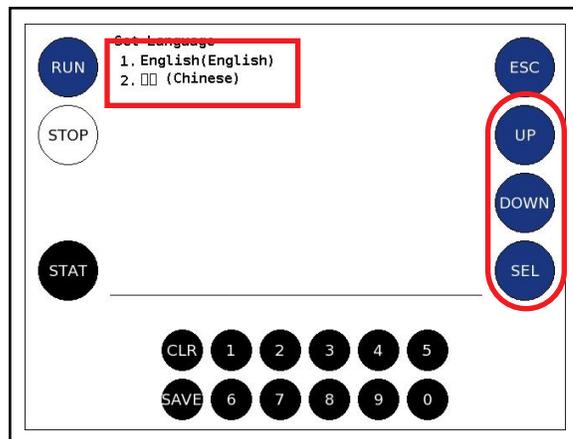
5 The **Set Language** screen is displayed. (See Figure 10-22.)

Figure 10-22 Set Language menu



6 To change language settings, tap **UP** or **DOWN** to highlight the desired language. Tap **SEL**. The system will restart and the desired language will be displayed. (See Figure 10-23.)

Figure 10-23 Changing language options



Chapter 11

Exit Function

11.1 Exit Function

Exit will restart the program or reboot the system.

- ◆ **Restart Program** turns off the system and then restarts it
- ◆ **Reboot System** resets the CMS5000 microprocessor and reloads drivers

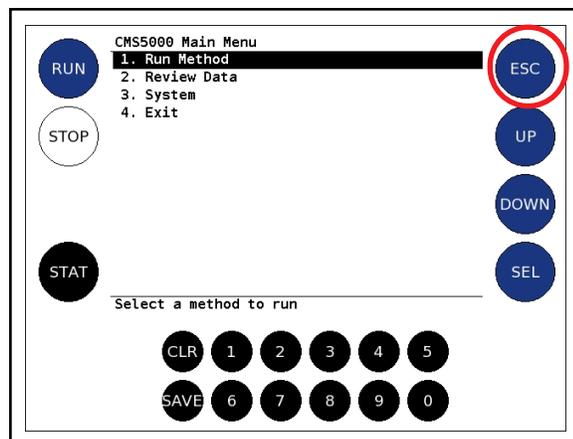
In the event of a power outage, CMS5000 will automatically restart when power becomes available. If the option to define a startup method has been selected, then CMS5000 will start that method after restarting. (See section 6.4, Defining Startup Methods, on page 6-12.)

CMS5000 will restart automatically after a software update.

11.2 Accessing Exit Options

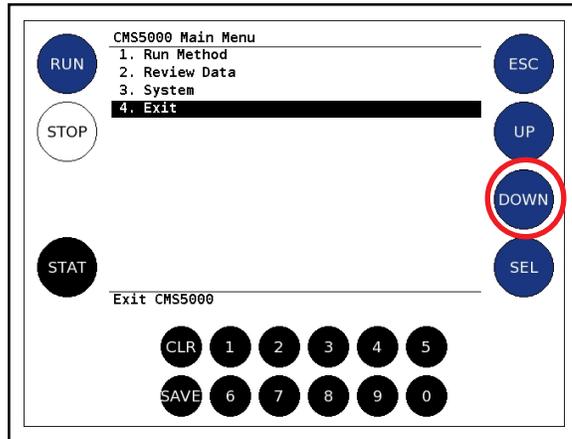
- 1 Tap **ESC** until the **CMS5000 Main Menu** is displayed. (See Figure 11-1.)

Figure 11-1 CMS5000 Main Menu



2 Tap **DOWN** to highlight **Exit**. (See Figure 11-2.)

Figure 11-2 Exit function



3 Tap **SEL**. (See Figure 11-3.)

NOTE: Alternately, tap **4** followed by **SEL**. (See Figure 11-4.)

Figure 11-3 Selecting Exit

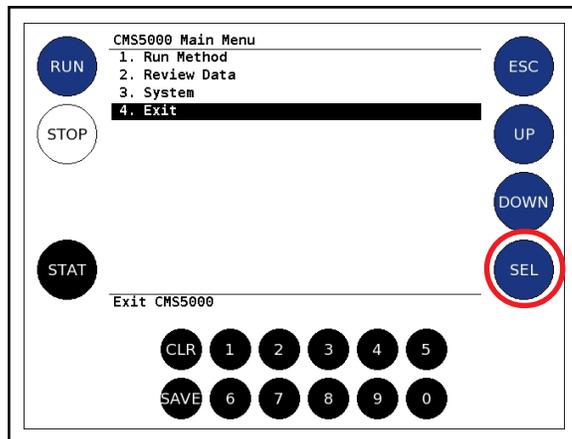
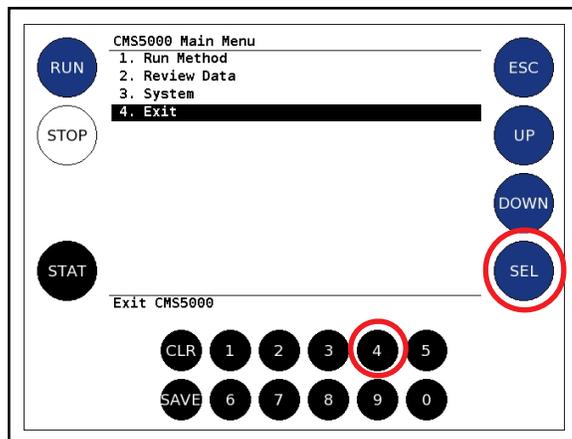


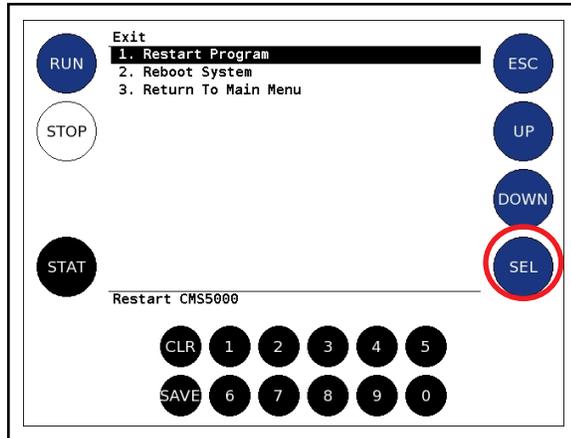
Figure 11-4 Using the number keys to select the Exit function



11.3 Restart System

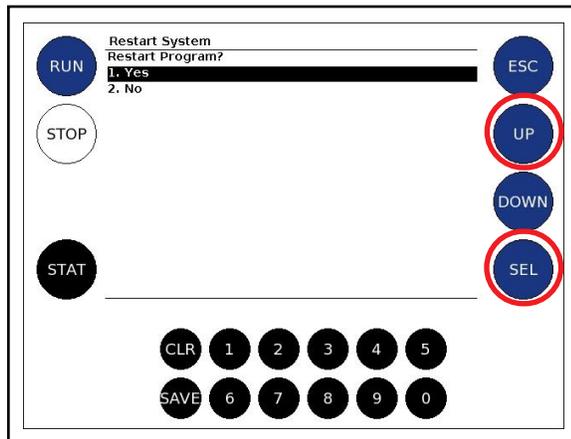
- 1 With **Restart Program** highlighted, tap **SEL**. (See Figure 11-5.)

Figure 11-5 Restart Program option



- 2 **Restart Program?** is displayed. Tap **UP** to highlight **Yes**. Tap **SEL**. (See Figure 11-6.)

Figure 11-6 Confirming Restart

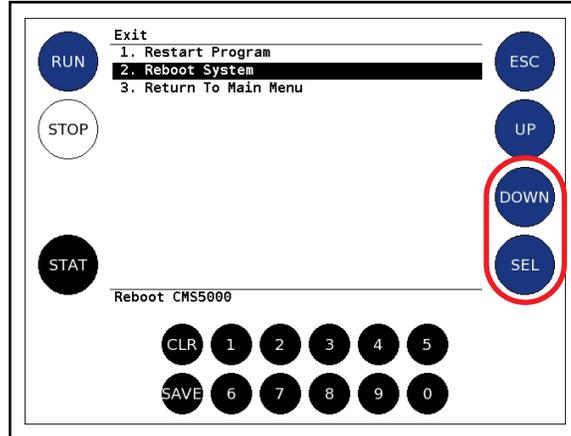


- 3 CMS5000 will restart.

11.4 Reboot System

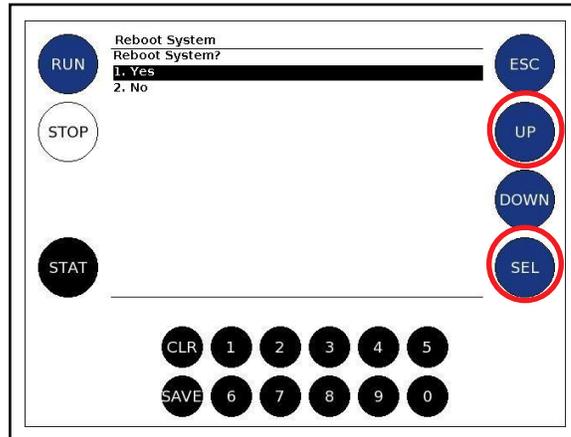
- 1 Tap **DOWN** to highlight **Reboot System**. Tap **SEL**. (See Figure 11-7.)

Figure 11-7 Reboot System option



- 2 **Reboot System?** will display. Tap **UP** to highlight **Yes**. Tap **SEL**. (See Figure 11-8.)

Figure 11-8 Confirming Reboot



- 3 CMS5000 will reboot.

11.5 Return to CMS5000 Main Menu

Select the **Return to Main Menu** option to display the **CMS5000 Main Menu**. Alternately, tap **ESC** until the **CMS5000 Main Menu** is displayed.

Chapter 12

CMS IQ System Setup

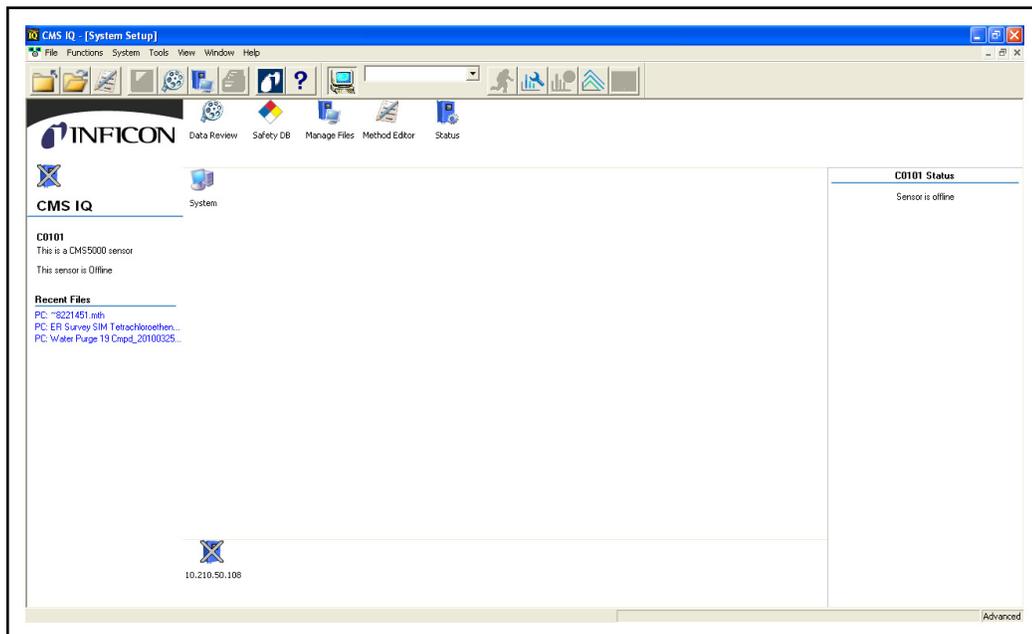
12.1 Introduction

The **System Setup** window controls instrument operation. **System Setup** is used to run analyses, access data files, create or edit methods, and set parameters of various CMS5000 components.

12.2 System Setup

To access **System Setup**, launch CMS IQ by double-clicking . The **System Setup** window is displayed. (See Figure 12-1.)

Figure 12-1 System Setup window

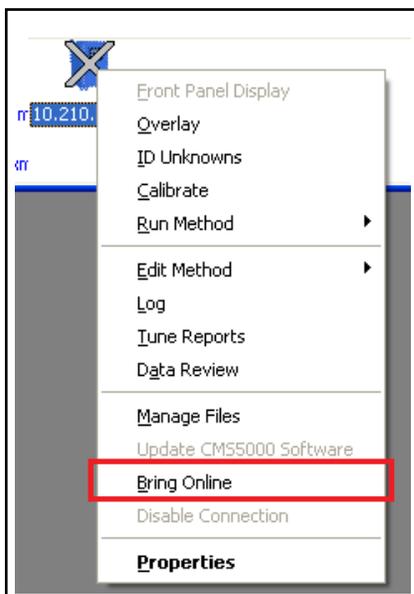


12.2.1 Connecting to CMS5000

When CMS IQ is launched, CMS5000 will not automatically connect. To connect to CMS5000, click the desired CMS5000 sensor status icon.

NOTE: If CMS IQ is configured to connect to multiple instruments, right click the desired CMS5000 sensor status icon and click **Bring Online**. (See Figure 12-2.)

Figure 12-2 Bringing CMS 5000 Online



12.2.2 System Setup Menu

The main menu toolbar includes **File**, **Functions**, **System**, **Tools**, **View**, **Window**, and **Help** options. (See Figure 12-3.)

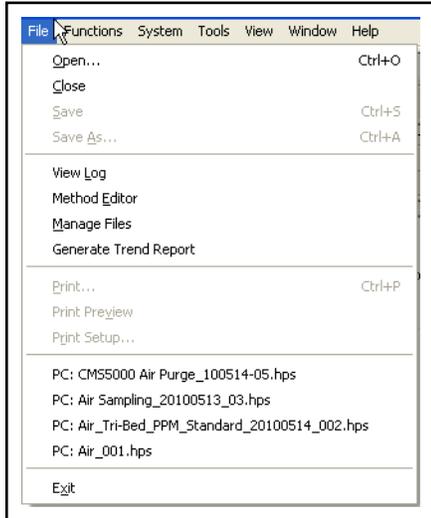
Figure 12-3 Main Menu toolbar



12.2.3 File Menu

The **File** menu is shown in Figure 12-4.

Figure 12-4 File menu



- Open** Opens a data file from either CMS5000 or the computer
- Close** Closes a data file
- Save** Unavailable when in the System Setup window. When a data file is opened, the Data Review window is displayed. See [section 13.2, Accessing the Data Review Feature, on page 13-1](#). **Save** is activated in the Data Review window. Changes to the data file can be saved
- Save As** Unavailable in the System Setup window. When a data file is opened, the Data Review window is displayed. **Save As** is activated in the Data Review window. The data file can be saved with a different name and/or to a different location
- View Log** Opens event log (*.evt) files. Examples of information logged are warnings, errors, events, and run history. See [section 12.6.6.2, Logged Items, on page 12-61](#)
- Method Editor** Functions the same as the **Method Editor** icon. See [Chapter 16, Method Editor](#)

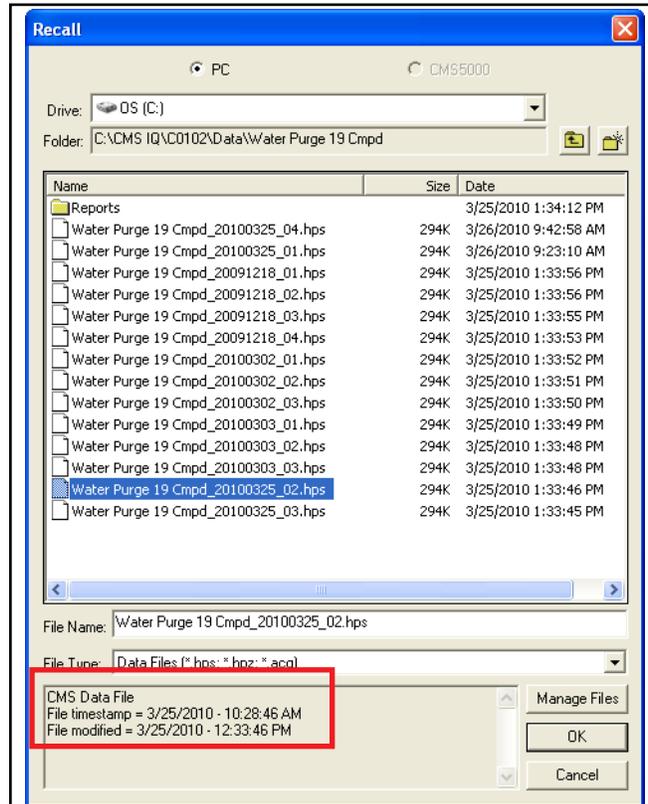
| | |
|--------------------------------------|---|
| Manage Files | Functions the same as the Manage Files icon. See section 12.5, Manage Files, on page 12-39 |
| Generate Trend Report | Analyzes data collected over a specified period of time. See section 12.2.3.1 |
| Print | Prints files and is active in the Data Review window |
| Print Preview | Displays a preview of the final print layout and is active in the Data Review window |
| Print Setup | Accesses the printer setup options |
| Recently Accessed Files | Displays a list of recently accessed files. Click a file name to open it in the Data Review window |
| Exit. | Closes CMS IQ software |

12.2.3.1 Generate Trend Report

To generate a trend report:

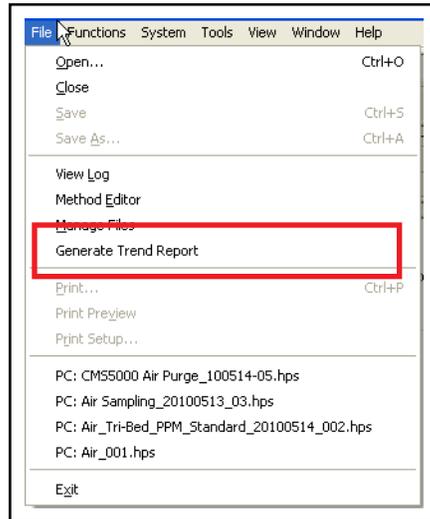
- 1 Determine the time period the trend report should cover. Alternatively, determine the date and time of the first and last data file to be used in the trend report. The date and time for the data file is displayed at the bottom of the **Recall** window. Take note of the date and time. (See Figure 12-5.) Click **Cancel**.

Figure 12-5 Recall data file date and time



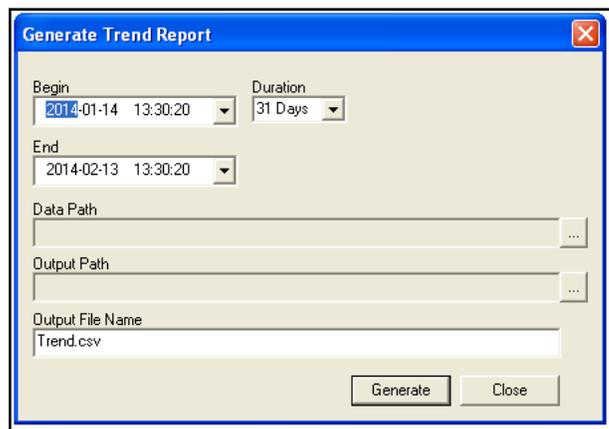
2 Click File and select Generate Trend Report. (See Figure 12-6.)

Figure 12-6 Select Generate Trend Report



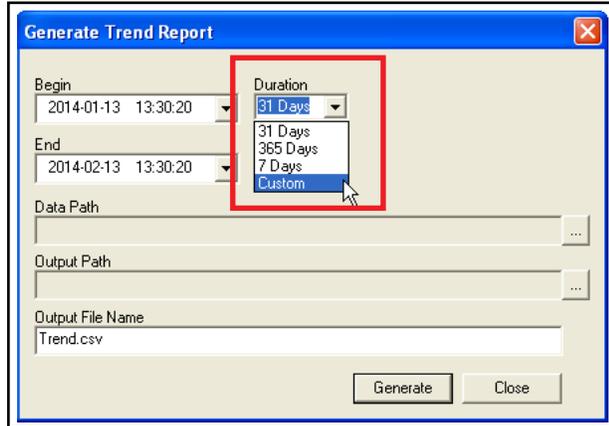
3 The Generate Trend Report window is displayed. (See Figure 12-7.)

Figure 12-7 Generate Trend Report



- Duration** sets the length of the trend report. There are three preset durations, **31 Days**, **365 Days**, and **7 Days**. For a duration of any different length, select **Custom**. (See Figure 12-8.)

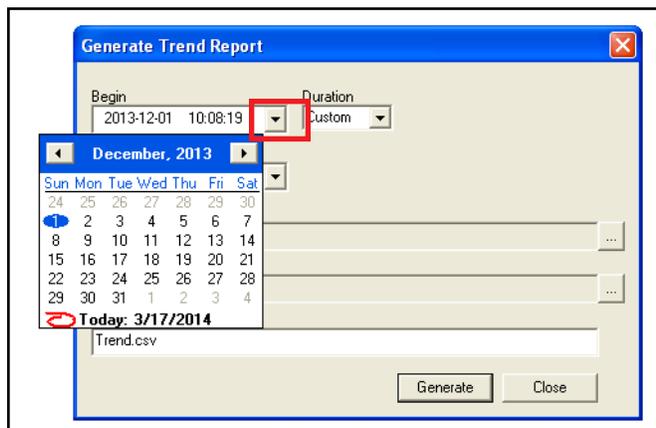
Figure 12-8 Duration



- Select **Begin** or **End** to set the date and time for the beginning or end of the trend report. The date and time can be entered by selecting each box and typing in the appropriate year, month, day, hour, minute, and second. The date can also be selected from the shortcut menu by selecting a calendar date. (See Figure 12-9.)

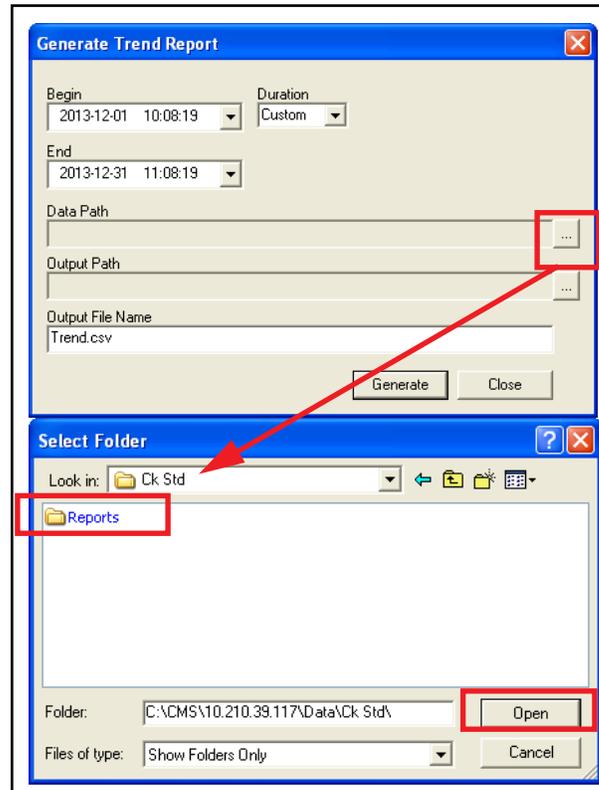
NOTE: If **Begin** is selected, **End** will adjust to fit the selected **Duration** and vice versa. If **Duration** is set to **Custom**, **Begin** and **End** must each be selected individually.

Figure 12-9 Begin and End



- 6 Click **Browse (...)** to set the **Data Path** to the **Reports** folder to contain the trend report data. (See Figure 12-10.)

Figure 12-10 Data Path/Reports folder

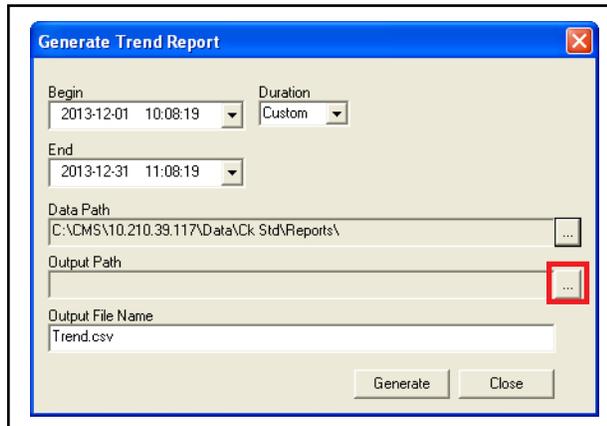


NOTE: The **Reports** folder may not contain all desired data reports. Data reports must be transferred from CMS5000 to the computer. See [section 12.5, Manage Files](#), on page 12-39 for information on transferring data files to the computer.

- 7 Double-click the **Reports** folder, or highlight the **Reports** folder and click **Open**. (Refer to Figure 12-10.)

- 8 Click **Browse (...)** to set the **Output Path** where the report file will be saved. (See Figure 12-11.)

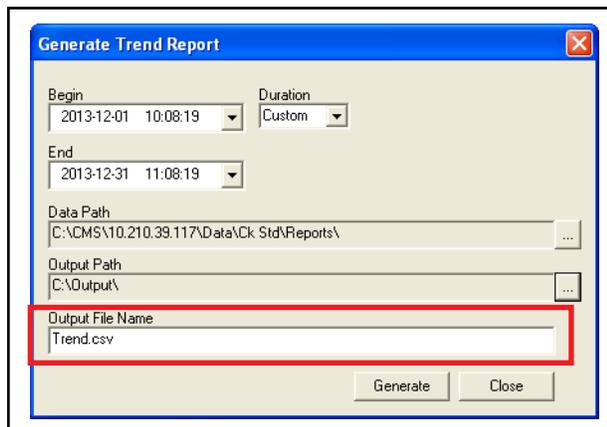
Figure 12-11 Output Path



The screenshot shows the 'Generate Trend Report' dialog box. It has a blue title bar with a close button. The main area is light beige. There are two date and time pickers: 'Begin' (2013-12-01 10:08:19) and 'End' (2013-12-31 11:08:19). A 'Duration' dropdown is set to 'Custom'. Below these are three text input fields: 'Data Path' (C:\CMS\10.210.39.117\Data\Ck Std\Reports\), 'Output Path' (empty), and 'Output File Name' (Trend.csv). Each of the first three fields has a small '...' button to its right. The 'Output Path' field's '...' button is highlighted with a red rectangle. At the bottom are 'Generate' and 'Close' buttons.

- 9 Enter the **Output File Name** for the trend report. The default report name is **Trend.csv**. The file can be renamed after it has been generated. (See Figure 12-12.)

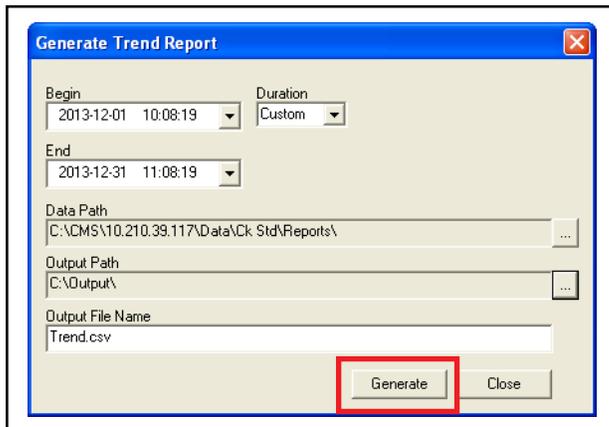
Figure 12-12 Output File Name



The screenshot shows the 'Generate Trend Report' dialog box, similar to Figure 12-11. In this view, the 'Output Path' field is filled with 'C:\Output\' and its '...' button is also highlighted with a red rectangle. The 'Output File Name' field is highlighted with a larger red rectangle, showing the text 'Trend.csv'. The 'Generate' and 'Close' buttons are at the bottom.

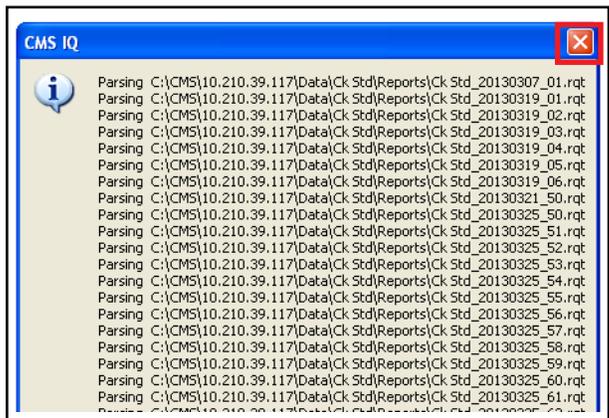
10 Click **Generate**. (See Figure 12-13.)

Figure 12-13 Generate the trend report



11 CMS IQ will parse every report within the data path and add reports with the appropriate dates to the trend report. A window displays the files being parsed and a trend report is generated. Depending on the number of files in the data path, the window may extend below the bottom of the screen. Click "X" to close the window. (See Figure 12-14.)

Figure 12-14 Parsing Files



- The trend report is saved as <Output File Name>.CSV in the Output Path folder and opened as a Microsoft Excel spreadsheet. (See Figure 12-15.)

Figure 12-15 Trend Report in Excel

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O |
|----|-----------------|------|------|-------------|----------|-----------|--------|-------------|-----------|-------------|------|----------------|------------------------------|-----------------------------|---|
| 1 | Date | REC# | CAS# | Target Name | Pred. RT | Actual RT | Area | Conc. (ppm) | No Adjust | Limit (ppm) | Flag | Water Temp (C) | Water Temp (Calibration) (C) | Argon Supply Pressure (kPa) | |
| 2 | 12/6/2013 10:07 | 1 | | Toluene | 06:17.7 | 06:14.7 | 396505 | 1 | 1.473 | --- | | | | 605 | |
| 3 | 12/6/2013 10:17 | 1 | | Toluene | 06:17.7 | 06:14.7 | 391399 | 1 | 1.454 | --- | | | | 605 | |
| 4 | 12/6/2013 10:27 | 1 | | Toluene | 06:17.7 | 06:13.2 | 518375 | 1 | 1.054 | --- | | | | 614 | |
| 5 | 12/6/2013 10:36 | 1 | | Toluene | 06:17.7 | 06:14.3 | 402414 | 1 | 1.495 | --- | | | | 607 | |
| 6 | 12/6/2013 10:46 | 1 | | Toluene | 06:17.7 | 06:14.4 | 399915 | 1 | 1.486 | --- | | | | 607 | |
| 7 | 12/6/2013 10:56 | 1 | | Toluene | 06:17.7 | 06:14.4 | 404451 | 1 | 1.503 | --- | | | | 607 | |
| 8 | 12/6/2013 11:06 | 1 | | Toluene | 06:17.7 | 06:14.4 | 401114 | 1 | 1.491 | --- | | | | 607 | |
| 9 | 12/6/2013 11:16 | 1 | | Toluene | 06:17.7 | 06:14.6 | 403602 | 1 | 1.5 | --- | | | | 607 | |
| 10 | 12/6/2013 11:26 | 1 | | Toluene | 06:17.7 | 06:14.6 | 405474 | 1 | 1.507 | --- | | | | 607 | |
| 11 | 12/6/2013 11:35 | 1 | | Toluene | 06:17.7 | 06:14.5 | 402327 | 1 | 1.495 | --- | | | | 607 | |
| 12 | 12/6/2013 11:45 | 1 | | Toluene | 06:17.7 | 06:15.0 | 396004 | 1 | 1.472 | --- | | | | 608 | |
| 13 | 12/6/2013 11:55 | 1 | | Toluene | 06:17.7 | 06:14.9 | 400674 | 1 | 1.489 | --- | | | | 608 | |
| 14 | 12/6/2013 12:05 | 1 | | Toluene | 06:17.7 | 06:14.9 | 400023 | 1 | 1.486 | --- | | | | 608 | |
| 15 | 12/6/2013 12:15 | 1 | | Toluene | 06:17.7 | 06:14.9 | 399406 | 1 | 1.484 | --- | | | | 608 | |
| 16 | 12/6/2013 12:25 | 1 | | Toluene | 06:17.7 | 06:15.0 | 399934 | 1 | 1.486 | --- | | | | 608 | |
| 17 | 12/6/2013 12:34 | 1 | | Toluene | 06:17.7 | 06:14.4 | 393125 | 1 | 1.461 | --- | | | | 605 | |
| 18 | 12/6/2013 12:44 | 1 | | Toluene | 06:17.7 | 06:14.6 | 398562 | 1 | 1.481 | --- | | | | 605 | |
| 19 | 12/6/2013 12:54 | 1 | | Toluene | 06:17.7 | 06:14.8 | 395131 | 1 | 1.468 | --- | | | | 608 | |
| 20 | 12/6/2013 13:04 | 1 | | Toluene | 06:17.7 | 06:14.5 | 412866 | 1 | 1.533 | --- | | | | 612 | |
| 21 | 12/6/2013 13:14 | 1 | | Toluene | 06:17.7 | 06:14.9 | 418012 | 1 | 1.553 | --- | | | | 612 | |

- Click **Close** to exit the **Generate Trend Report** window. (See Figure 12-16.)

Figure 12-16 Close Generate Trend Data window

Generate Trend Report

Begin: 2013-12-01 10:08:19 | Duration: Custom

End: 2013-12-31 11:08:19

Data Path: C:\CMS\10.210.39.117\Data\Ck Std\Reports\

Output Path: C:\Output\

Output File Name: Trend.csv

Buttons: Generate, Close

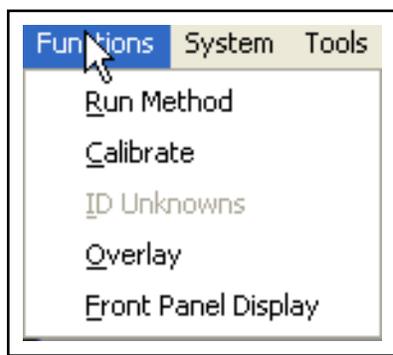
12.2.4 Functions Menu

The **Functions** menu contains **Run Method**, **Calibrate**, **Overlay**, and **Front Panel Display**. (See Figure 12-17.) These options behave identically to their icons on the toolbar. See:

- ♦ Chapter 14, Run Method
- ♦ Chapter 17, Calibration
- ♦ Chapter 15, Chromatogram Overlay
- ♦ section 12.7, Front Panel Display Icon, on page 12-70

NOTE: ID Unknowns is unavailable.

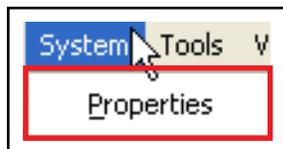
Figure 12-17 Functions menu



12.2.5 System

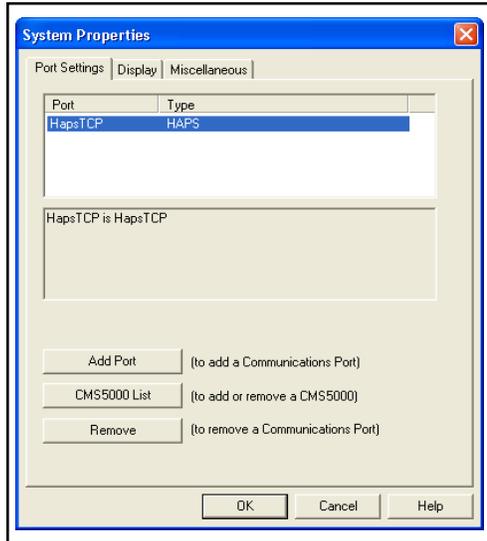
The **System** menu is shown in Figure 12-18.

Figure 12-18 System menu



Click **Properties** to display the **System Properties** window. (See Figure 12-19.)

Figure 12-19 System Properties window



12.2.5.1 Port Settings

The **Port Settings** tab is displayed. (See Figure 12-20.)

NOTE: **Add Port** and **Remove** should only be used by INFICON personnel.

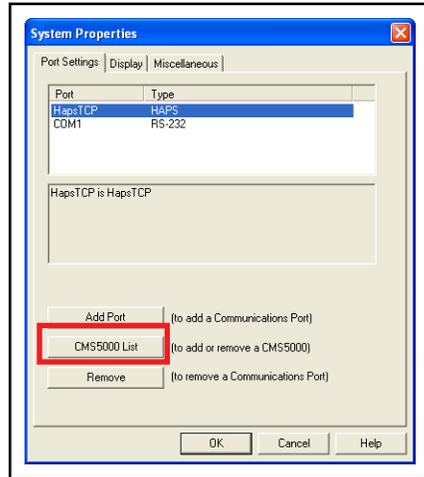
CMS5000 List is used to:

- ◆ add, change, or delete a CMS5000 instrument from **CMS IQ**. The instrument name is displayed in the **CMS IQ System Setup** window
- ◆ connect CMS5000 to the computer via TCP/IP. Refer to [Chapter 4, Setting Up Computer Communication](#)

To change the system name:

- 1 Click **CMS5000 List**. (See Figure 12-20.)

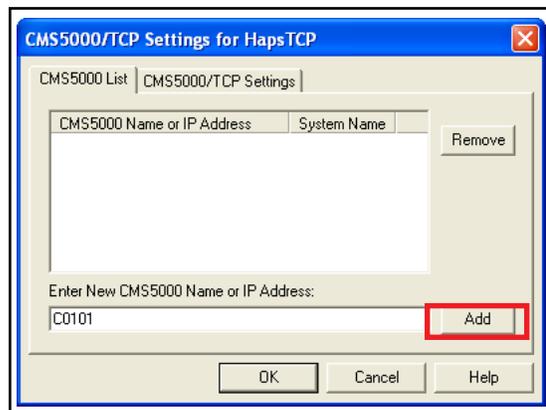
Figure 12-20 System Properties window



- 2 If a CMS5000 has not been previously connected, the list will be blank. Type in the CMS5000 Name (C#####) or IP address. Click **Add**. (See Figure 12-21.)

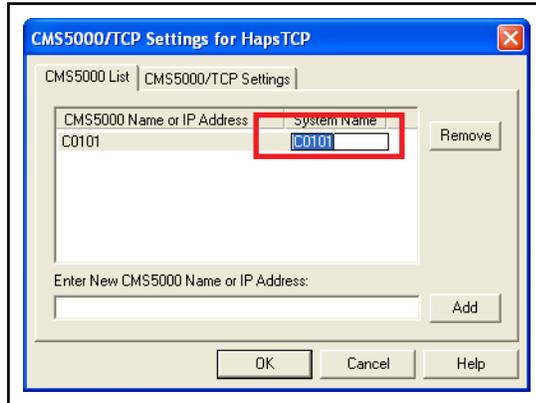
NOTE: To find the CMS5000 Name or IP address, refer to section 4.2, Configuring the Computer for CMS5000 Communication, on page 4-1.

Figure 12-21 Adding CMS5000



- 3 Double-click **System Name** to highlight, then edit the text to change the Host Name or IP address. (See Figure 12-22.)

Figure 12-22 CMS5000 list



- 4 Click **OK**. The new CMS5000 **System Name** for CMS5000 is displayed in the **System Setup** window. (See Figure 12-23 and Figure 12-24.)

Figure 12-23 New system name

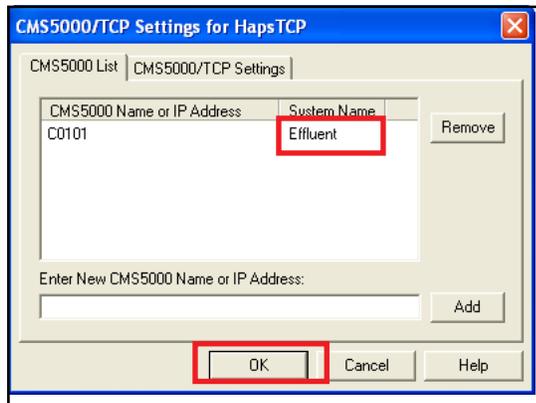


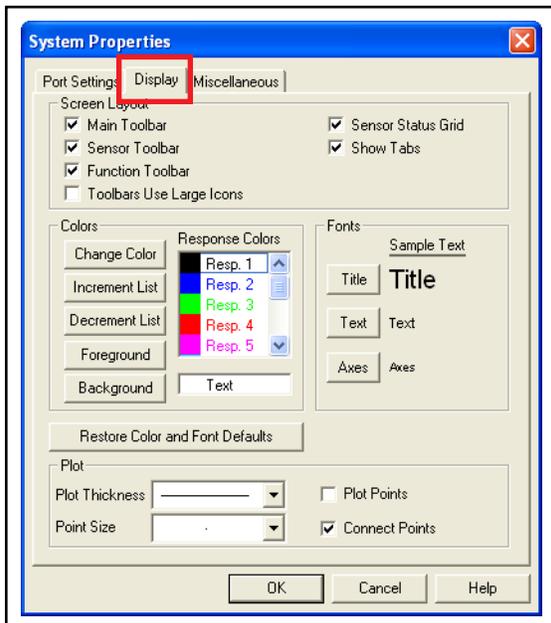
Figure 12-24 Renamed CMS5000



12.2.5.2 Display

The **Display** tab is used to change the appearance of CMS IQ, including screen layout, color, font, and plot parameters. (See Figure 12-25.)

Figure 12-25 Display tab



12.2.5.2.1 Screen Layout

The **Screen Layout** pane sets the configuration of the main CMS IQ window. (See Figure 12-26.)

Figure 12-26 Screen layout section



Main Toolbar Selecting or clearing the Main Toolbar checkbox displays or hides the toolbar icons for Close, Open, Method Editor, Save As, Data Review, Manage Files, Print, About, and Help

Sensor Toolbar Selecting or clearing the Sensor Toolbar checkbox displays or hides the toolbar icons for System Setup, Sensors shortcut menu, Run Method, Calibrate, Chromatogram Overlay, and Front Panel Display

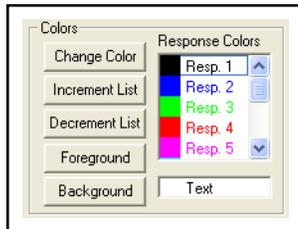
Function Toolbar Unavailable

- Toolbars Use Large Icons** Selecting or clearing the Toolbars Use Large Icons checkbox displays large or small toolbar icons
- Sensor Status Grid** Selecting or clearing the Sensor Status Grid checkbox displays or hides grids displaying information pertaining to the current state of valves and heaters
- Show Tabs** Selecting or clearing the Show Tabs checkbox will enable or disable the appearance of tabs in the software

12.2.5.2.2 Colors

Colors sets the color displayed when using **Data Review** and **Chromatogram Overlay**. (See Figure 12-27.)

Figure 12-27 Colors section

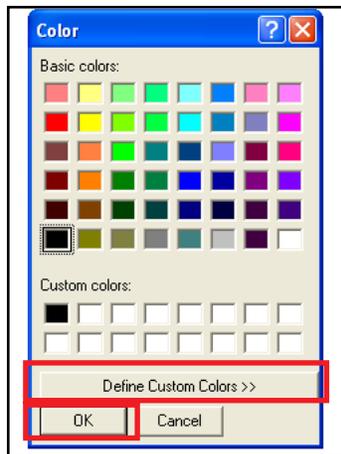


- Change Color** Select a color used when displaying data files. See section 12.2.5.2.3, *Selecting Colors*, on page 12-18
- Increment List** Adds an additional Resp # to the Response Colors list that can be assigned a color
- Decrement List** Removes a Resp # from the Response Colors list
- Foreground** Select the color used for text and axes displayed when using the Data Review and Chromatogram Overlay functions. See section 12.2.5.2.3, *Selecting Colors*, on page 12-18
- Background** Select the background color when using the Data Review and Chromatogram Overlay functions. See section 12.2.5.2.3, *Selecting Colors*, on page 12-18

12.2.5.2.3 Selecting Colors

To select a new color, click the desired color and click **OK**. (See Figure 12-28.)

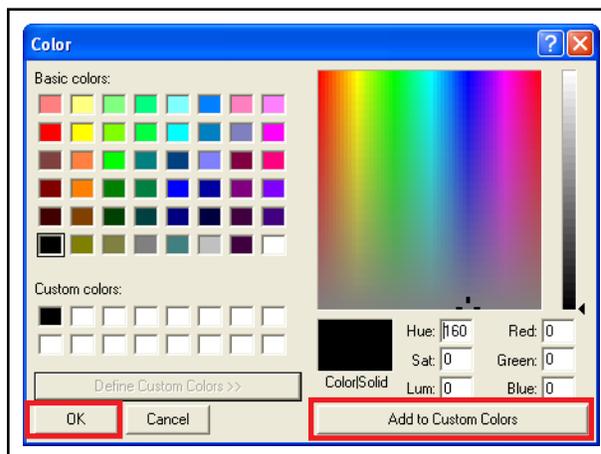
Figure 12-28 Changing colors



To create custom colors:

- 1 Click **Define Custom Colors >>**. An expanded color selection is displayed.
- 2 Define the desired color with the color palette; Red, Green, and Blue values; or Hue, Saturation, and Tone. Click **Add to Custom Colors**, select the color in the **Custom colors:** menu, then click **OK**. (See Figure 12-29.)

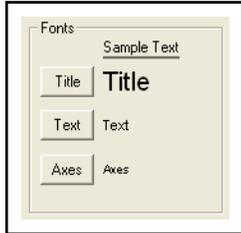
Figure 12-29 Defining custom colors



12.2.5.2.4 Fonts

Fonts sets the fonts displayed when using the **Data Review** and **Chromatogram Overlay** functions. (See [Figure 12-30](#).)

Figure 12-30 Fonts section



- Title** Unavailable
- Text** Changes the font displayed for Response_Max, Response/Response_Max, Response, etc.
- Axes** Changes the font displayed for the axis text

12.2.5.2.5 Restore Colors and Fonts Defaults

Restore Colors and Fonts Defaults reverts colors and fonts back to their default settings. (See [Figure 12-31](#).)

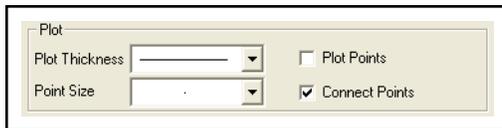
Figure 12-31 Restore Colors and Fonts Defaults button



12.2.5.2.6 Plot

The **Plot** pane sets the plot options that will be displayed when using the **Data Review** and **Chromatogram Overlay** functions. (See [Figure 12-32](#).)

Figure 12-32 Plot section



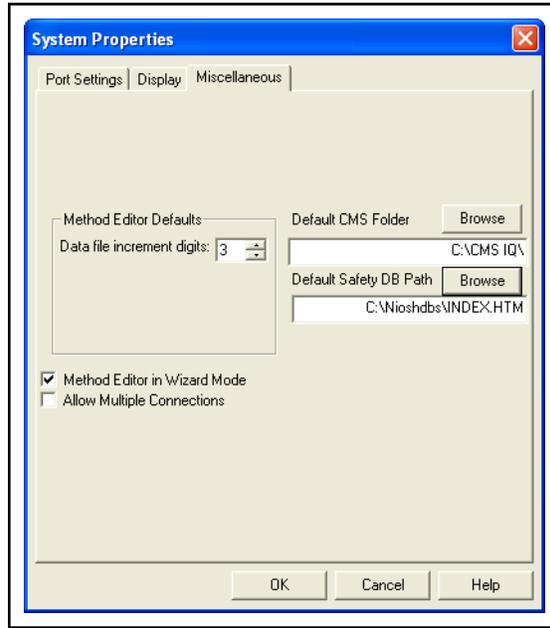
- Plot Thickness** Changes the thickness of the chromatogram trace

NOTE: **Point Size**, **Plot Points**, and **Connect Points** are unavailable.

12.2.5.3 Miscellaneous

The **Miscellaneous** tab is used to change default pathways, method editor defaults, and select the options **Method Editor in Wizard Mode** and **Allow Multiple Connections**. (See Figure 12-33.)

Figure 12-33 Miscellaneous tab



12.2.5.3.1 Data File Increment Digits

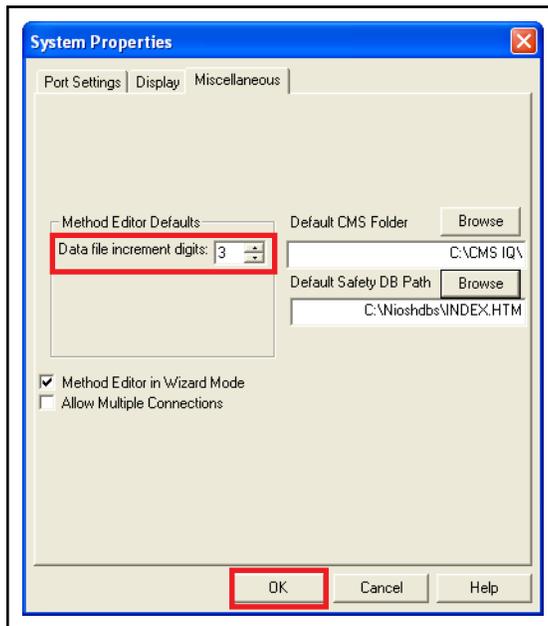
Data file increment digits sets the default number of digits (#) to be appended to a data file name in sequential order. For example:

- ♦ selecting 2 would set up the file name to read *method_yearmonthday_##*
- ♦ selecting 3 would set the file name to read *method_yearmonthday_###*

Click **OK** to save changes. (See Figure 12-34.)

Data file increments can also be set in Method Editor. See section 16.8, Data, on page 16-20.

Figure 12-34 Data File Increment digits

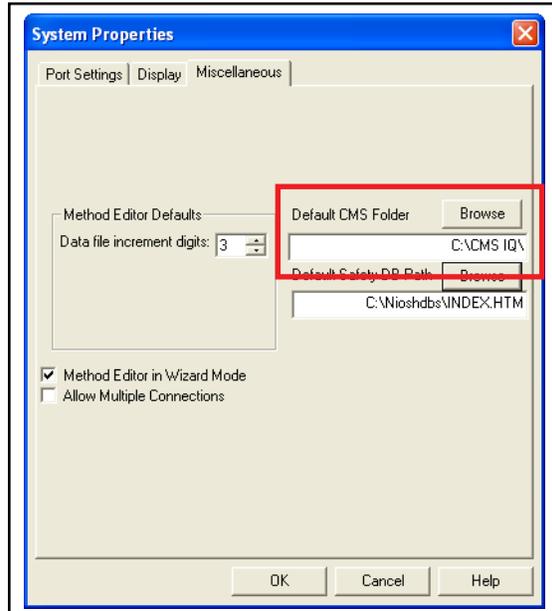


12.2.5.3.2 Default Pathways

Two default software pathways are displayed:

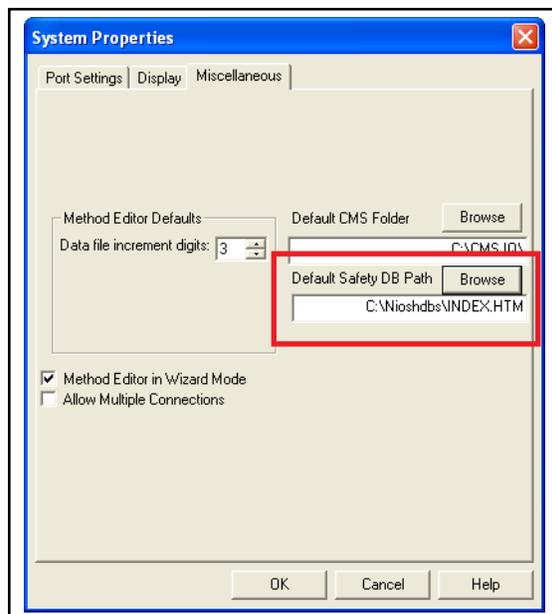
- ◆ **Default CMS Folder** displays the pathway to the folder where CMS IQ software is installed (See Figure 12-35.)

Figure 12-35 Default CMS Folder



- ◆ **Default Safety DB Path** displays the pathway to the NIOSH database (See Figure 12-36.)

Figure 12-36 Default Safety DB Path

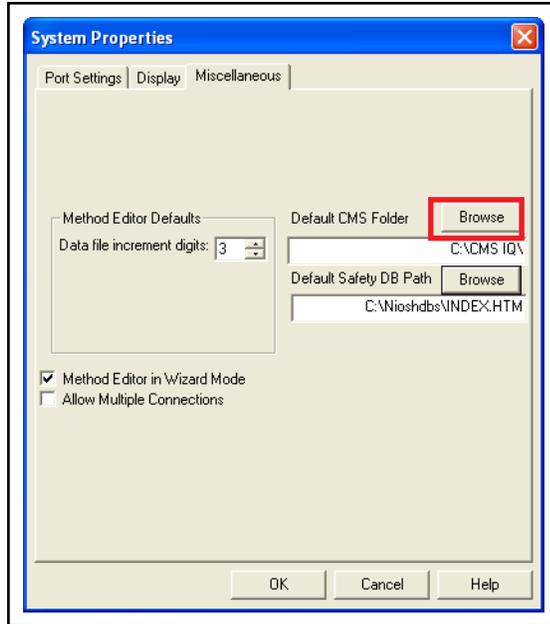


These pathways are automatically configured during software installation.

12.2.5.3.3 Changing Default CMS Folder

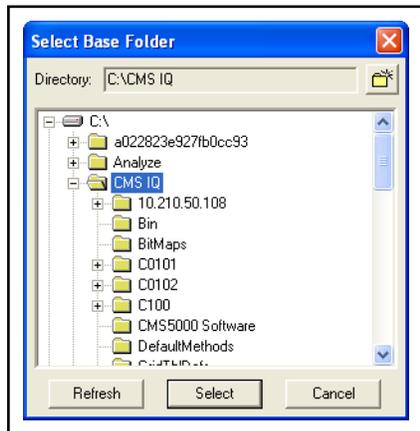
- 1 Click **Browse** for the **Default CMS Folder**. (See Figure 12-37.)

Figure 12-37 Browse button



- 2 The **Select Base Folder** window is displayed. (See Figure 12-38.)

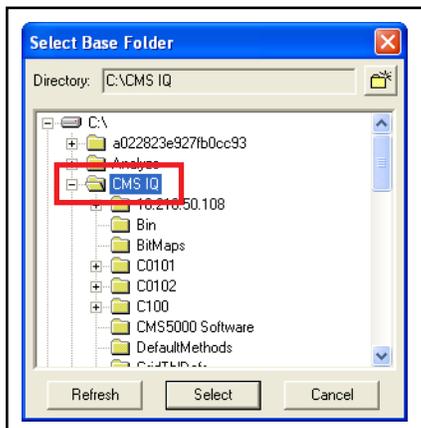
Figure 12-38 Select Base Folder window



- 3 Click to highlight the desired folder. (See Figure 12-39.)

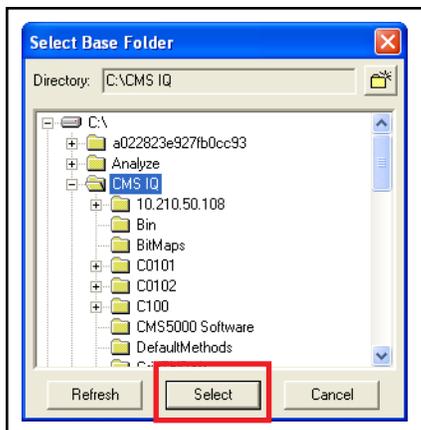
NOTE: Click **Refresh** if the desired folder is not displayed.

Figure 12-39 Selecting desired folder



- 4 Click **Select** to set the pathway and close the window. (See Figure 12-40.)

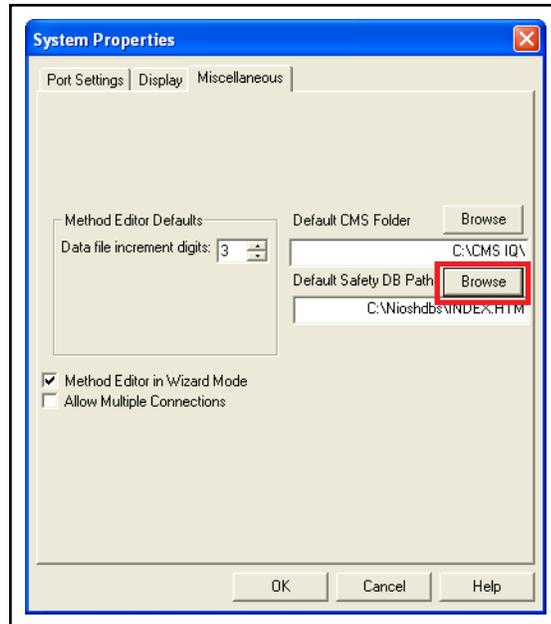
Figure 12-40 Selecting the pathway



12.2.5.3.4 Changing Default NIOSH Database Folder

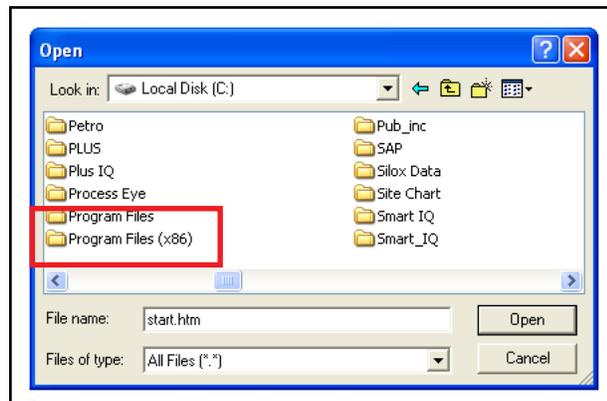
- 1 Click **Browse** for the **Default CMS Folder**. (See Figure 12-41.)

Figure 12-41 Browse button



- 2 The **Open** window is displayed.
- 3 Click **Up One Level**  until the desired folder is visible.
- 4 Double-click the folder. (See Figure 12-42.) Alternately, highlight the folder and click **Open**.

Figure 12-42 Selecting desired folder



- 5 The folder opens. Click **Open** and navigate to the correct folder. Select the folder and click **Select**. (See Figure 12-43 and Figure 12-44.)

Figure 12-43 Selecting the pathway

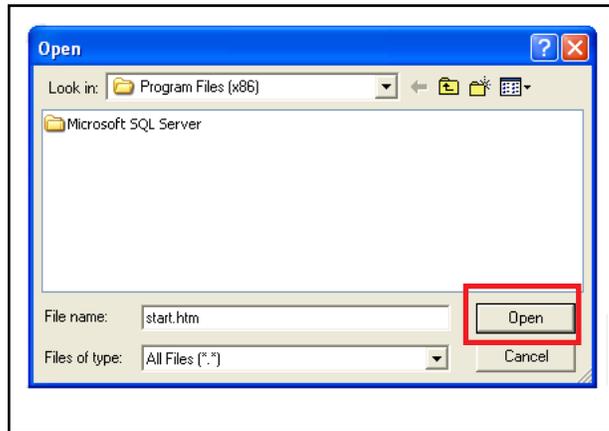
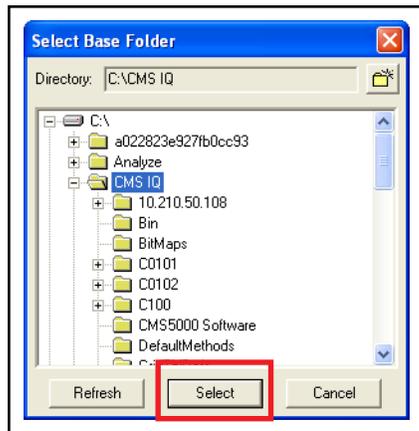


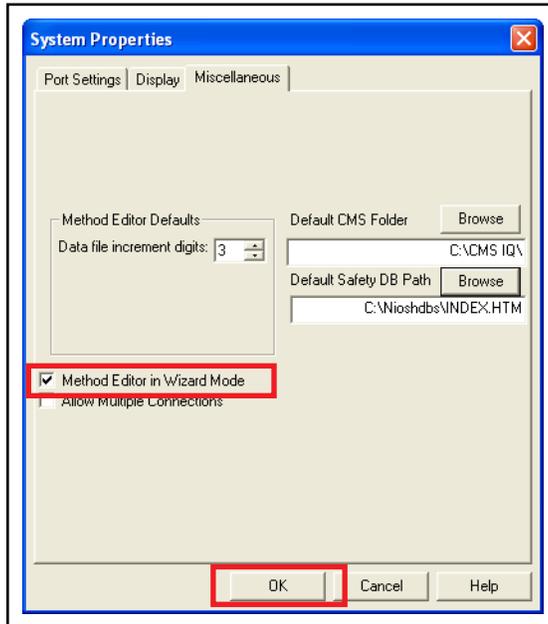
Figure 12-44 Selecting the folder



12.2.5.3.5 Method Editor in Wizard Mode

Select **Method Editor in Wizard Mode** to enable Wizard Mode for method editing. Click **OK** to save changes. (See Figure 12-45.) See section 16.2, Wizard Mode, on page 16-2.

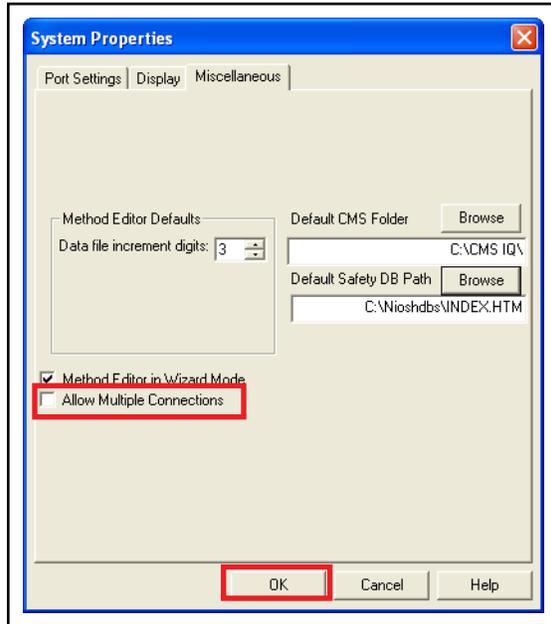
Figure 12-45 Method Editor in Wizard Mode checkbox



12.2.5.3.6 Allow Multiple Connections

Select **Allow Multiple Connections** to connect to multiple CMS5000. When clear, connection is available to only one CMS5000. Click **OK** to save changes. (See Figure 12-46.)

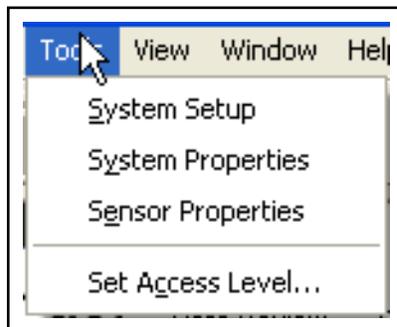
Figure 12-46 Connect to multiple systems



12.2.6 Tools Menu

The **Tools** menu is shown in Figure 12-47.

Figure 12-47 Tools menu



12.2.6.1 System Setup

System Setup opens and closes the **System Setup** window.

12.2.6.2 System Properties

System Properties behaves identically to **Properties** in the **System** menu. Refer to section 12.2.5, System, on page 12-12.

12.2.6.3 Sensor Properties

Sensor Properties behaves identically to the **Status** icon on the **System Setup** window. See section 12.6, Status Icon, on page 12-46.

12.2.6.4 Set Access Level

Set Access Level... sets software access levels. There are two access levels: **Normal** and **Advanced**. Neither access level has a factory set password.

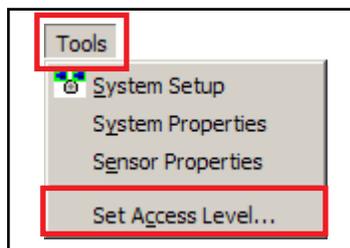
- ◆ **Normal** level allows running samples, viewing results and basic CMS5000 operations
- ◆ **Advanced** provides access to normal user functions plus method creation and editing, file deletion, changing alarm parameters and changing network settings

If desired, set an advanced access level password to restrict access to advanced functions. Once a password is set, it must be entered each time CMS IQ is run in advanced mode, or whenever the access level is changed from normal to advanced. See section 12.2.6.4.2, Setting or Changing the Access Level Password, on page 12-31.

12.2.6.4.1 Changing Access Levels

- 1 In System Setup, click **Tools >> Set Access Level....** (See Figure 12-48.)

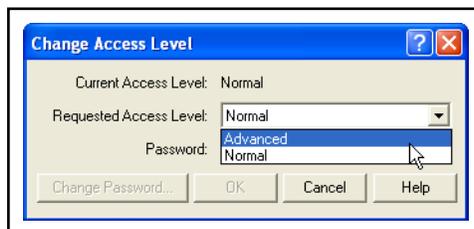
Figure 12-48 Set Access Level... option



- 2 Select the desired option (**Normal** or **Advanced**) from the **Requested Access Level** shortcut menu. Click **OK** to save changes. (See Figure 12-49.)

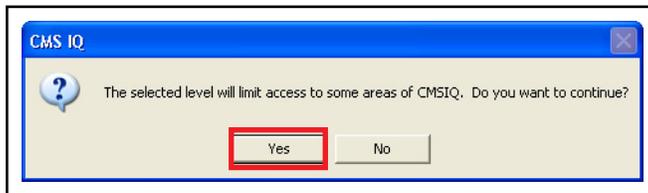
NOTE: If a password has been defined (for **Advanced** access only), type the password in the **Password** box before clicking **OK**.

Figure 12-49 Change Access Level window



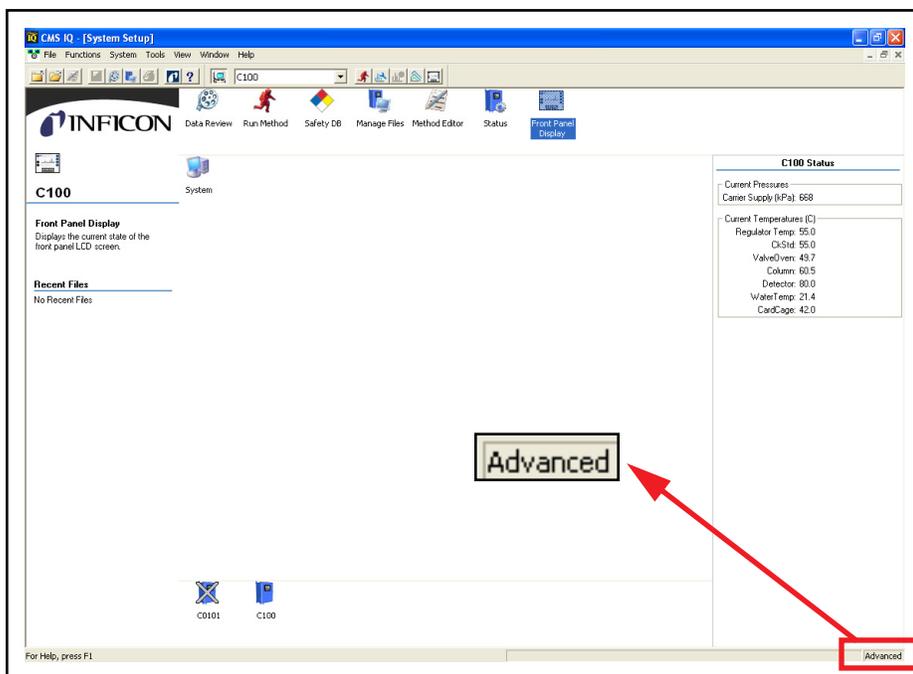
NOTE: When in **Advanced** access level, if **Normal** access level is selected, a prompt will appear stating that some areas of CMS IQ will have restricted access. Click **Yes** to continue. (See Figure 12-50.)

Figure 12-50 Restricted access prompt



3 The selected access level of the software is indicated in the bottom right corner of the CMS IQ program. (See Figure 12-51.)

Figure 12-51 Current access level shown in System Setup window



12.2.6.4.2 Setting or Changing the Access Level Password

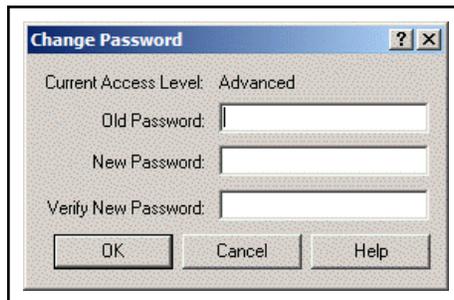
- 1 Select **Advanced** from the **Requested Access Level** shortcut menu.
- 2 Click **Change Password**. (See Figure 12-52.)

Figure 12-52 Change Password... button



- 3 The **Change Password** window will display. (See Figure 12-53.)

Figure 12-53 Change Password window



- 4 Type the current password in the **Old Password** box. The **Old Password** box should be left blank when creating a password for the first time.
- 5 Type the new password in **New Password** and **Verify New Password** box.
- 6 Click **OK** to set the new password, or click **Cancel** to exit without setting the new password.
- 7 Click **OK** to close the **Change Access Level** window.

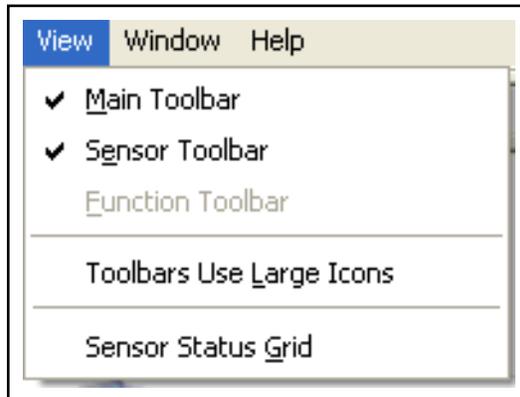
NOTE: When closed, CMS IQ retains the last access level. Upon re-opening the program, CMS IQ will return to the last access level utilized. If CMS IQ opens in advanced level, and a password has been set, the correct password is required to obtain advanced access. If the password is unknown, select normal access.

NOTE: If password is lost or forgotten, contact INFICON to reset it.

12.2.7 View Menu

View menu sets the toolbars to display. (See Figure 12-54.)

Figure 12-54 View menu



12.2.7.1 Main Toolbar

Select to display the **Main Toolbar**, the default condition. (See Figure 12-55.) See Table 12-1, System Setup icons, on page 12-34.

Figure 12-55 Main toolbar



12.2.7.2 Sensor Toolbar

Select to display the **Sensor Toolbar**, the default condition. (See Figure 12-56.) See Table 12-1 on page 12-34, **System Setup icons**.

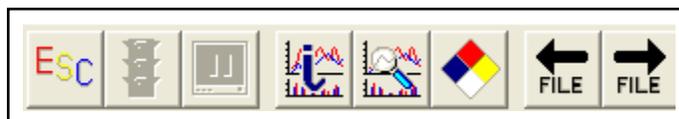
Figure 12-56 Sensor toolbar



12.2.7.3 Function Toolbar

Function Toolbar is only available when the **Data Review** window is open. (See Figure 12-57.) Refer to section 13.4, Data Review Toolbar, on page 13-5.

Figure 12-57 Function toolbar



12.2.7.4 Toolbars Use Large Icons

Toolbars Use Large Icons increases the size of toolbar icons.

12.2.7.5 Sensor Status Grid

Sensor Status Grid will display the current status of CMS5000 **Gas/Valves** and **Heaters**.

The **Gas/Valves** tab displays the current status (on or off) for:

- ◆ CMS5000 valves
- ◆ GC column pressure
- ◆ carrier gas supply pressure

The **Heaters** tab displays the current temperatures and set points of the heated components. (See Figure 12-58.)

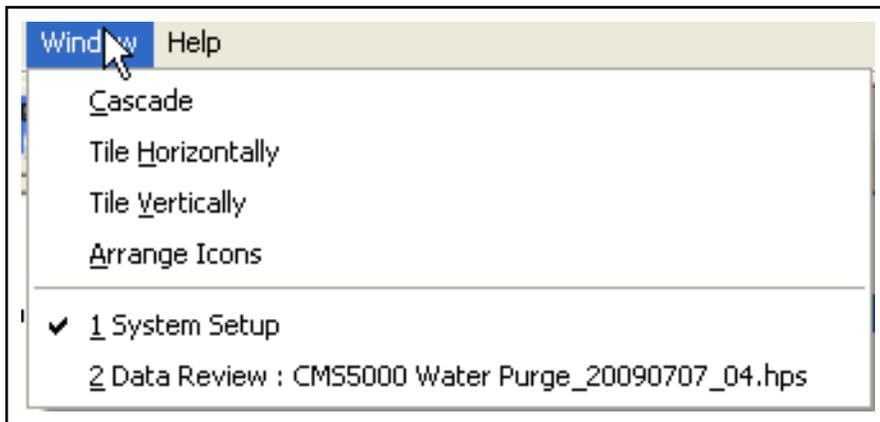
Figure 12-58 Sensor Status Grid

| Sensor | Status | Process | Process Status | GC Flow | HSFlow | Sample | Purge | Ck Std | Sample Pump | VSD | VSDrive | GC Col Pr |
|---------------|---------|---------|----------------|---------|--------|--------|-------|--------|-------------|-----|---------|-----------|
| 10.210.70.108 | Offline | None | | | | | | | | | 0 | 0 |

12.2.8 Window Menu

Window Menu will display various window configuration options. (See Figure 12-59.)

Figure 12-59 Window menu



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

Arrange Icons aligns the icons along the top row.

Windows currently open are listed. The current view is the selected view.

12.2.9 Help Menu

Please contact INFICON at www.inficon.com for assistance.

12.3 System Setup Icons

Table 12-1 System Setup icons

| Icon | Name | Description |
|---|---------------|---|
|  | Close | Closes a data file |
|  | Open | Opens a data file |
|  | Method Editor | See Chapter 16, Method Editor |
|  | Save As | Saves a data file to the computer. Will be unavailable when a data file is not selected |
|  | Data Review | See Chapter 13, Data Review |
|  | Manage Files | See section 12.5, Manage Files, on page 12-39 |
|  | Print | Prints a copy of the chromatogram of the selected data file. Will be unavailable when a data file is not selected |
|  | About | Displays the installed software version |
|  | Help | Unavailable. Contact INFICON at www.inficon.com for assistance |
|  | System Setup | Switches between the System Setup and either the Data Review or Run Method views |

Table 12-1 System Setup icons

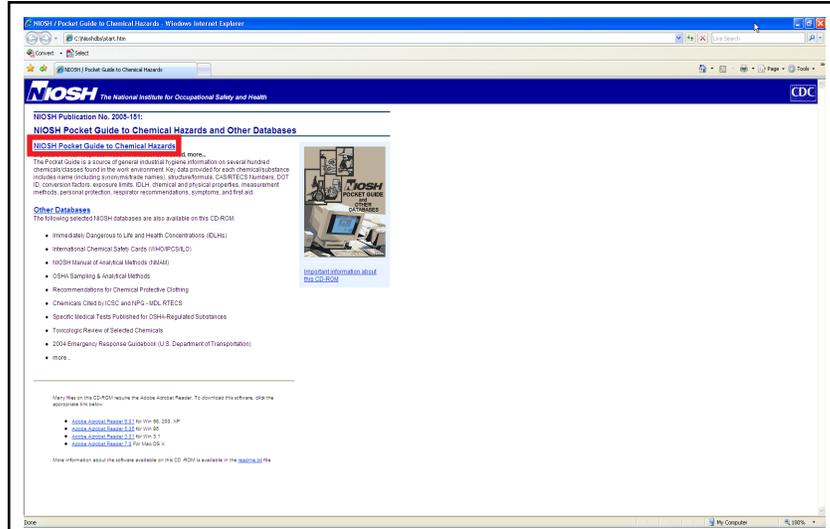
| Icon | Name | Description |
|--|---------------------|---|
|  Run Method | Run Method | See Chapter 14, Run Method |
|  Calibrate | Calibrate | See Chapter 17, Calibration |
|  ID Unknowns | ID Unknowns | Unavailable |
|  Overlay | Overlay | See Chapter 15, Chromatogram Overlay |
|  Front Panel Display | Front Panel Display | See section 12.7, Front Panel Display Icon, on page 12-70 |
|  Safety DB | Safety Database | See section 12.4, Safety DB, on page 12-36 |
|  Status | Status | See section 12.6, Status Icon, on page 12-46 |
|  System | System | Refer to section 12.2.5, System, on page 12-12 |
|  Sensor Status | Sensor Status | See section 12.8, CMS5000 Sensor Status Icon, on page 12-71 |

12.4 Safety DB

Safety DB accesses the NIOSH Safety Database used to locate NIOSH REL, OSHA PEL, CAS Numbers, synonyms, IDLH's, and safety recommendations.

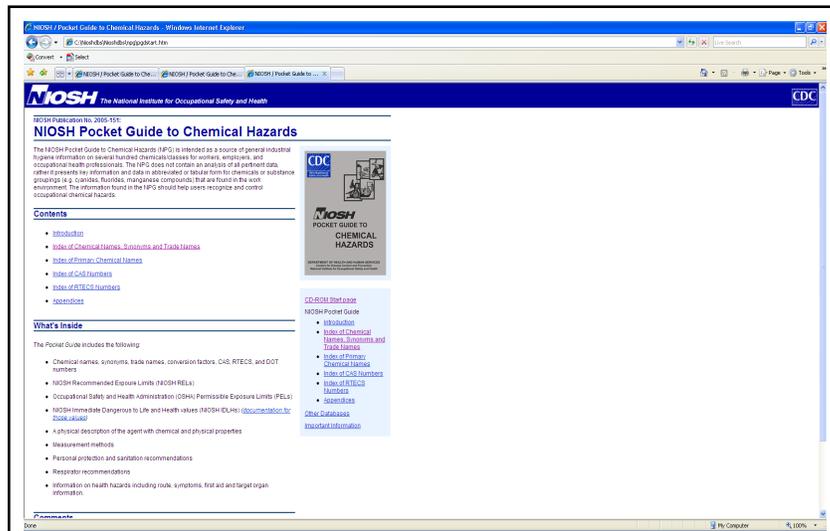
- 1 Double-click **Safety DB** . The **NIOSH Pocket Guide to Chemical Hazards and Other Databases** window is displayed. (See Figure 12-60.)

Figure 12-60 NIOSH / Pocket Guide to Chemical Hazards and Other Databases window



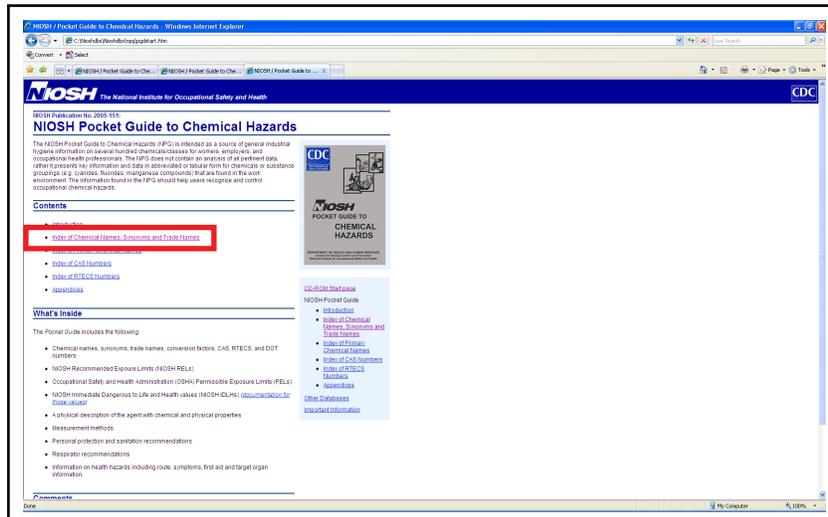
- 2 Click **NIOSH Pocket Guide to Chemical Hazards**. The **NIOSH Pocket Guide to Chemical Hazards** window is displayed. (See Figure 12-61.)

Figure 12-61 NIOSH Pocket Guide to Chemical Hazards link



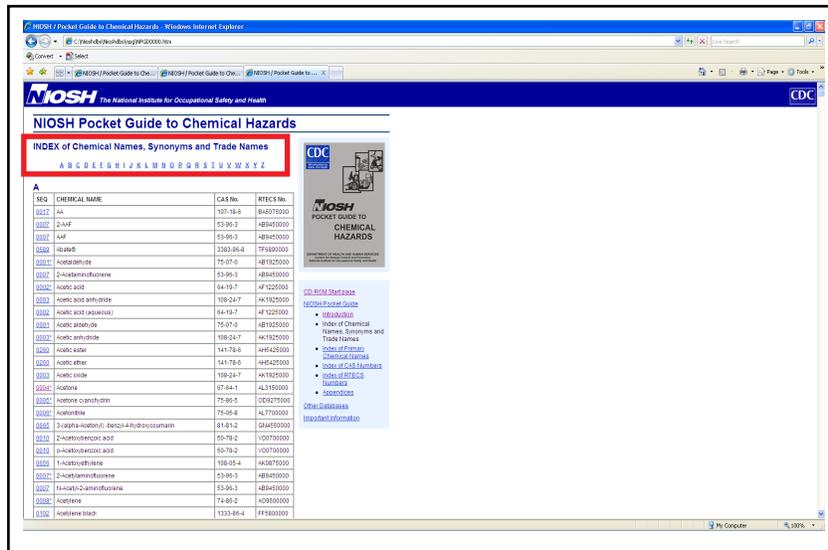
3 Click Index of Chemical Names, Synonyms, and Trade Names.
(See Figure 12-62.)

Figure 12-62 Index of Chemical Names, Synonyms and, Trade Names



4 The Index Of Chemical Names, Synonyms, and Trade Names List window
with the components of the database listed in alphabetical order is displayed.
(See Figure 12-63.)

Figure 12-63 Index Of Chemical Names, Synonyms, and Trade Names List



- 5 In Figure 12-64, benzene is selected by clicking **B** and clicking the **SEQ** number (0049*) associated with benzene.

Figure 12-64 benzene example

| SEQ | CHEMICAL NAME | CAS No. | ITECS No. |
|------|-----------------|-----------|-----------|
| 0012 | Baobab seed | 1395-21-7 | CO9450000 |
| 0013 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0014 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0015 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0016 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0017 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0018 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0019 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0020 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0021 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0022 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0023 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0024 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0025 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0026 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0027 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0028 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0029 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0030 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0031 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0032 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0033 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0034 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0035 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0036 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0037 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0038 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0039 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0040 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0041 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0042 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0043 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0044 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0045 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0046 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0047 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0048 | Baobab seed oil | 1395-21-7 | CO9450000 |
| 0049 | Benzene | 62-53-3 | BH0550000 |
| 0050 | Benzene | 71-42-2 | CH1400000 |
| 0051 | Benzene | 106-60-7 | CD1750000 |
| 0052 | 1,4-Dioxane | 106-60-3 | EG0500000 |
| 0053 | 1,3-Dioxane | 625-17-6 | CE1900000 |
| 0054 | 1,2-Dioxane | 65-44-9 | TD1500000 |
| 0055 | 1,3-Dioxane | 1477-55-0 | PF0970000 |
| 0056 | 1,2-Dioxane | 106-60-7 | UN1900000 |
| 0057 | 1,3-Dioxane | 106-60-3 | UN2620000 |
| 0058 | 1,4-Dioxane | 106-60-3 | UN3000000 |
| 0059 | m-Benzenediol | 108-45-3 | VG0250000 |

- 6 The benzene window is displayed. (See Figure 12-65.)

Figure 12-65 benzene information window

NIOSH Pocket Guide to Chemical Hazards

Benzene CAS 71-42-2

Synonyms & Trade Names Benzene, Benzol

Exposure Limits NIOSH REL: Ca TWA 0.1 ppm ST 1 ppm See Appendix E
OSHA PEL: 100% TWA 1 ppm ST 5 ppm See Appendix E

Physical Description Colorless to light-yellow liquid with an aromatic odor (Note: A solid below 42°F)

Health Hazards Irritant to eyes, nose, throat, and skin. May cause dizziness and headache. May cause respiratory irritation. May cause skin irritation. May cause allergic reactions. May cause sensitization by inhalation. May cause cancer.

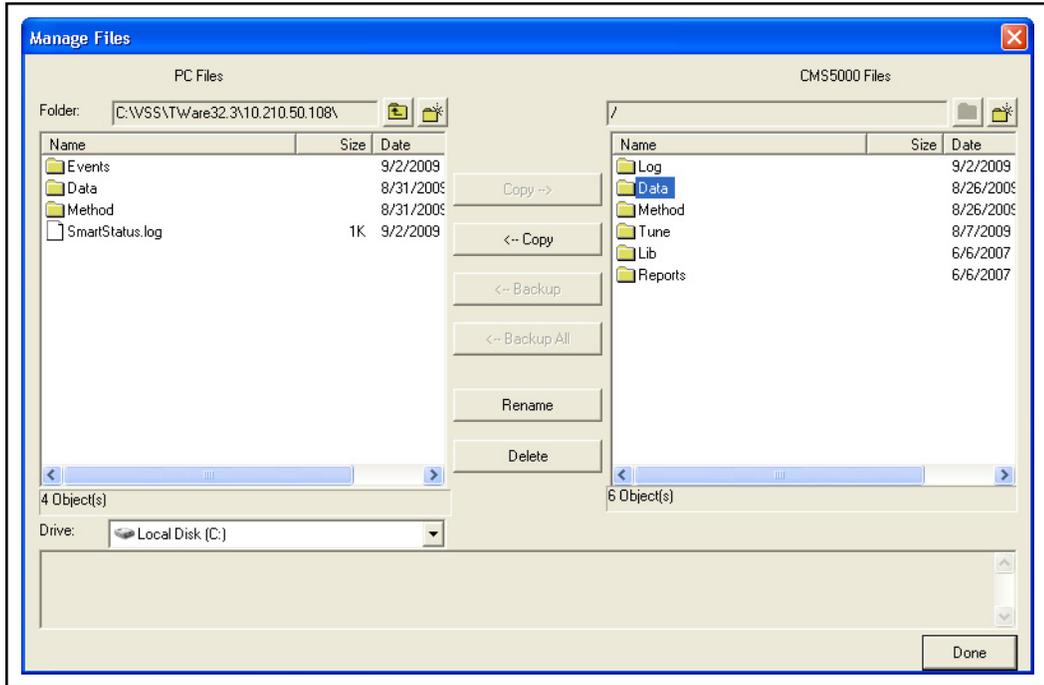
Measurement Methods NIOSH Method 1515, 1520, 1521, 1522, 1523, 1524, 1525, 1526, 1527, 1528, 1529, 1530, 1531, 1532, 1533, 1534, 1535, 1536, 1537, 1538, 1539, 1540, 1541, 1542, 1543, 1544, 1545, 1546, 1547, 1548, 1549, 1550, 1551, 1552, 1553, 1554, 1555, 1556, 1557, 1558, 1559, 1560, 1561, 1562, 1563, 1564, 1565, 1566, 1567, 1568, 1569, 1570, 1571, 1572, 1573, 1574, 1575, 1576, 1577, 1578, 1579, 1580, 1581, 1582, 1583, 1584, 1585, 1586, 1587, 1588, 1589, 1590, 1591, 1592, 1593, 1594, 1595, 1596, 1597, 1598, 1599, 1600, 1601, 1602, 1603, 1604, 1605, 1606, 1607, 1608, 1609, 1610, 1611, 1612, 1613, 1614, 1615, 1616, 1617, 1618, 1619, 1620, 1621, 1622, 1623, 1624, 1625, 1626, 1627, 1628, 1629, 1630, 1631, 1632, 1633, 1634, 1635, 1636, 1637, 1638, 1639, 1640, 1641, 1642, 1643, 1644, 1645, 1646, 1647, 1648, 1649, 1650, 1651, 1652, 1653, 1654, 1655, 1656, 1657, 1658, 1659, 1660, 1661, 1662, 1663, 1664, 1665, 1666, 1667, 1668, 1669, 1670, 1671, 1672, 1673, 1674, 1675, 1676, 1677, 1678, 1679, 1680, 1681, 1682, 1683, 1684, 1685, 1686, 1687, 1688, 1689, 1690, 1691, 1692, 1693, 1694, 1695, 1696, 1697, 1698, 1699, 1700, 1701, 1702, 1703, 1704, 1705, 1706, 1707, 1708, 1709, 1710, 1711, 1712, 1713, 1714, 1715, 1716, 1717, 1718, 1719, 1720, 1721, 1722, 1723, 1724, 1725, 1726, 1727, 1728, 1729, 1730, 1731, 1732, 1733, 1734, 1735, 1736, 1737, 1738, 1739, 1740, 1741, 1742, 1743, 1744, 1745, 1746, 1747, 1748, 1749, 1750, 1751, 1752, 1753, 1754, 1755, 1756, 1757, 1758, 1759, 1760, 1761, 1762, 1763, 1764, 1765, 1766, 1767, 1768, 1769, 1770, 1771, 1772, 1773, 1774, 1775, 1776, 1777, 1778, 1779, 1780, 1781, 1782, 1783, 1784, 1785, 1786, 1787, 1788, 1789, 1790, 1791, 1792, 1793, 1794, 1795, 1796, 1797, 1798, 1799, 1800, 1801, 1802, 1803, 1804, 1805, 1806, 1807, 1808, 1809, 1810, 1811, 1812, 1813, 1814, 1815, 1816, 1817, 1818, 1819, 1820, 1821, 1822, 1823, 1824, 1825, 1826, 1827, 1828, 1829, 1830, 1831, 1832, 1833, 1834, 1835, 1836, 1837, 1838, 1839, 1840, 1841, 1842, 1843, 1844, 1845, 1846, 1847, 1848, 1849, 1850, 1851, 1852, 1853, 1854, 1855, 1856, 1857, 1858, 1859, 1860, 1861, 1862, 1863, 1864, 1865, 1866, 1867, 1868, 1869, 1870, 1871, 1872, 1873, 1874, 1875, 1876, 1877, 1878, 1879, 1880, 1881, 1882, 1883, 1884, 1885, 1886, 1887, 1888, 1889, 1890, 1891, 1892, 1893, 1894, 1895, 1896, 1897, 1898, 1899, 1900, 1901, 1902, 1903, 1904, 1905, 1906, 1907, 1908, 1909, 1910, 1911, 1912, 1913, 1914, 1915, 1916, 1917, 1918, 1919, 1920, 1921, 1922, 1923, 1924, 1925, 1926, 1927, 1928, 1929, 1930, 1931, 1932, 1933, 1934, 1935, 1936, 1937, 1938, 1939, 1940, 1941, 1942, 1943, 1944, 1945, 1946, 1947, 1948, 1949, 1950, 1951, 1952, 1953, 1954, 1955, 1956, 1957, 1958, 1959, 1960, 1961, 1962, 1963, 1964, 1965, 1966, 1967, 1968, 1969, 1970, 1971, 1972, 1973, 1974, 1975, 1976, 1977, 1978, 1979, 1980, 1981, 1982, 1983, 1984, 1985, 1986, 1987, 1988, 1989, 1990, 1991, 1992, 1993, 1994, 1995, 1996, 1997, 1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020, 2021, 2022, 2023, 2024, 2025, 2026, 2027, 2028, 2029, 2030, 2031, 2032, 2033, 2034, 2035, 2036, 2037, 2038, 2039, 2040, 2041, 2042, 2043, 2044, 2045, 2046, 2047, 2048, 2049, 2050, 2051, 2052, 2053, 2054, 2055, 2056, 2057, 2058, 2059, 2060, 2061, 2062, 2063, 2064, 2065, 2066, 2067, 2068, 2069, 2070, 2071, 2072, 2073, 2074, 2075, 2076, 2077, 2078, 2079, 2080, 2081, 2082, 2083, 2084, 2085, 2086, 2087, 2088, 2089, 2090, 2091, 2092, 2093, 2094, 2095, 2096, 2097, 2098, 2099, 2100, 2101, 2102, 2103, 2104, 2105, 2106, 2107, 2108, 2109, 2110, 2111, 2112, 2113, 2114, 2115, 2116, 2117, 2118, 2119, 2120, 2121, 2122, 2123, 2124, 2125, 2126, 2127, 2128, 2129, 2130, 2131, 2132, 2133, 2134, 2135, 2136, 2137, 2138, 2139, 2140, 2141, 2142, 2143, 2144, 2145, 2146, 2147, 2148, 2149, 2150, 2151, 2152, 2153, 2154, 2155, 2156, 2157, 2158, 2159, 2160, 2161, 2162, 2163, 2164, 2165, 2166, 2167, 2168, 2169, 2170, 2171, 2172, 2173, 2174, 2175, 2176, 2177, 2178, 2179, 2180, 2181, 2182, 2183, 2184, 2185, 2186, 2187, 2188, 2189, 2190, 2191, 2192, 2193, 2194, 2195, 2196, 2197, 2198, 2199, 2200, 2201, 2202, 2203, 2204, 2205, 2206, 2207, 2208, 2209, 2210, 2211, 2212, 2213, 2214, 2215, 2216, 2217, 2218, 2219, 2220, 2221, 2222, 2223, 2224, 2225, 2226, 2227, 2228, 2229, 2230, 2231, 2232, 2233, 2234, 2235, 2236, 2237, 2238, 2239, 2240, 2241, 2242, 2243, 2244, 2245, 2246, 2247, 2248, 2249, 2250, 2251, 2252, 2253, 2254, 2255, 2256, 2257, 2258, 2259, 2260, 2261, 2262, 2263, 2264, 2265, 2266, 2267, 2268, 2269, 2270, 2271, 2272, 2273, 2274, 2275, 2276, 2277, 2278, 2279, 2280, 2281, 2282, 2283, 2284, 2285, 2286, 2287, 2288, 2289, 2290, 2291, 2292, 2293, 2294, 2295, 2296, 2297, 2298, 2299, 2300, 2301, 2302, 2303, 2304, 2305, 2306, 2307, 2308, 2309, 2310, 2311, 2312, 2313, 2314, 2315, 2316, 2317, 2318, 2319, 2320, 2321, 2322, 2323, 2324, 2325, 2326, 2327, 2328, 2329, 2330, 2331, 2332, 2333, 2334, 2335, 2336, 2337, 2338, 2339, 2340, 2341, 2342, 2343, 2344, 2345, 2346, 2347, 2348, 2349, 2350, 2351, 2352, 2353, 2354, 2355, 2356, 2357, 2358, 2359, 2360, 2361, 2362, 2363, 2364, 2365, 2366, 2367, 2368, 2369, 2370, 2371, 2372, 2373, 2374, 2375, 2376, 2377, 2378, 2379, 2380, 2381, 2382, 2383, 2384, 2385, 2386, 2387, 2388, 2389, 2390, 2391, 2392, 2393, 2394, 2395, 2396, 2397, 2398, 2399, 2400, 2401, 2402, 2403, 2404, 2405, 2406, 2407, 2408, 2409, 2410, 2411, 2412, 2413, 2414, 2415, 2416, 2417, 2418, 2419, 2420, 2421, 2422, 2423, 2424, 2425, 2426, 2427, 2428, 2429, 2430, 2431, 2432, 2433, 2434, 2435, 2436, 2437, 2438, 2439, 2440, 2441, 2442, 2443, 2444, 2445, 2446, 2447, 2448, 2449, 2450, 2451, 2452, 2453, 2454, 2455, 2456, 2457, 2458, 2459, 2460, 2461, 2462, 2463, 2464, 2465, 2466, 2467, 2468, 2469, 2470, 2471, 2472, 2473, 2474, 2475, 2476, 2477, 2478, 2479, 2480, 2481, 2482, 2483, 2484, 2485, 2486, 2487, 2488, 2489, 2490, 2491, 2492, 2493, 2494, 2495, 2496, 2497, 2498, 2499, 2500, 2501, 2502, 2503, 2504, 2505, 2506, 2507, 2508, 2509, 2510, 2511, 2512, 2513, 2514, 2515, 2516, 2517, 2518, 2519, 2520, 2521, 2522, 2523, 2524, 2525, 2526, 2527, 2528, 2529, 2530, 2531, 2532, 2533, 2534, 2535, 2536, 2537, 2538, 2539, 2540, 2541, 2542, 2543, 2544, 2545, 2546, 2547, 2548, 2549, 2550, 2551, 2552, 2553, 2554, 2555, 2556, 2557, 2558, 2559, 2560, 2561, 2562, 2563, 2564, 2565, 2566, 2567, 2568, 2569, 2570, 2571, 2572, 2573, 2574, 2575, 2576, 2577, 2578, 2579, 2580, 2581, 2582, 2583, 2584, 2585, 2586, 2587, 2588, 2589, 2590, 2591, 2592, 2593, 2594, 2595, 2596, 2597, 2598, 2599, 2600, 2601, 2602, 2603, 2604, 2605, 2606, 2607, 2608, 2609, 2610, 2611, 2612, 2613, 2614, 2615, 2616, 2617, 2618, 2619, 2620, 2621, 2622, 2623, 2624, 2625, 2626, 2627, 2628, 2629, 2630, 2631, 2632, 2633, 2634, 2635, 2636, 2637, 2638, 2639, 2640, 2641, 2642, 2643, 2644, 2645, 2646, 2647, 2648, 2649, 2650, 2651, 2652, 2653, 2654, 2655, 2656, 2657, 2658, 2659, 2660, 2661, 2662, 2663, 2664, 2665, 2666, 2667, 2668, 2669, 2670, 2671, 2672, 2673, 2674, 2675, 2676, 2677, 2678, 2679, 2680, 2681, 2682, 2683, 2684, 2685, 2686, 2687, 2688, 2689, 2690, 2691, 2692, 2693, 2694, 2695, 2696, 2697, 2698, 2699, 2700, 2701, 2702, 2703, 2704, 2705, 2706, 2707, 2708, 2709, 2710, 2711, 2712, 2713, 2714, 2715, 2716, 2717, 2718, 2719, 2720, 2721, 2722, 2723, 2724, 2725, 2726, 2727, 2728, 2729, 2730, 2731, 2732, 2733, 2734, 2735, 2736, 2737, 2738, 2739, 2740, 2741, 2742, 2743, 2744, 2745, 2746, 2747, 2748, 2749, 2750, 2751, 2752, 2753, 2754, 2755, 2756, 2757, 2758, 2759, 2760, 2761, 2762, 2763, 2764, 2765, 2766, 2767, 2768, 2769, 2770, 2771, 2772, 2773, 2774, 2775, 2776, 2777, 2778, 2779, 2780, 2781, 2782, 2783, 2784, 2785, 2786, 2787, 2788, 2789, 2790, 2791, 2792, 2793, 2794, 2795, 2796, 2797, 2798, 2799, 2800, 2801, 2802, 2803, 2804, 2805, 2806, 2807, 2808, 2809, 2810, 2811, 2812, 2813, 2814, 2815, 2816, 2817, 2818, 2819, 2820, 2821, 2822, 2823, 2824, 2825, 2826, 2827, 2828, 2829, 2830, 2831, 2832, 2833, 2834, 2835, 2836, 2837, 2838, 2839, 2840, 2841, 2842, 2843, 2844, 2845, 2846, 2847, 2848, 2849, 2850, 2851, 2852, 2853, 2854, 2855, 2856, 2857, 2858, 2859, 2860, 2861, 2862, 2863, 2864, 2865, 2866, 2867, 2868, 2869, 2870, 2871, 2872, 2873, 2874, 2875, 2876, 2877, 2878, 2879, 2880, 2881, 2882, 2883, 2884, 2885, 2886, 2887, 2888, 2889, 2890, 2891, 2892, 2893, 2894, 2895, 2896, 2897, 2898, 2899, 2900, 2901, 2902, 2903, 2904, 2905, 2906, 2907, 2908, 2909, 2910, 2911, 2912, 2913, 2914, 2915, 2916, 2917, 2918, 2919, 2920, 2921, 2922, 2923, 2924, 2925, 2926, 2927, 2928, 2929, 2930, 2931, 2932, 2933, 2934, 2935, 2936, 2937, 2938, 2939, 2940, 2941, 2942, 2943, 2944, 2945, 2946, 2947, 2948, 2949, 2950, 2951, 2952, 2953, 2954, 2955, 2956, 2957, 2958, 2959, 2960, 2961, 2962, 2963, 2964, 2965, 2966, 2967, 2968, 2969, 2970, 2971, 2972, 2973, 2974, 2975, 2976, 2977, 2978, 2979, 2980, 2981, 2982, 2983, 2984, 2985, 2986, 2987, 2988, 2989, 2990, 2991, 2992, 2993, 2994, 2995, 2996, 2997, 2998, 2999, 3000, 3001, 3002, 3003, 3004, 3005,

12.5 Manage Files

Manage Files  transfers files between CMS5000 and the computer. Files can be renamed or deleted.

Double-click  to open the **Manage Files** window. (See Figure 12-66.)

Figure 12-66 Manage Files window



12.5.1 Copy Function

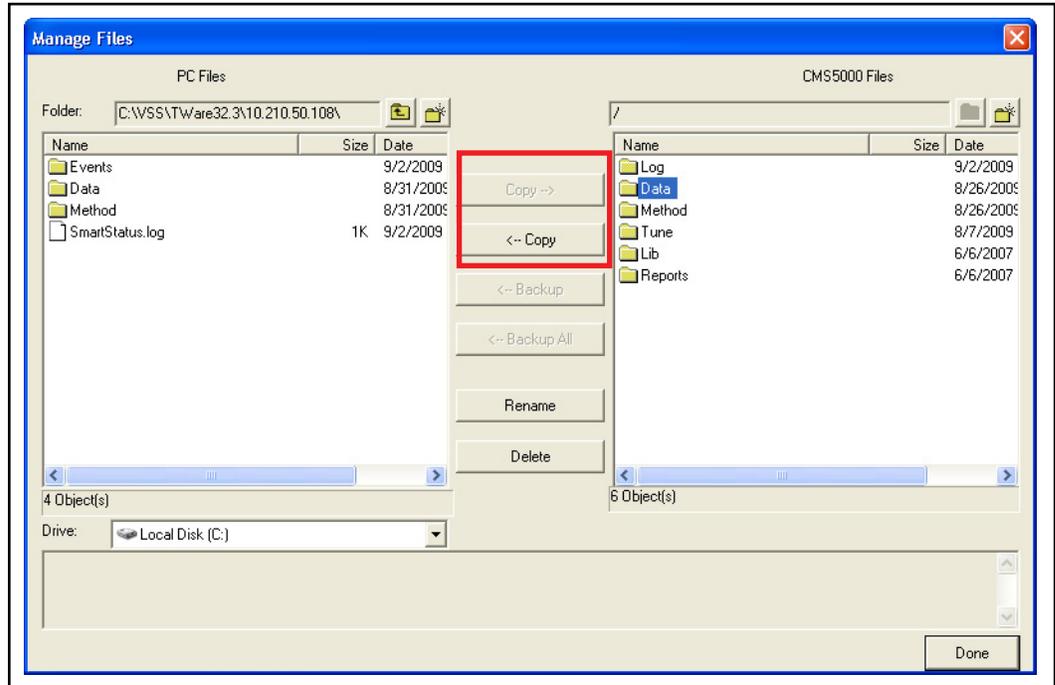
Copy--> will copy methods from the computer to CMS5000.

<--Copy will copy methods, data reports, and data files from CMS5000 to the computer. (See Figure 12-67.)

NOTE: Data reports are located inside the **Data** subfolder.

NOTE: Data files cannot be copied from the computer to CMS5000.

Figure 12-67 Copy function



12.5.2 Backup Function

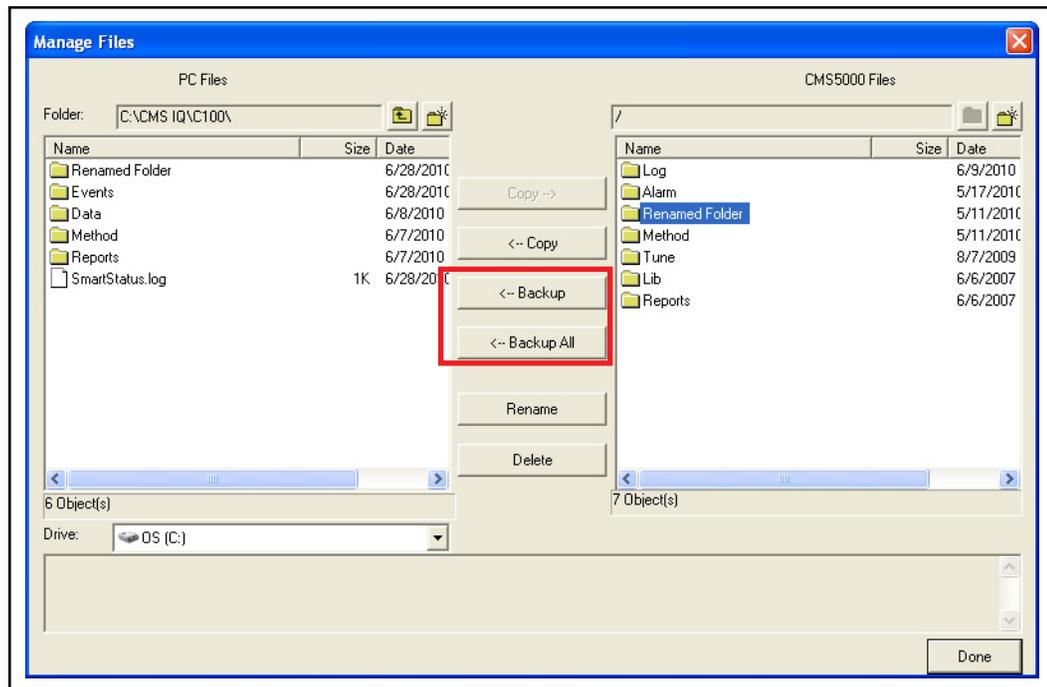
<--Backup will backup selected files from CMS5000 to the computer.

<--Backup All will backup all files from CMS5000 to the computer.

NOTE: Advanced level permission is required to backup files. Refer to section 12.2.6.4, Set Access Level, on page 12-29 to change access levels.

- ◆ **Backup** will copy and compress files into <backupfilename>.tgz
- ◆ **Copy** does not compress files and keeps their <originalfilename>.hps or <originalfilename>.mth (See Figure 12-68.)

Figure 12-68 Backup function



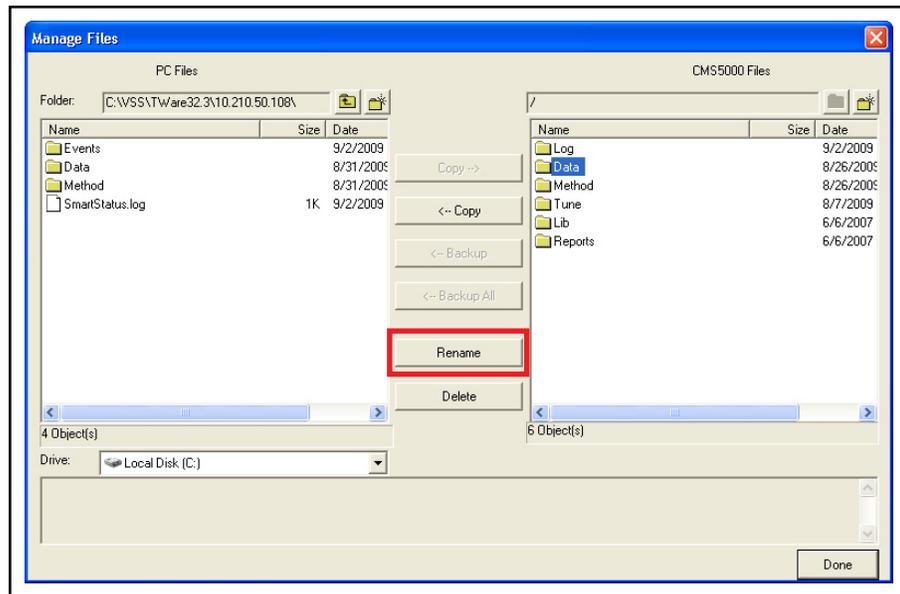
12.5.3 Rename Function

Rename will rename folders or files.

NOTE: Advanced level permission is required to rename folders or files. Refer to section 12.2.6.4, Set Access Level, on page 12-29 to change access levels.

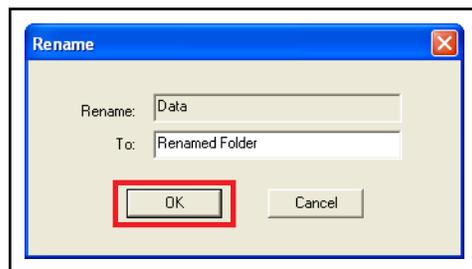
- 1 To rename a folder or file, click the desired folder or file and click **Rename**. (See Figure 12-69.)

Figure 12-69 Rename function



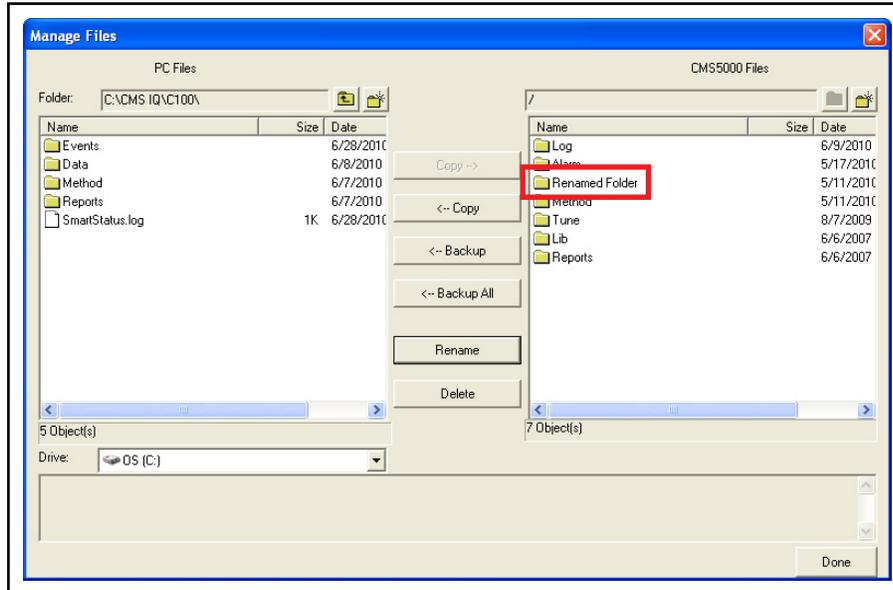
- 2 The **Rename** window is displayed. **Rename:** displays the current folder name. Type the new name in the **To:** box and click **OK**. (See Figure 12-70.)

Figure 12-70 Renaming folder



- 3 The renamed folder will appear in the Manage Files window. (See Figure 12-71.)

Figure 12-71 Renamed folder



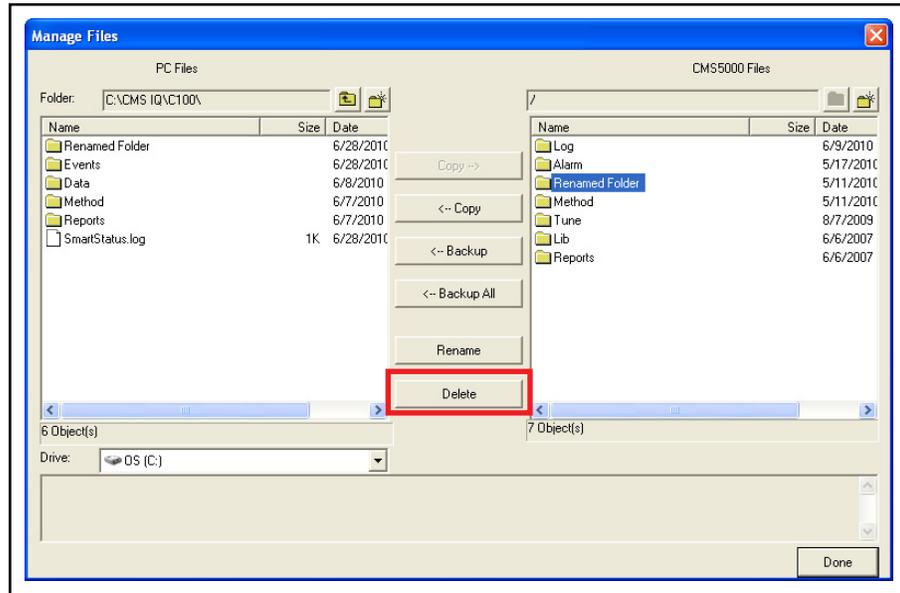
12.5.4 Delete Function

Delete removes folders or files.

NOTE: Advanced level permission is required to delete folders or files. Refer to section 12.2.6.4, Set Access Level, on page 12-29 to change access levels.

- 1 Highlight the desired folder or file and click **Delete**. (See Figure 12-72.)

Figure 12-72 Delete function



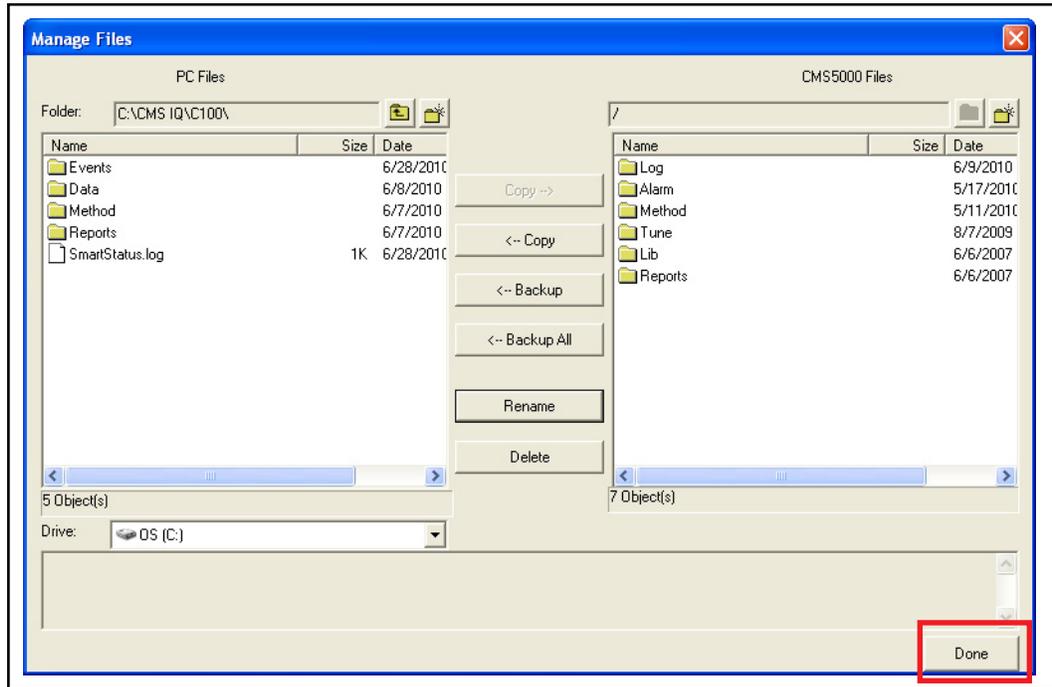
- 2 A confirmation message is displayed. Click **Yes** to delete the folder or file. (See Figure 12-73.)

Figure 12-73 Warning message



3 Click **Done** to exit the **Manage Files** window. (See Figure 12-74.)

Figure 12-74 Folder or file deleted



12.6 Status Icon

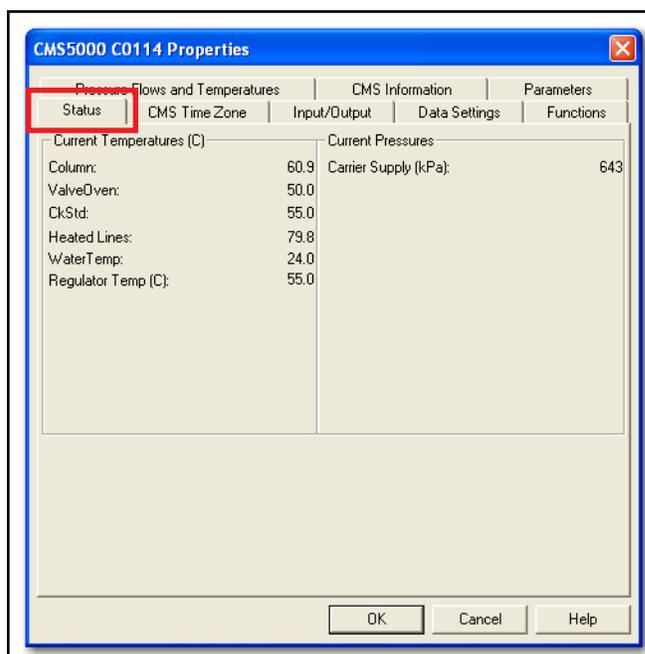


Double-click **Status** to display the **Properties** window. Several parameters such as CMS5000 time, Input/Output, and data settings can be accessed.

12.6.1 Status

The **Status** tab displays current temperatures of the column, valve oven, check standard, heated lines, sample water (if running a water method), and regulator. Carrier gas pressure is displayed. (See Figure 12-75.)

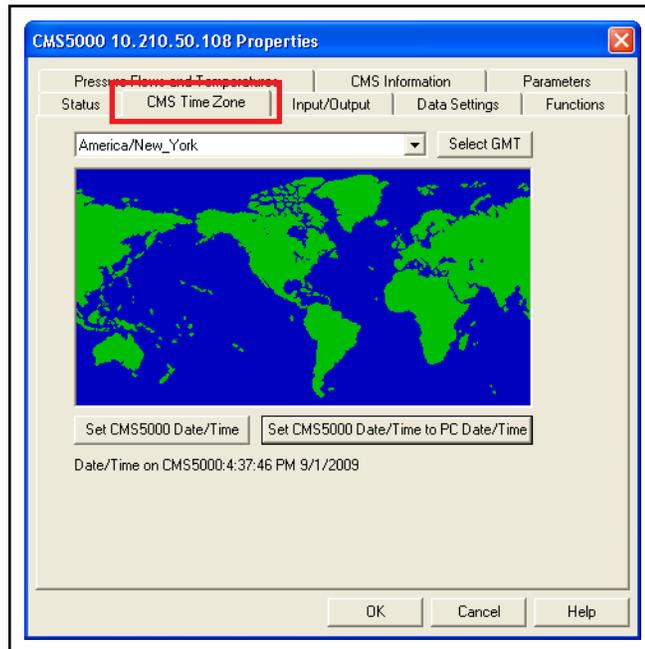
Figure 12-75 Status tab



12.6.2 CMS5000 Time Zone

The **CMS5000 Time Zone** tab sets CMS5000 date and time. Data files are stamped with date and time based on the **CMS5000 Time Zone** setting. (See Figure 12-76.)

Figure 12-76 CMS5000 Time Zone tab

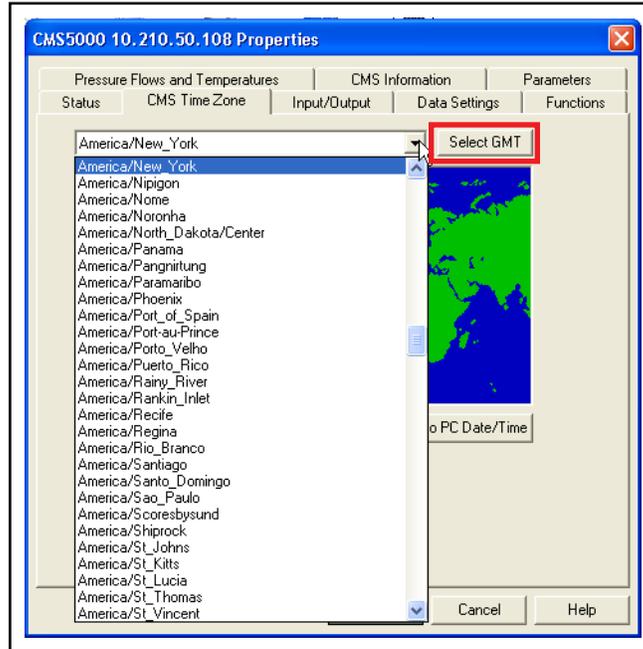


12.6.2.1 Setting the Time Zone

To set the time zone, select the desired time zone from the shortcut menu.
(See Figure 12-77.)

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

Figure 12-77 Selecting time zone



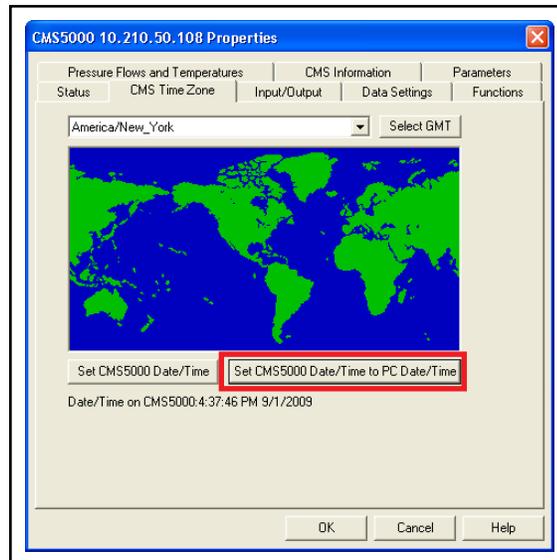
12.6.2.2 Setting Date and Time

There are two options to set the date and time.

12.6.2.2.1 Sync Date and Time to Computer

Click **Set CMS5000 Date/Time to PC Date/Time** to automatically synchronize CMS5000 to the computer date and time. (See Figure 12-78.)

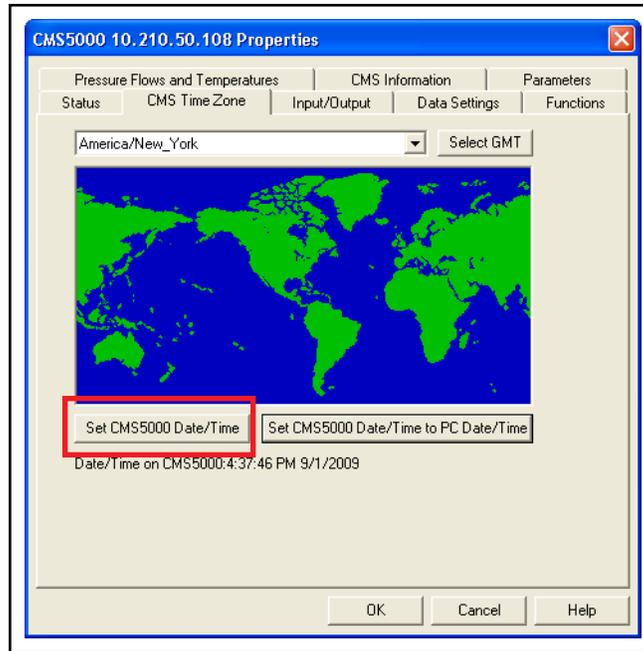
Figure 12-78 Set CMS5000 Date/Time to computer Date/Time button



12.6.2.2.2 Enter Date and Time Manually

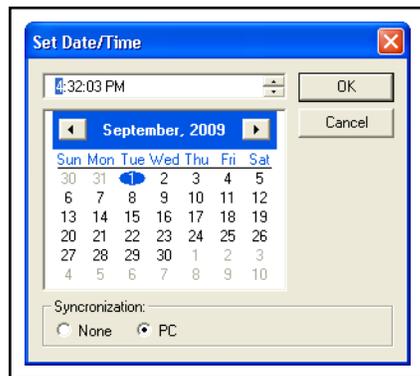
- 1 Click **Set CMS5000 Date/Time**. (See Figure 12-79.)

Figure 12-79 Set CMS5000 Date/Time button



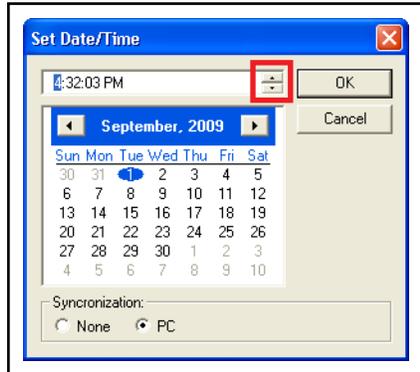
- 2 The **Set Date/Time** window will display. (See Figure 12-80.)

Figure 12-80 Set Date/Time



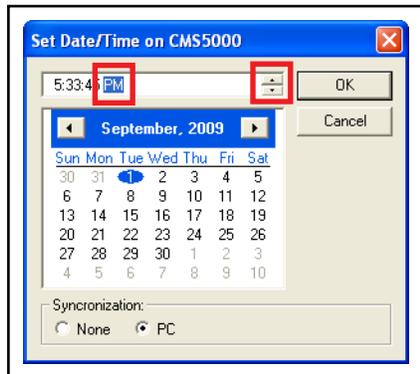
- Use the top arrow buttons, to the right of the displayed time, to select the desired time. (See Figure 12-81.)

Figure 12-81 Time selection arrow buttons



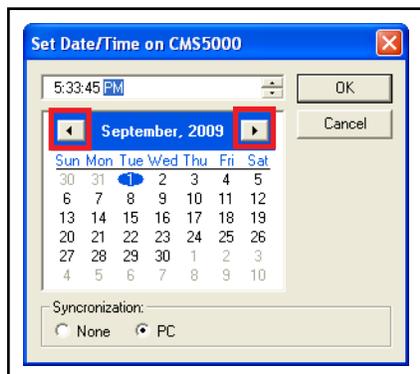
- Highlight minutes, seconds, or AM/PM. Use the arrow buttons to change the highlighted value. (See Figure 12-82.)

Figure 12-82 Setting the time



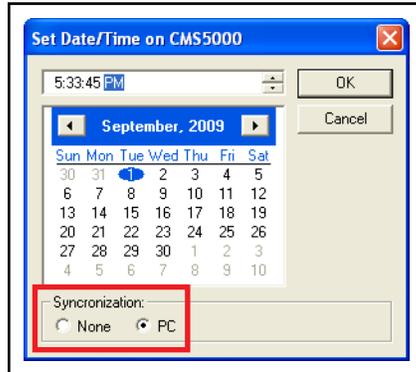
- Click the arrow to scroll to the desired month. Click the desired date. (See Figure 12-83.)

Figure 12-83 Setting date



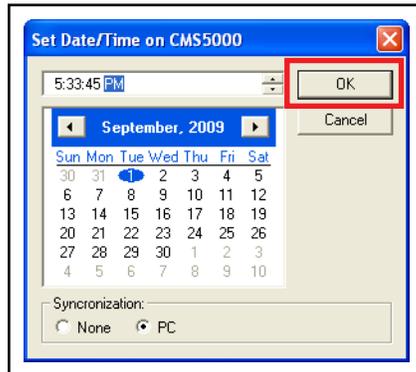
- 6 Select **PC** to synchronize CMS5000 time with the computer time. Select **None** if synchronization is not required. (See Figure 12-84.)

Figure 12-84 Synchronization



- 7 Click **OK** to close the window. (See Figure 12-85.)

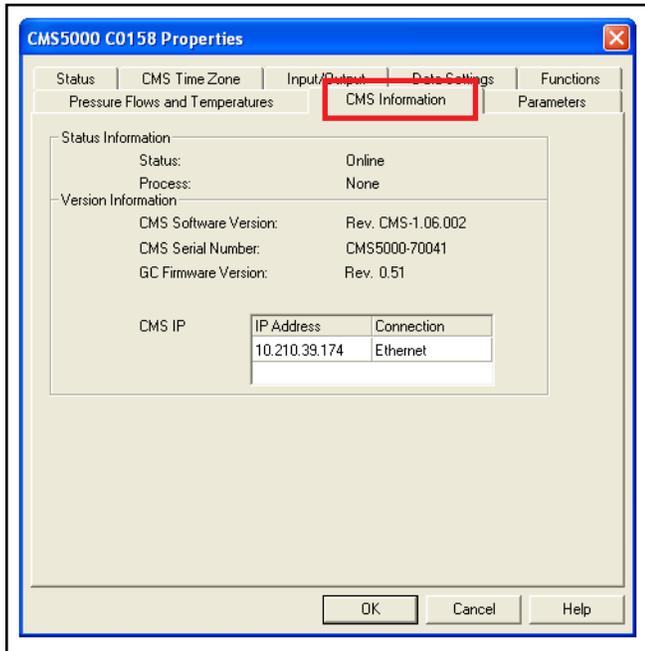
Figure 12-85 Setting date and time



12.6.3 CMS5000 Information

The **CMS Information** tab displays CMS5000 system information.
(See Figure 12-86.)

Figure 12-86 CMS Information tab



Status Indicates if CMS5000 is online or offline

Process Displays **None** when CMS5000 is idle.
Displays **Run Method** when CMS5000 is running a method or is preparing the next method

NOTE: Process will not refresh until the CMS5000 Properties window is closed and reopened.

CMS Software Version Current version of software loaded on CMS5000

CMS Serial Number Serial number of the connected CMS5000

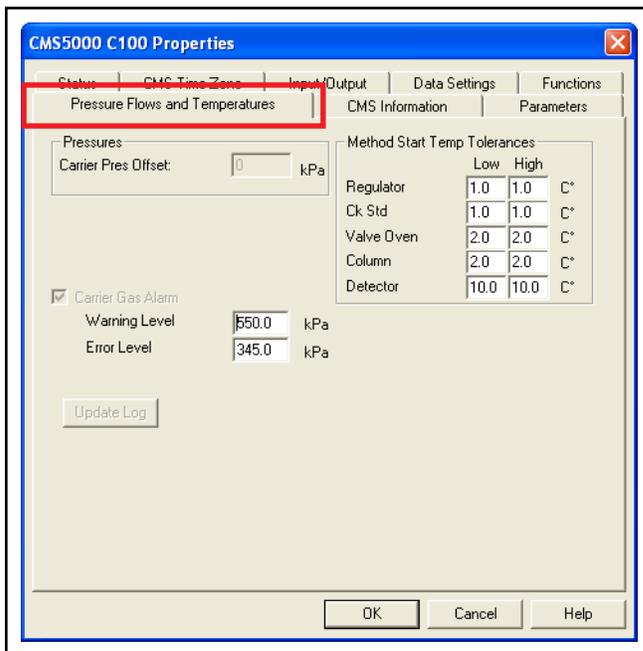
GC Firmware Version Current version of GC card firmware

CMS IP Displays the IP address and Connection type

12.6.4 Pressure Flows and Temperatures

The **Pressure Flows and Temperatures** tab displays carrier gas **Pressures**, **Method Start Temp Tolerances**, and **Carrier Gas Alarm** information. (See Figure 12-87.)

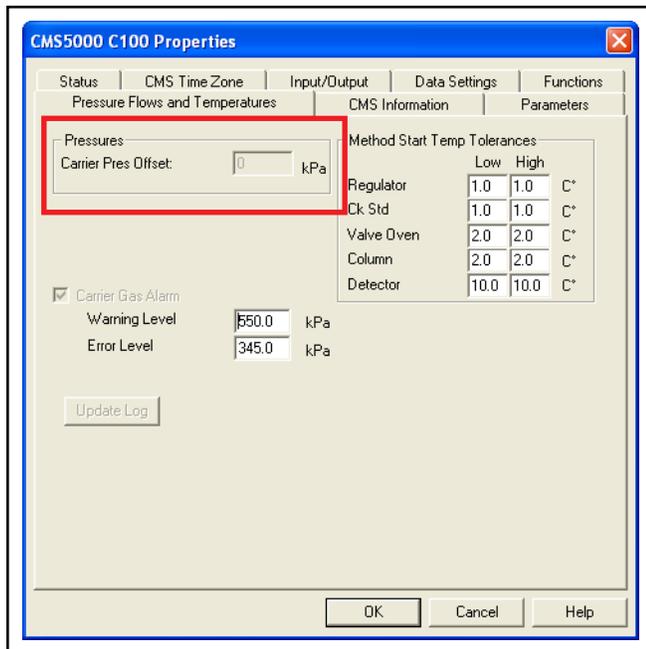
Figure 12-87 Pressure Flows and Offsets tab



12.6.4.1 Pressures

The **Pressures** pane displays the **Carrier Pres Offset**. This value is set at the factory and cannot be changed. (See Figure 12-88.)

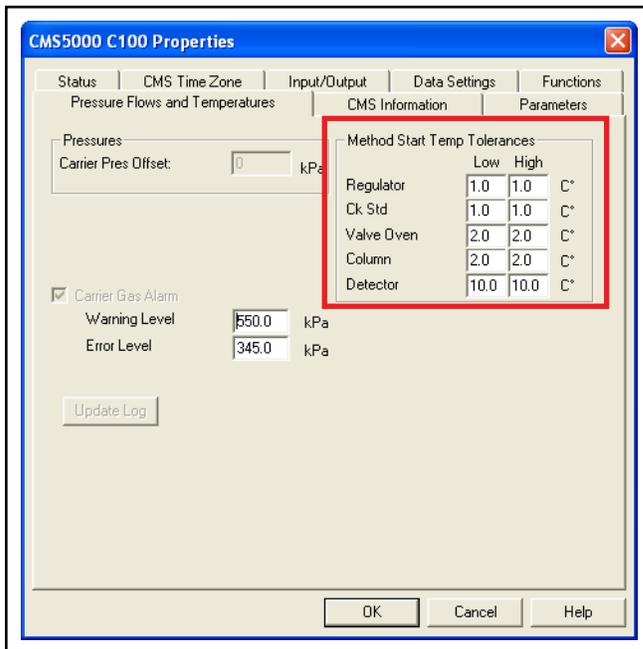
Figure 12-88 Pressures



12.6.4.2 Method Start Temperature Tolerances

The **Method Start Temp Tolerances** pane sets the operating temperature range for temperature regulated components. (See Figure 12-89.)

Figure 12-89 Method Start Temperature Tolerances



12.6.4.3 Carrier Gas Alarm

The **Warning Level 550.0 kPa** (default) and **Error Level 345.0 kPa** (default) are displayed. (See Figure 12-90.)

Carrier gas warning and error level values are adjustable.

When the carrier gas pressure reaches the **Warning Level**, an **Argon Pressure Low!** warning message is displayed on the CMS5000 front panel.

Refer to Figure 7-6 on page 7-4.

When the carrier gas pressure reaches the **Error Level**, a **REPLACE ARGON CYLINDER!** error message is displayed on the CMS5000 front panel.

Refer to Figure 7-7 on page 7-4.

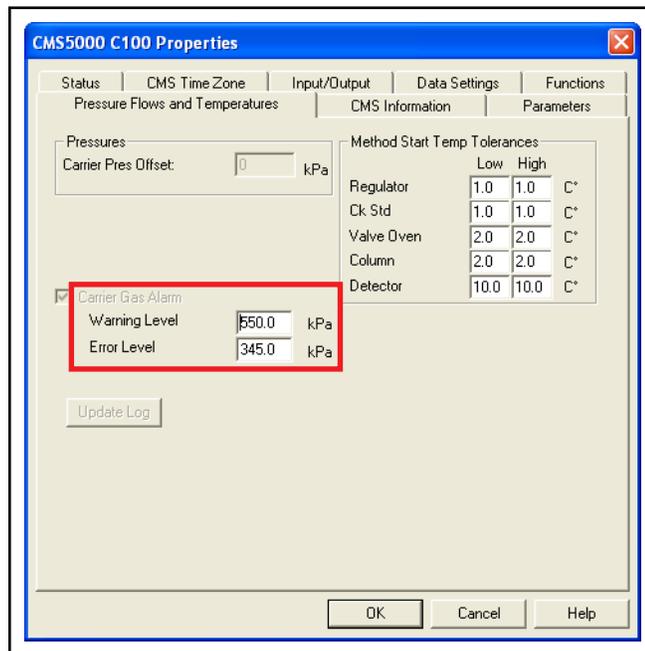
When **Error Level** is reached, the column heater will turn off, preventing operation.



CAUTION

Do not set Carrier Gas Alarm Error Level below 345 kPa. Levels below 345 kPa will not provide sufficient carrier gas flow and will damage the column.

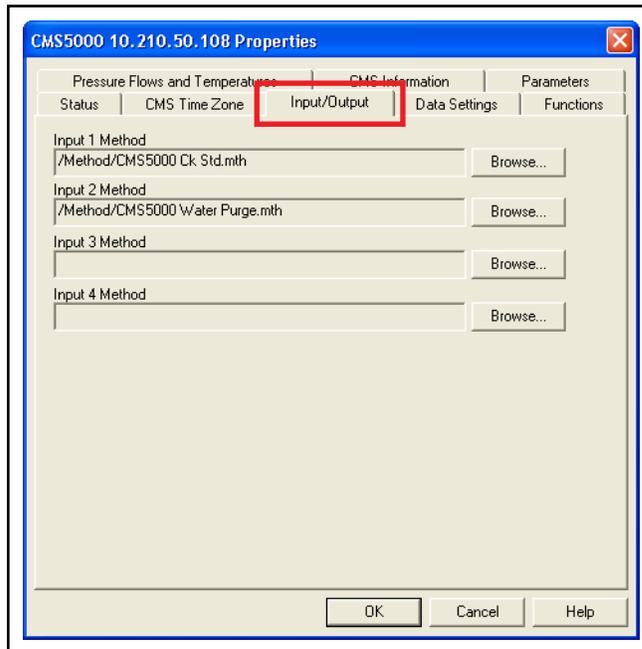
Figure 12-90 Carrier Gas Alarm



12.6.5 Input/Output

The desired methods for input triggers are entered in the **Input/Output** tab. (See Figure 12-91.) For instructions on defining input methods, refer to section 6.3, System Integration, on page 6-12.

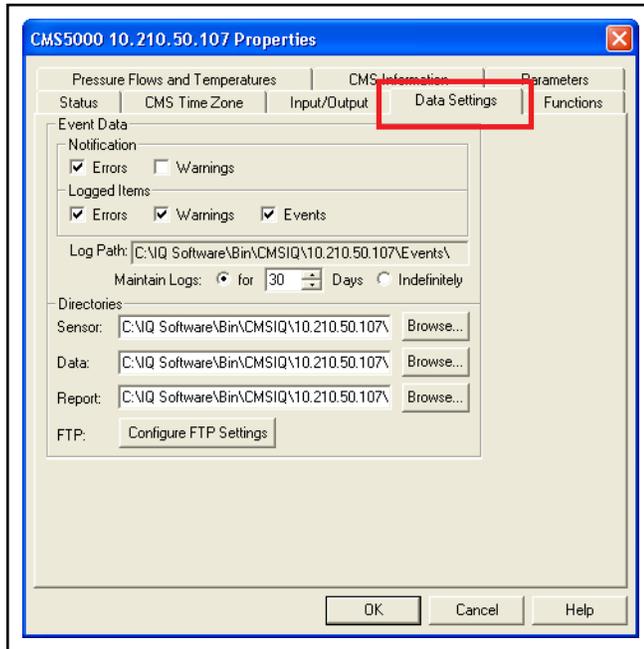
Figure 12-91 Input/Output tab



12.6.6 Data Settings

The **Data Settings** tab **Event Data** pane provides settings for **Notification**, **Logged Items**, the **Log Path**, and **Directories**. (See Figure 12-92.)

Figure 12-92 Data Settings tab

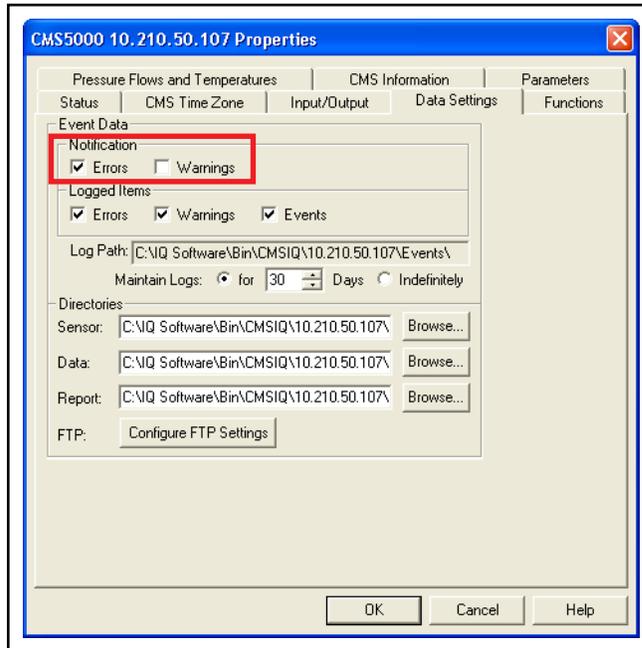


12.6.6.1 Notification

The **Notification** pane establishes whether errors, events and warnings will be displayed on the front panel. (See Figure 12-93.)

- ◆ When the **Errors** checkbox is selected, all error messages are displayed on the front panel, as they occur
- ◆ When the **Warnings** checkbox is selected, all error warnings are displayed on the front panel, as they occur

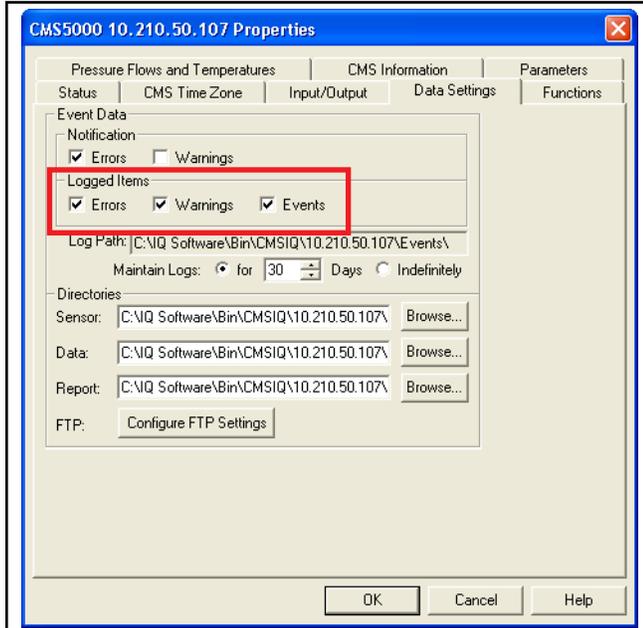
Figure 12-93 Notification pane



12.6.6.2 Logged Items

Select a checkbox in the **Logged Items** pane to add item(s) to the system log. (See Figure 12-94.) To view logged items, refer to section 12.2.3 on page 12-3.

Figure 12-94 Logged items pane

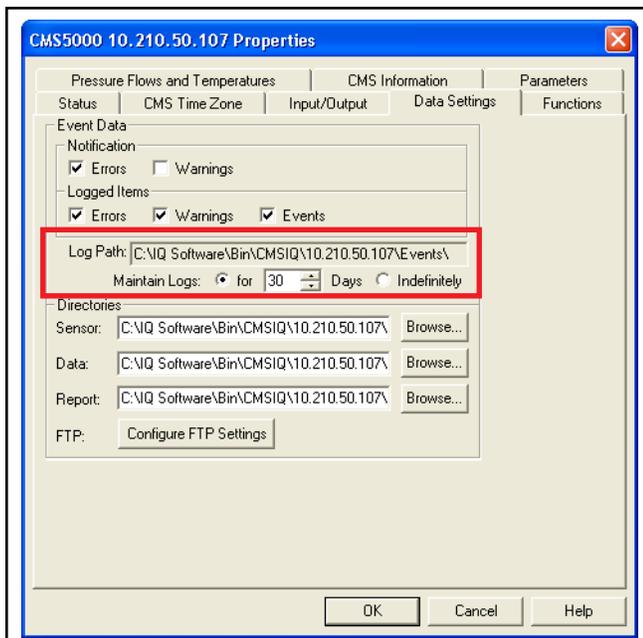


12.6.6.3 Log Path and Maintain Logs

Log Path displays the pathway to the folder where logged events are stored.

Maintain Logs defines the period of time that must expire before the logged events are deleted. (See Figure 12-95.)

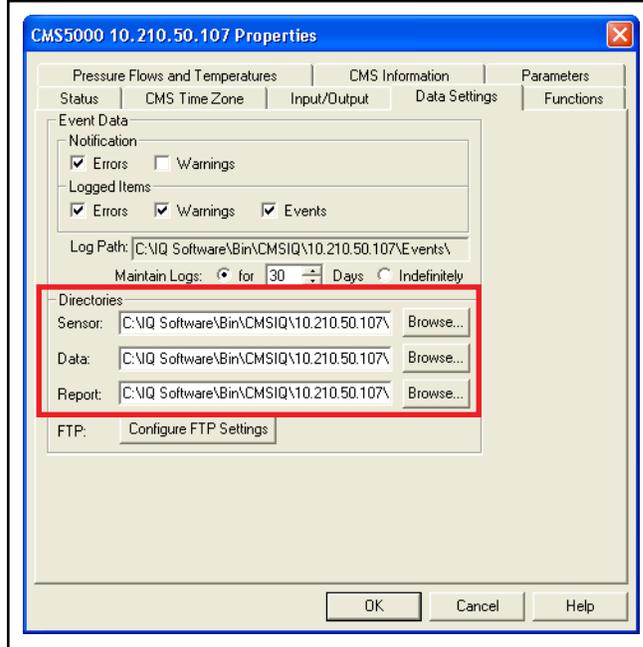
Figure 12-95 Log Path and Maintain Logs sections



12.6.6.4 Directories

The **Directories** pane is set during CMS IQ installation. Do not change the pathways. (See Figure 12-96.)

Figure 12-96 Directories



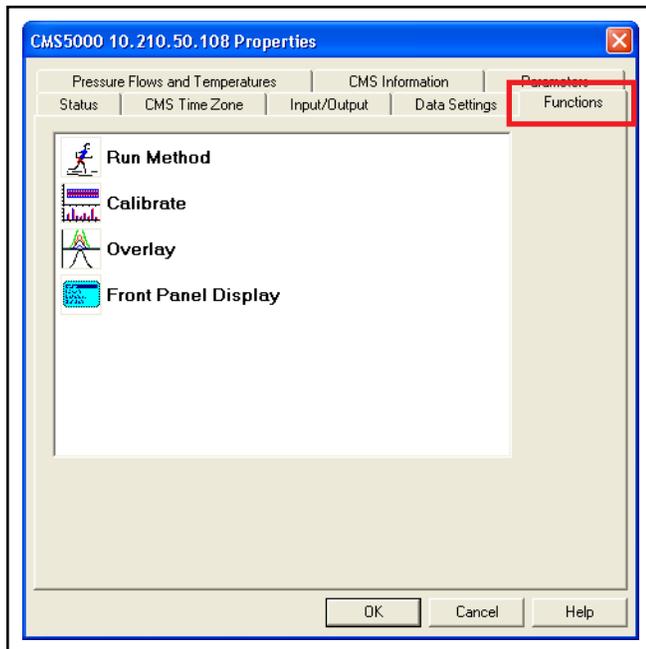
12.6.6.5 Configure FTP Settings

Refer to section 6.2, FTP Connection, on page 6-1.

12.6.7 Functions

The icons on the **Functions** tab behave the same as the icons on the **Sensor** toolbar in the **System Setup** window. (See Figure 12-97.)

Figure 12-97 Functions tab



Run Method icon, see Chapter 14, Run Method

Calibrate icon, see Chapter 17, Calibration

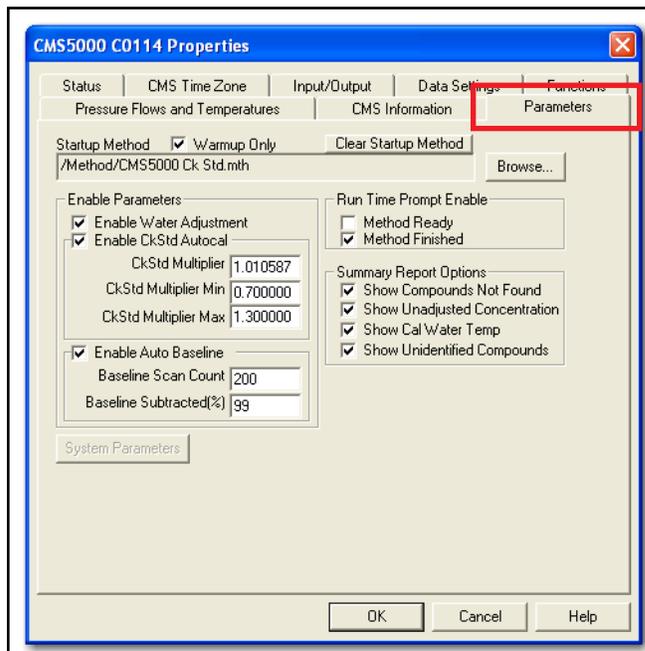
Overlay icon, see Chapter 15, Chromatogram Overlay

Front Panel Display icon, see section 12.7, Front Panel Display Icon, on page 12-70

12.6.8 Parameters

The **Parameters** tab includes setting a startup method, enabling the water adjustment, check standard auto calibration, auto baseline parameters, the run time prompt, and the summary report options. (See Figure 12-98.)

Figure 12-98 Parameters tab



12.6.8.1 Startup Method

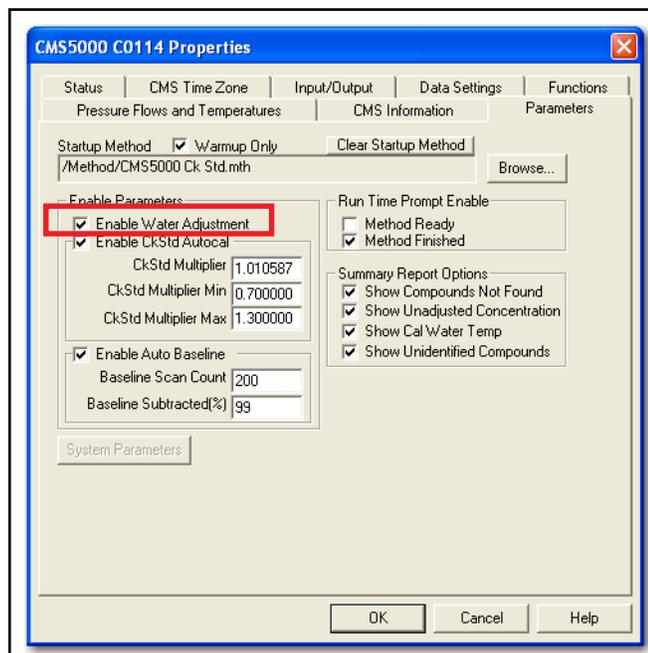
For instructions on defining and clearing the Startup method, refer to section 6.4, Defining Startup Methods, on page 6-12.

12.6.8.2 Enable Water Adjustment

Select the **Enable Water Adjustment** checkbox to calculate the difference in partition coefficient between the sample and calibration due to the difference in water temperature. (See Figure 12-99.)

NOTE: For more information on partition coefficient, see section 17.7, Water Beta, on page 17-36.

Figure 12-99 Enable Water Adjustment checkbox



12.6.8.3 Enable CkStd Autocal

Select the **Enable CkStd Autocal** checkbox to adjust calculations of all methods based on shifts in response of toluene from the **Check Standard** method. (See Figure 12-100.)

Once the **Check Standard** method is calibrated, the changes in response when running the method account for detector drift. Refer to section 17.4, Calibrating the Check Standard, on page 17-2 for calibrating the **Check Standard**.

CkStd Multiplier The multiple (i.e., factor) that analytes are adjusted by to account for detector drift. This value is automatically updated after each check standard method run

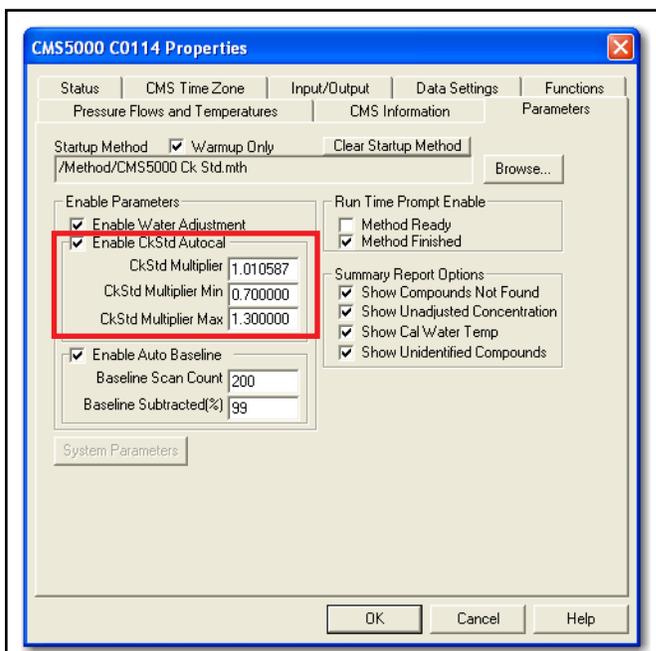
CkStd Multiplier Min. Defines the minimum allowable multiplier value. If the CkStd Multiplier is close to or equal to the CkStd Multiplier Min, the check standard and analytical method must be recalibrated

CkStd Multiplier Max Defines the maximum allowable multiplier value. If the CkStd Multiplier is close to or equal to the CkStd Multiplier Max, the check standard and analytical method must be recalibrated

NOTE: CMS5000 will not warn when **CkStd Multiplier** is at the **Min** or **Max** level. **CkStd Multiplier** must be checked weekly to determine if recalibration is necessary.

NOTE: The Check Standard Multiplier Min and Max is defined as $\pm 30\%$ of the true value. This is based on the USEPA standard tolerance for acceptance of continuing calibration verification standards. This value can be changed if desired.

Figure 12-100 Enable CkStd Autocal checkbox



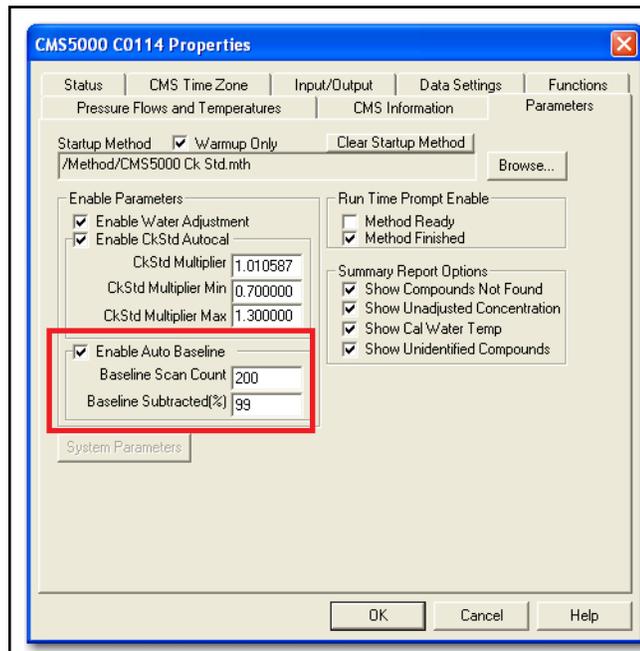
12.6.8.4 Auto Baseline Function

Auto Baseline normalizes detector response to make chromatograms easier to evaluate visually. (See Figure 12-101.)

Baseline Scan Count Number of scans used at the beginning of a chromatogram to determine the baseline response

Baseline Subtracted(%) Percent of the baseline response subtracted from all scans to normalize chromatogram

Figure 12-101 Enable Auto Baseline Correct checkbox



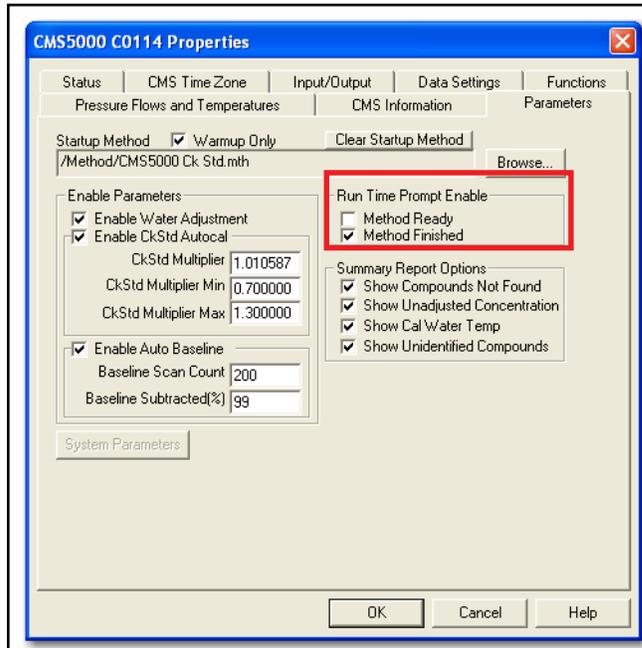
12.6.8.5 Run Time Prompt Enable

The **Run Time Prompt Enable** pane determines when CMS5000 waits for user input. (See Figure 12-102.)

Method Ready System will not start a method until RUN is selected from the front panel or in IQ

Method Finished System will keep the data file of a method run open until closed by the user

Figure 12-102 Run Time Prompt Enable



12.6.8.6 Summary Report Options

The **Summary Report Options** pane sets options to appear in a quantitative report. (See Figure 12-103.)

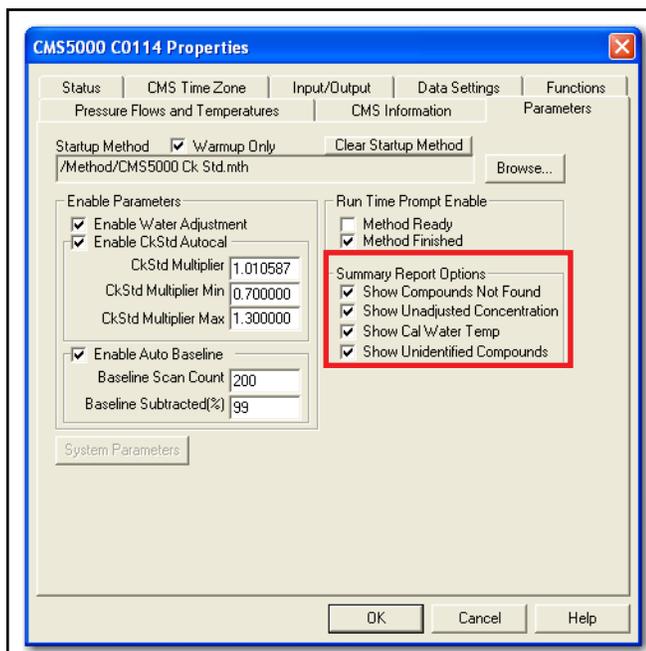
Show Compounds Not Found Display compounds that are part of the calibration library but were not detected in the sample

Show Unadjusted Concentration For water manifolds only. Display the concentration of a compound prior to adjustment by the check standard multiplier and water temperature compensation

Show Cal Water Temp For water methods only. Display the water temperature at the time of calibration

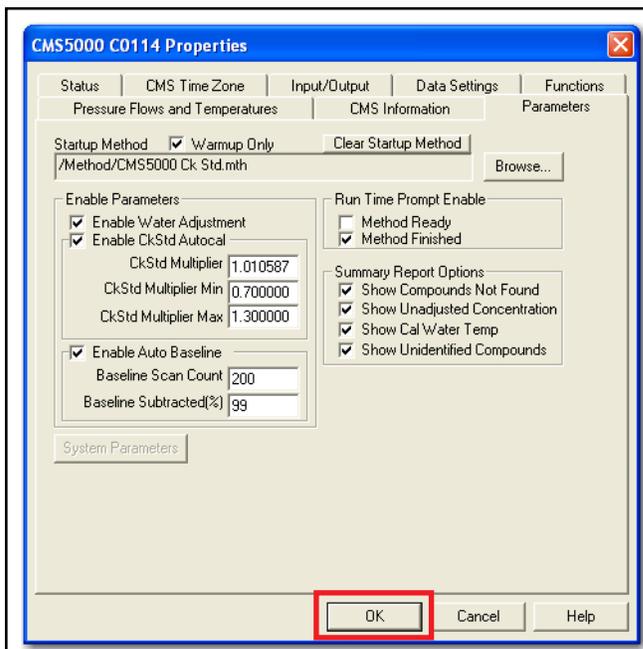
Show Unidentified Compounds Display the retention times of peaks that were found in the chromatogram but were not included in the calibration library

Figure 12-103 Summary Report Options pane



Click **OK** to close the **CMS5000 Properties** window. (See Figure 12-104.)

Figure 12-104 Closing CMS5000 Properties window

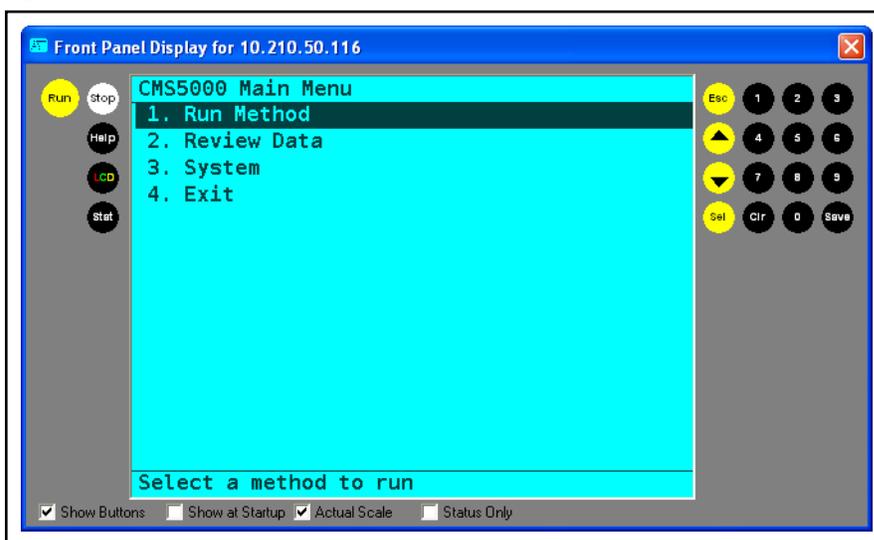


12.7 Front Panel Display Icon



Double-click **Front Panel Display** to open the **Front Panel Display** emulator. (See Figure 12-105.) The **Front Panel Display** emulator operates identically to the front panel.

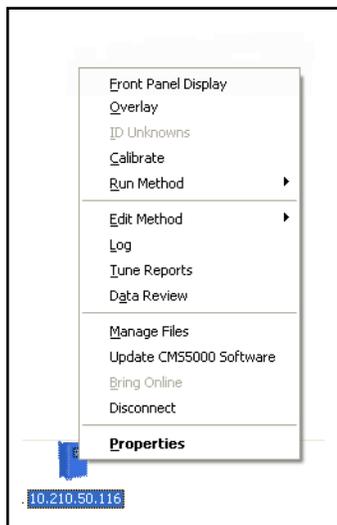
Figure 12-105 Front Panel Display emulation



12.8 CMS5000 Sensor Status Icon

Right-click **CMS5000 Sensor Status**  to display the following menu. (See Figure 12-106.)

Figure 12-106 Sensor Status menu



- Front Panel Display** Refer to section 12.7, Front Panel Display Icon, on page 12-70
- Overlay** See Chapter 15, Chromatogram Overlay
- ID Unknowns**. Unavailable
- Calibrate** See Chapter 17, Calibration
- Run Method**. Lists recent methods to run (See Chapter 14, Run Method)
- Edit Method**. Lists recent methods to edit (See Chapter 16, Method Editor)
- Log**. Opens event log (*.evt) files. Information logged are warnings, errors, events and run history. Refer to section 12.6.6.2, Logged Items, on page 12-61
- Tune Reports** Unavailable
- Data Review** See Chapter 13, Data Review
- Manage Files**. Refer to section 12.5, Manage Files, on page 12-39
- Update CMS5000 Software** See section 12.8.1, Update CMS5000 Software, on page 12-72

- Bring Online** See section 12.8.2, Bring Online, on page 12-72
- Disconnect** See section 12.8.3, Disconnect, on page 12-72

12.8.1 Update CMS5000 Software

For complete installation instructions, refer to the Software Installation Instructions that accompany the update. When a software or method update for CMS5000 is available for download, **Update CMS5000 Software** selects the update (*.upd) file. Once selected, the update will be loaded onto the analytical module and the analytical module will restart.

12.8.2 Bring Online

If the connection has been disabled using CMS IQ **Disconnect**, click **Bring Online** to enable the connection.

12.8.2.1 Communication Messages

If the computer is not communicating with CMS5000, there are three colors of "X"s that may be displayed over the instrument icon. (See Table 12-2.)

Table 12-2 Colored "x"s indicating communication state

| Icon | Description |
|---|--|
|  | Communication OK. |
|  | (1) Communication has yet to be established. (2) Communication has been disabled using the CMS IQ Disconnect, see section 12.8.3, Disconnect, on page 12-72 |
|  | Communication was lost |
|  | Communication cannot be established |

12.8.3 Disconnect

Disconnect will disconnect computer communication from CMS5000. Click **Bring Online** to enable communication.

Chapter 13

Data Review

13.1 Introduction to Data Review

Data Review provides access to previously acquired data for review and analysis.

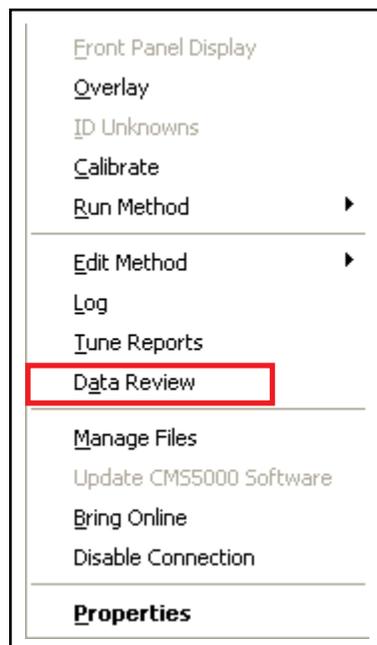
- ◆ Reviewing Data File information
- ◆ Viewing Summary and Quantitative reports
- ◆ Zooming in/out of chromatogram
- ◆ Labeling peaks
- ◆ Viewing the method used to acquire data

13.2 Accessing the Data Review Feature

- 1 Double-click **Data Review** .

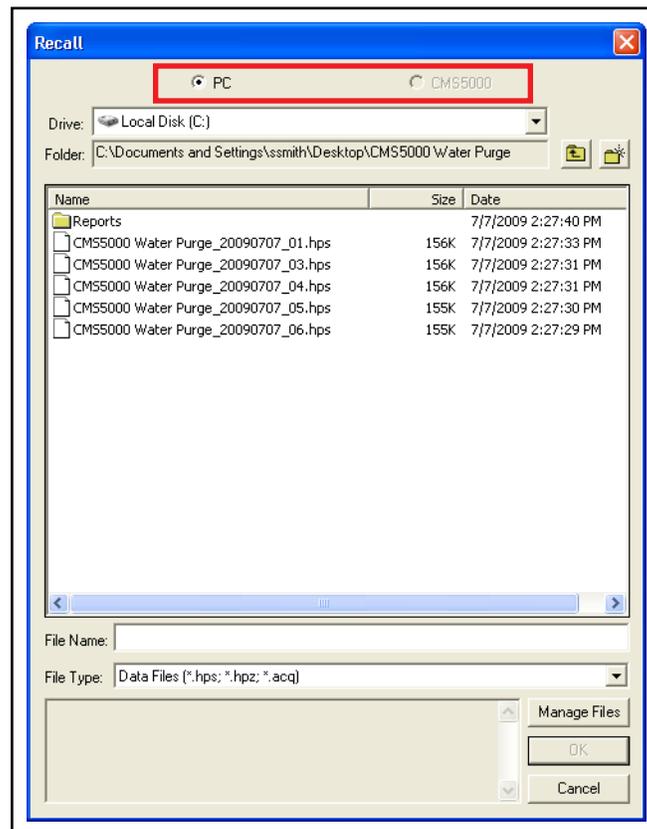
Alternately, right-click **CMS5000 Sensor Status**  to display the menu displayed in Figure 13-1. Select **Data Review**.

Figure 13-1 Data Review menu



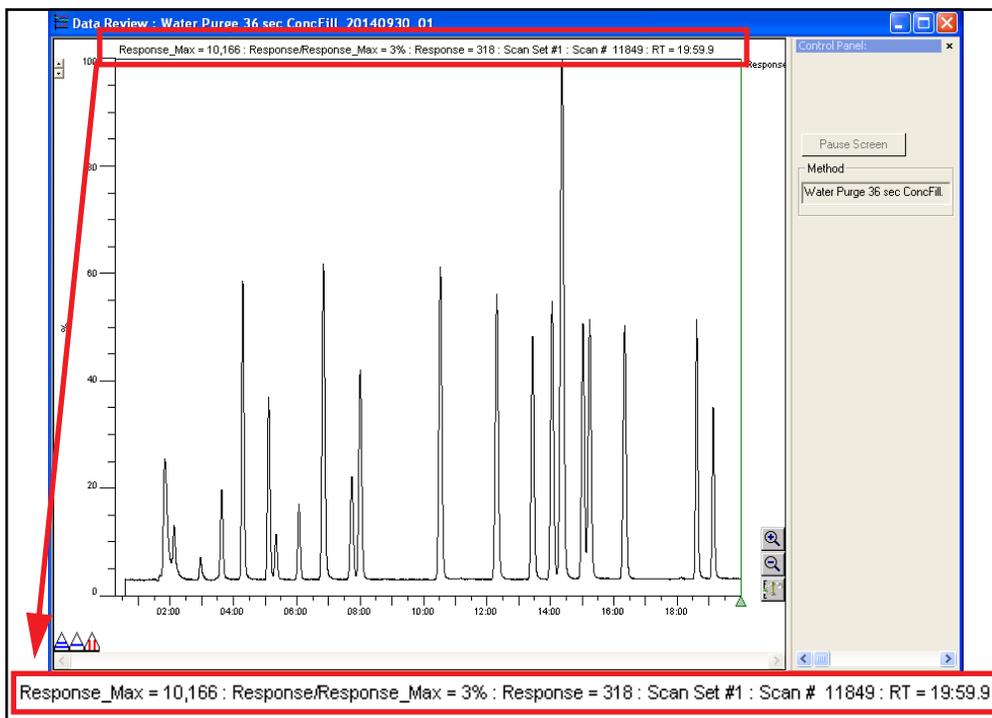
- 2 The **Recall** window is displayed. Select the desired data file, either from the computer or CMS5000. (See Figure 13-2.)
- ◆ Select **PC** or **CMS5000** to access the appropriate file storage location. **CMS5000** will be unavailable if CMS5000 is not connected to the computer
 - ◆ Methods and data files are saved on CMS5000. Methods will only be available on the computer after they have been manually transferred to the computer
 - ◆ Data files will automatically transfer to the computer if CMS IQ was open and connected to CMS5000 when the data file was collected

Figure 13-2 Recall window



- 3 Double-click the desired data file to display in the **Data Review** window. (See Figure 13-3.)

Figure 13-3 Data Review window



The **Data Review** window displays the data file’s chromatogram.

The x-axis displays the retention time of peaks.

The y-axis displays the signal intensity as a percent of the largest peak.

Response_Max The highest intensity signal on the chromatogram

Response/Response_Max The percent difference between the signal intensity at the location of the Scan Cursor and the highest intensity signal on the chromatogram

Response The signal intensity at the location of the Scan Cursor

Scan # The number of data points taken since the beginning of data collection from the location of the Scan Cursor

RT The retention time in minutes and seconds at the location of the Scan Cursor

NOTE: See section 13.8, How to Access the Scan Cursor, on page 13-28 for more information on the Scan Cursor.

13.3 Menu Bar

When a data file is selected, the menu bar at the top of CMS IQ displays the **Data Review** option. (See Figure 13-4.)

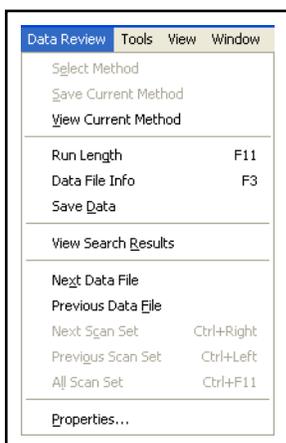
Figure 13-4 Data Review option in menu bar



13.3.1 Data Review Menu

Selecting **Data Review** opens the **Data Review** menu. (See Figure 13-5.)

Figure 13-5 Data Review menu



View Current Method Opens the method used to create the current data file

Run Length Displays full chromatogram

Data File Info Opens the Data File Information window. See section 13.5, Data File Information Window, on page 13-6

Save Data Saves changes to the data file

NOTE: Changed data files can be saved to the computer, not CMS5000.

View Search Results Opens summary and quantitative reports for the selected data file. See section 13.6, Reports, on page 13-7

Next Data File Opens the next saved data file in the data folder

Previous Data File Opens the previously saved data file in the data folder

13.4 Data Review Toolbar

Figure 13-6 Data Review toolbar



Table 13-1 Data review toolbar icons

| Icon | Name | Description |
|---|-----------------------|--|
|  | Abort | Aborts a running method |
|  | Start/Stop | Stops a method |
|  | Pause | Pauses the chromatogram in CMS IQ. The method will continue to run |
|  | Data File Information | Contains method and sample information. Refer to Figure 13-4 on page 13-4 |
|  | View Search Results | Accesses data reports for this data file |
|  | Safety Database | Accesses the NIOSH Database. Refer to section 12.4, Safety DB, on page 12-36 |
|  | Previous File | Opens the previous data file in the current data folder |
|  | Next File | Opens the next data file in the current data folder |

Table 13-1 Data review toolbar icons

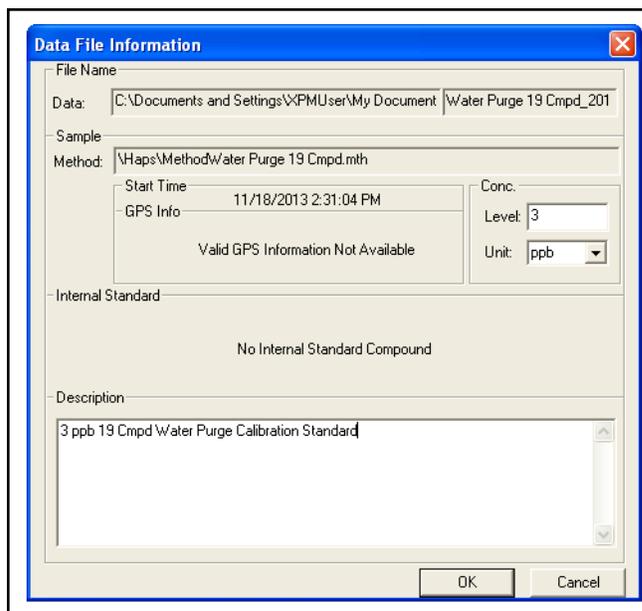
| Icon | Name | Description |
|---|---------------|---|
|  | Previous Peak | Moves to previous peak when Search for Peaks is selected |
|  | Next Peak | Moves to next peak when Search for Peaks is selected |
|  | All Peaks | Returns to the full chromatogram view |

NOTE: The **Set** buttons are unavailable.

13.5 Data File Information Window

The **Data File Information** window is shown in Figure 13-7. To access, click **Data File Information** .

Figure 13-7 Data File Information window



- Data:** The file location and filename of the data file
- Method:** The method associated with the data file
- Start Time** The date and time when the sample was collected
- GPS Info** Unavailable

- Conc.** For data files with known concentrations, the concentration and units of concentration can be entered into the **Level:** and **Unit:** boxes
- Internal Standard** Unavailable
- Description** Sampling information or notes can be entered into the **Description** box
 - ◆ If description or concentration information is entered while a run is in progress, the information will be saved with the data file in CMS IQ
 - ◆ If information is entered after the run has finished, the information is saved as a copy on the computer

13.6 Reports

Two data reports are available at the completion of a sample run:

- ◆ **Summary** report provides a brief description of the compounds identified
- ◆ **Quantitative** report is more detailed and based upon the calibration library

13.6.1 Access Reports

1 To access reports, click **View Search Results** .

Alternately, select **View Search Results** from the **Data Review** menu on the **Data Review** window. (See Figure 13-8.)

Figure 13-8 View Search Results from Data Review menu



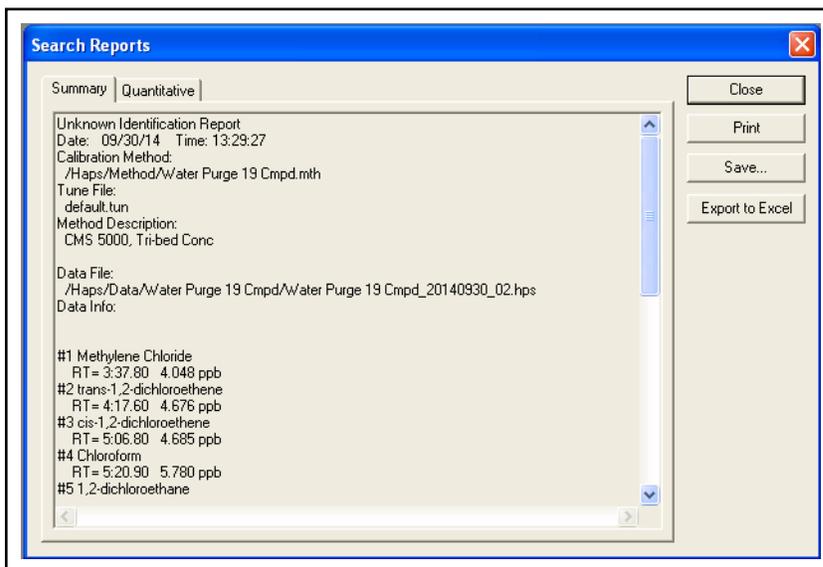
2 The **Search Reports** window will open with the **Summary** report tab selected. (See Figure 13-9.)

- ◆ Reports can be saved, printed, or exported to Excel
- ◆ Summary Reports are saved as *.rql_sum files
- ◆ Quantitative Reports are saved as *.rqt files

13.6.2 Summary Reports

The **Summary** report provides the method start date and time, name of the method file, a description of the method, name of the data file and the sample description if entered into the **Data File Information** window (refer to section 13.5, [Data File Information Window](#), on page 13-6). A list of compounds identified, retention times and concentrations are also displayed. The compounds are listed in retention time order. (See Figure 13-9.)

Figure 13-9 Summary Report



13.6.3 Quantitative Reports

A **Quantitative** report is displayed for methods containing a calibration library. The report will show the method start date and time, compounds identified, predicted retention time, actual retention time, peak area, concentration, and limit. (See Chapter 16, [Method Editor](#).)

<=== ALARM ===> is displayed in the flag column if the concentration is above a defined limit. (See Figure 13-10.)

Area too low is displayed in the flag column if the area of the peak was lower than the method limit for the peak area. (See Figure 13-10.)

Not found with current search parameters is displayed in the flag column if the peak width is too small or larger than the method permits. (See Figure 13-10.)

Figure 13-10 Flag column

| Pred. RT | Actual RT | Area | Conc. (ppb) | No Adjust | Limit (ppb) | Flag |
|----------|-----------|-------|-------------|-----------|-------------|--|
| 3:27.80 | 3:28.00 | 603 | --- | --- | --- | --- |
| 4:10.01 | 4:09.60 | 1338 | 0.09150 | [0.09341] | --- | --- |
| 5:02.50 | --- | --- | --- | --- | --- | Area too low |
| 7.60 | 5:16.20 | 32278 | 2.944 | [3.352] | --- | Area too low |
| 5:02.40 | --- | --- | --- | --- | --- | Area too low |
| 1.70 | --- | --- | --- | --- | --- | Not found with current search parameters |
| 7:48.30 | --- | --- | --- | --- | --- | Area too low |
| 05.50 | --- | --- | --- | --- | --- | Area too low |
| 4.20 | --- | --- | --- | --- | --- | Area too low |
| 2:35.00 | --- | --- | --- | --- | --- | Area too low |
| 3:45.90 | 13:48.00 | 1618 | 0.1331 | [0.1355] | --- | --- |
| 4:25.00 | 14:27.80 | 1576 | 0.2204 | [0.2224] | --- | --- |
| 4:44.30 | --- | --- | --- | --- | --- | Area too low |
| 5.60 | 15:27.40 | 1821 | 0.2963 | [0.2993] | --- | --- |
| 8.70 | 15:40.60 | 1643 | 0.2004 | [0.2027] | --- | --- |
| 16:45.00 | 16:47.70 | 2844 | 0.2877 | [0.2915] | --- | --- |
| 18:55.80 | 18:57.60 | 12019 | 0.4628 | [0.4670] | --- | --- |
| 19:28.30 | 19:28.00 | 8502 | 0.5153 | [0.4153] | 0.5000 | <== ALARM ==> |

If a calibration library was not present in the method run, the **Quantitative** window will display **No Report**.

To export the Quantitative report to Excel, click **Export to Excel**. (See Figure 13-11.)

Click **Close**.

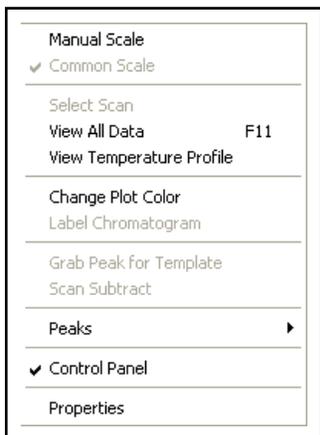
Figure 13-11 Quantitative Report

| REC # | CAS # | Target Name | Pred. RT | Actual RT | Area | Conc. (ppb) |
|-------|-------|--------------------------|----------|-----------|----------|-------------|
| 1 | | Methylene Chloride | 3:29.30 | 3:33.06 | 1551090 | 4.092 |
| 2 | | trans-1,2-dichloroethene | 4:12.00 | 4:16.31 | 5238601 | 4.092 |
| 3 | | cis-1,2-dichloroethene | 5:03.30 | 5:08.83 | 2992998 | 4.092 |
| 4 | | Chloroform | 5:18.50 | 5:24.19 | 1083007 | 4.092 |
| 5 | | 1,2-dichloroethane | 6:03.60 | 6:09.83 | 1022729 | 4.092 |
| 6 | | Benzene | 6:53.70 | 6:59.63 | 5225006 | 4.092 |
| 7 | | 1,2-dichloropropane | 7:50.00 | 7:57.11 | 1502544 | 4.092 |
| 8 | | trichloroethene | 8:07.60 | 8:14.33 | 3445660 | 4.092 |
| 9 | | Toluene | 10:49.20 | 10:55.33 | 5321976 | 4.092 |
| 10 | | tetrachloroethene | 12:40.50 | 12:47.35 | 5242850 | 4.092 |
| 11 | | chlorobenzene | 13:51.40 | 13:58.14 | 3565123 | 4.092 |
| 12 | | ethylbenzene | 14:31.00 | 14:37.24 | 4568416 | 4.092 |
| 13 | | m-xylene, p-xylene | 14:51.50 | 14:56.79 | 14200043 | 4.092 |
| 14 | | styrene | 15:32.00 | 15:37.67 | 3558637 | 4.092 |
| 15 | | o-xylene | 15:45.60 | 15:50.77 | 4080458 | 4.092 |

13.7 Chromatogram Window Options

Right-click anywhere in the chromatogram window to display the menu shown in Figure 13-12.

Figure 13-12 Chromatogram Window menu



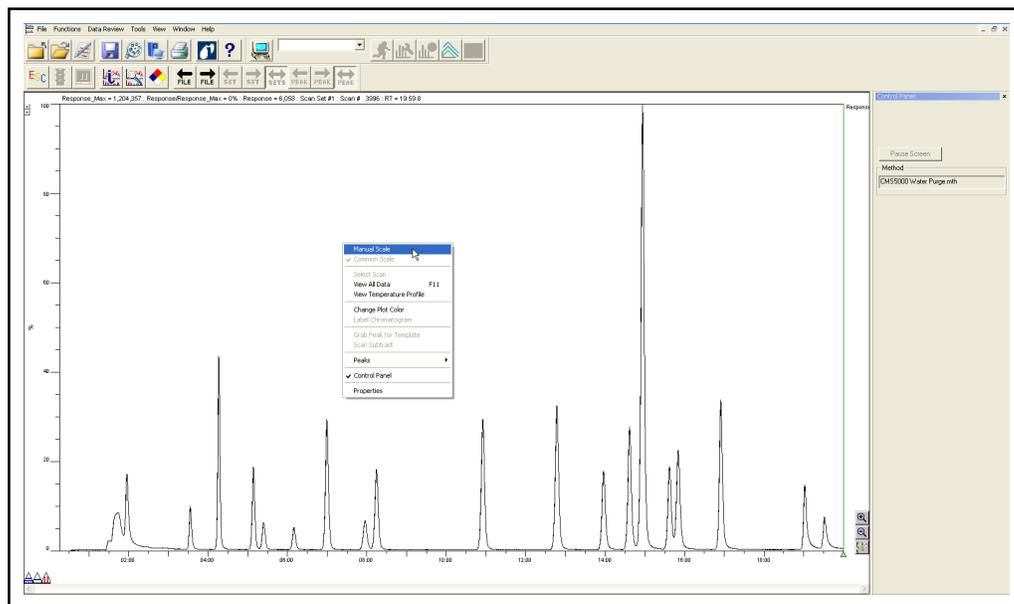
13.7.1 Manual Scale

Manual Scale will rescale the y-axis of the chromatogram to a desired intensity.

NOTE: By default, the graph will scale to the highest peak of the chromatogram.

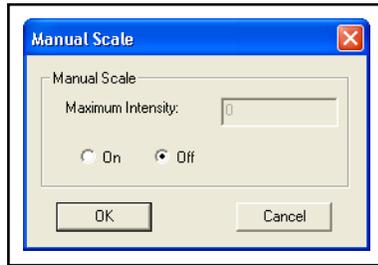
- 1 Right-click in the chromatogram window and select **Manual Scale**. (See Figure 13-13.)

Figure 13-13 Manual Scale



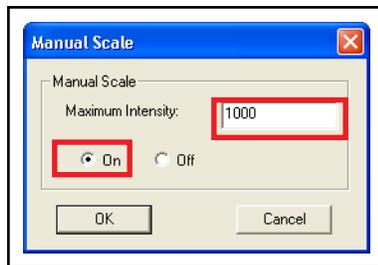
- The **Manual Scale** window is displayed. (See Figure 13-14.)

Figure 13-14 Manual Scale window



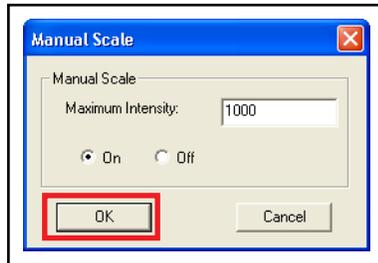
- Select **On** and type a value into the **Maximum Intensity** box. (See Figure 13-15.)

Figure 13-15 Enter the intensity



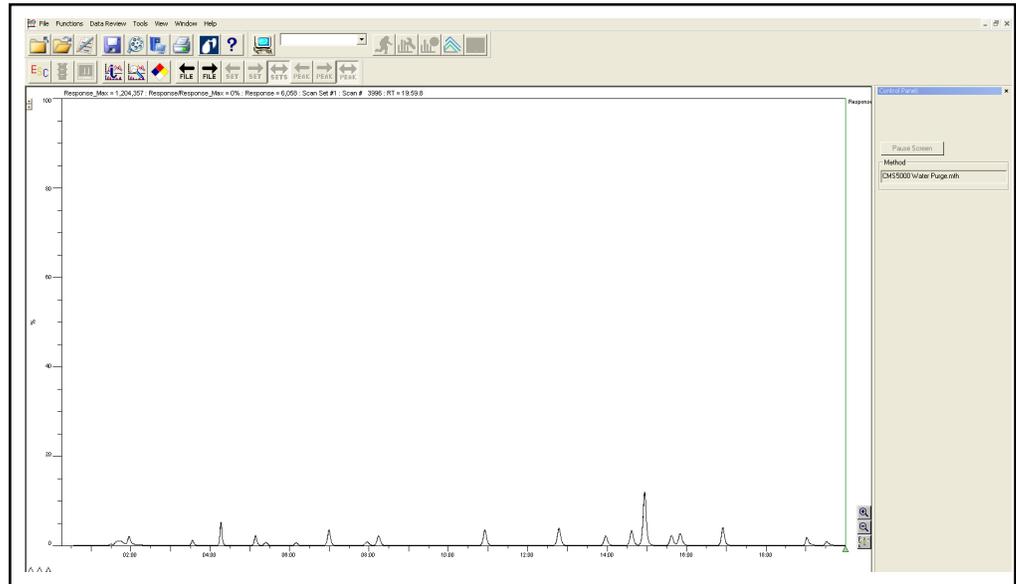
- Click **OK** to close the window and activate Manual Scale. (See Figure 13-16.)

Figure 13-16 Activate Manual Scale



5 The chromatogram is rescaled. (See Figure 13-17.)

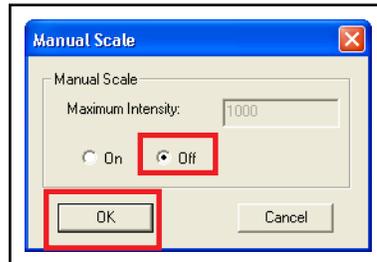
Figure 13-17 Rescaled chromatogram



NOTE: The y-axis is labelled in percent of maximum intensity. The intensity selected from **Manual Scale** will not be displayed on the chromatogram.

6 To view the original scale, refer to steps 1 and 2. Select **Off** and click **OK**. (See Figure 13-18.)

Figure 13-18 Deactivate Manual Scale

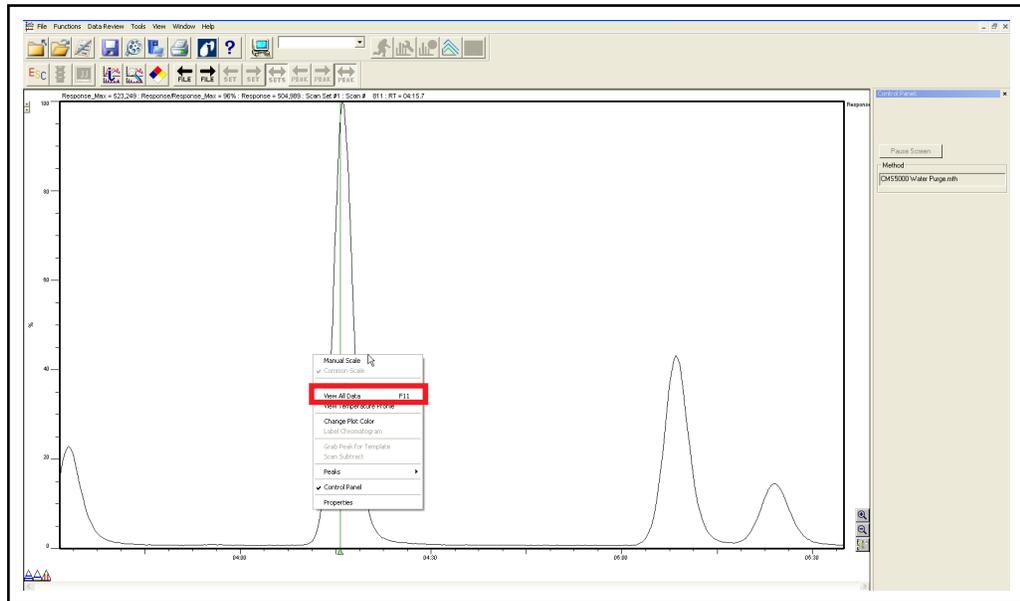


13.7.2 View All Data

View All Data function is used to view the entire chromatogram. See section 13.9, Using the Zoom Function, on page 13-29 for instructions on using Zoom.

- 1 Right-click anywhere in the zoomed chromatogram and select **View All Data**. (See Figure 13-19.) Alternately, **View All Data** can be activated by pressing **F11** on the computer keyboard.

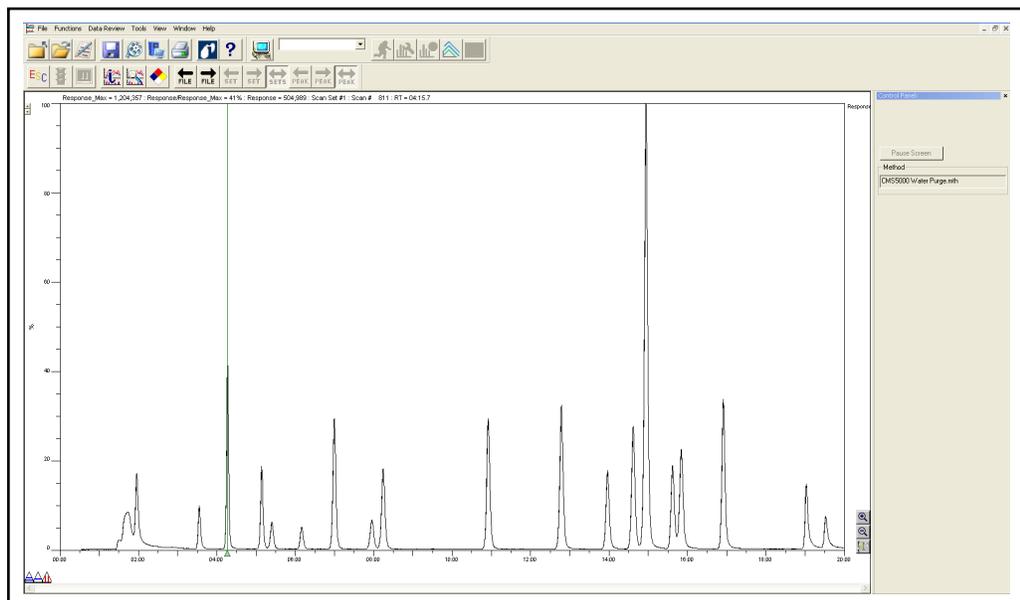
Figure 13-19 View All Data function



- 2 The full method run will be displayed. (See Figure 13-20.)

NOTE: **View All Data** will not adjust the y-axis scale.

Figure 13-20 View All Data screen



13.7.3 View Temperature Profile

View Temperature Profile displays the GC temperature profile of the method. Right-click anywhere in the chromatogram window and select **View Temperature Profile**. To remove the profile, right-click in the chromatogram window and clear the **View Temperature Profile** option. (See Figure 13-21 and Figure 13-22.)

Figure 13-21 View Temperature Profile function

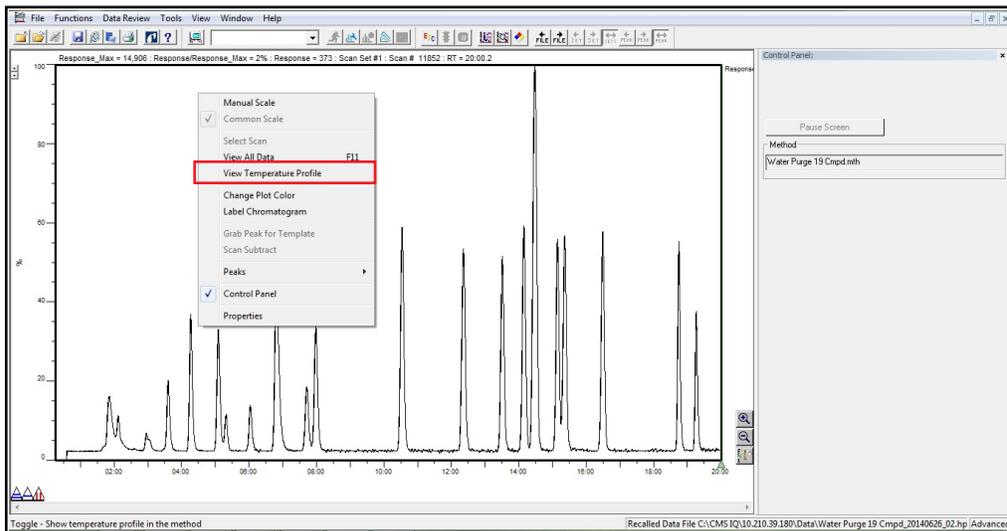
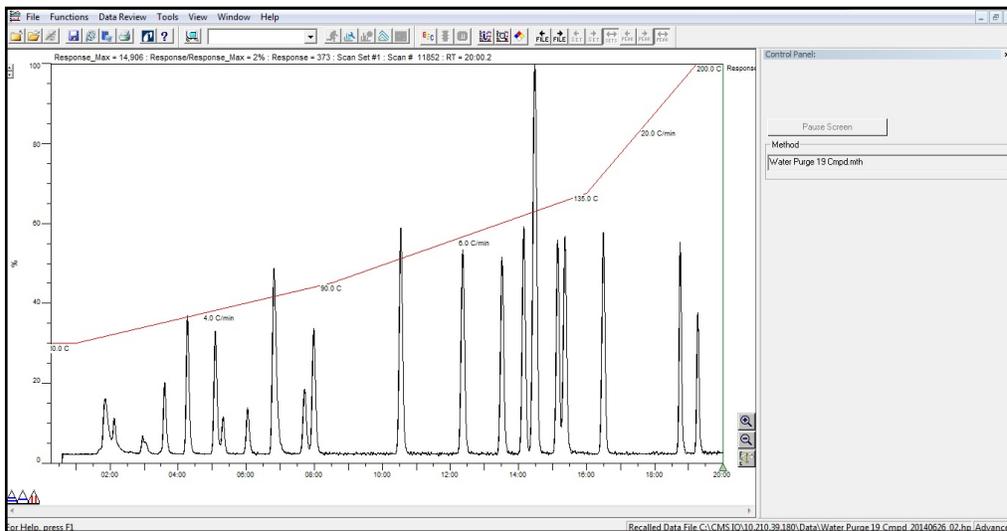


Figure 13-22 View Temperature Profile screen

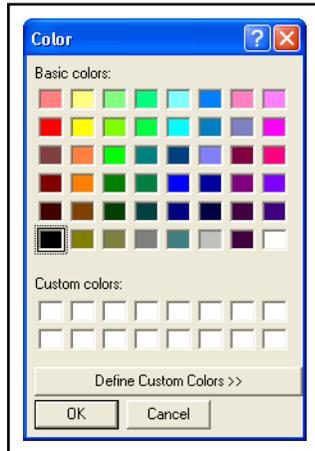


13.7.4 Change Plot Color

Change Plot Color changes the color of the plot utilized in the chromatogram.

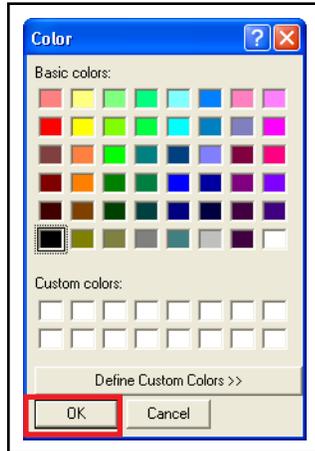
- 1 Right-click anywhere in the chromatogram window and select **Change Plot Color**. The **Color** window is displayed. (See Figure 13-23.)

Figure 13-23 Color window



- 2 Click the desired color and click **OK**. The chromatogram plot will appear in the selected color. (See Figure 13-24.)

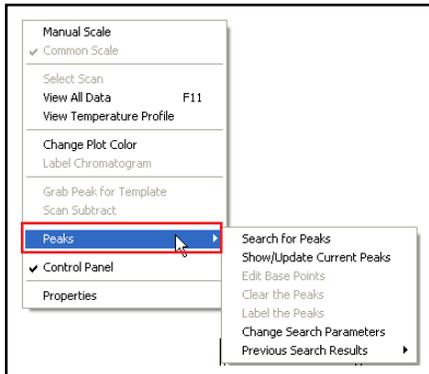
Figure 13-24 Selecting color



13.7.5 Peaks

Right click anywhere in the chromatogram window and select **Peaks** to display the Peaks menu. (See Figure 13-25.)

Figure 13-25 Peaks menu



13.7.5.1 Search for Peaks

Search for Peaks searches the entire chromatogram to locate peaks that meet the default search criteria.

- 1 Right-click in the chromatogram window. (See Figure 13-26.) Select **Peaks >> Search for Peaks**.
- 2 The **Peaks Found** window is displayed. (See Figure 13-27.)

The peaks meeting the criteria will be denoted with arrows, and the Peaks Found window will appear. (See Figure 13-26.)

Figure 13-26 Chromatogram after Search for Peaks is selected

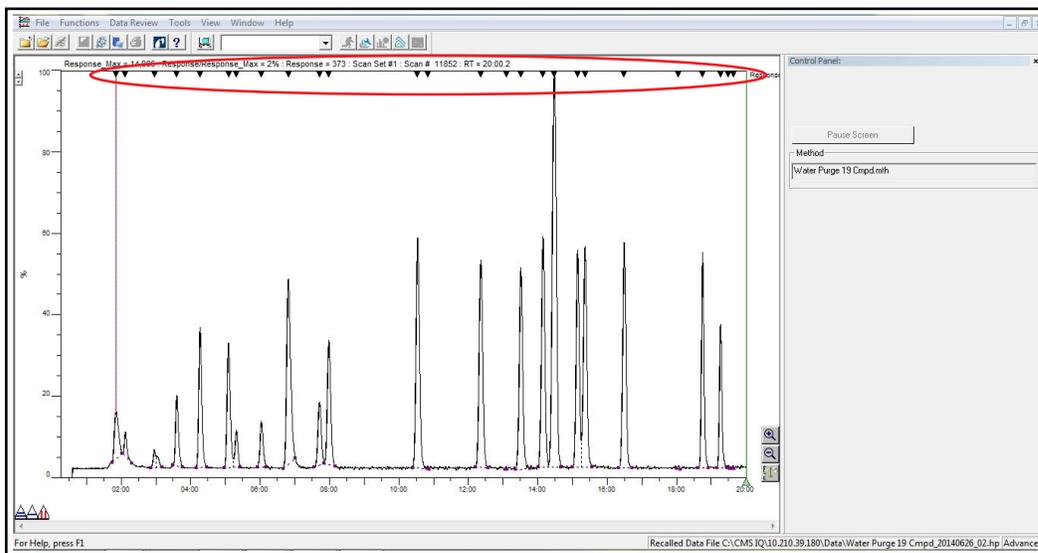
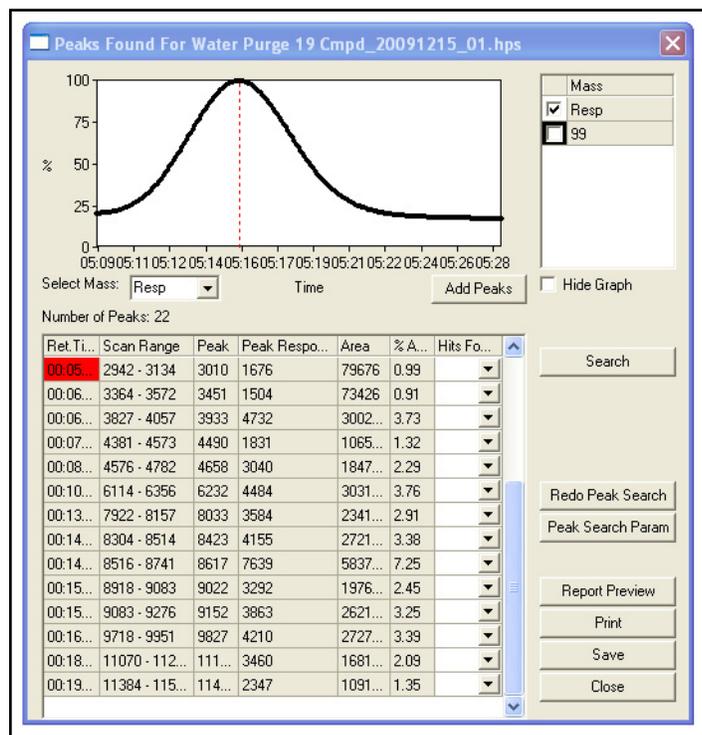


Figure 13-27 Peaks found



Data regarding each identified peak is displayed.

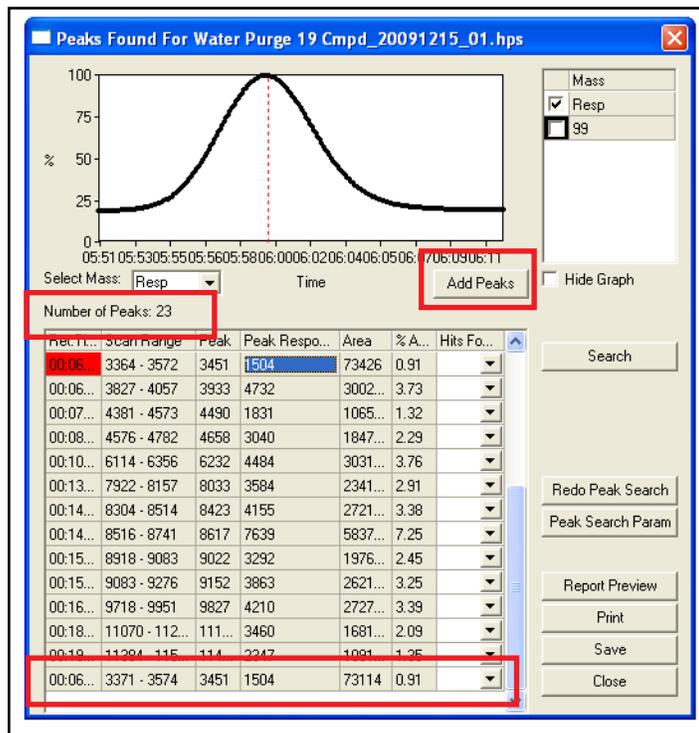
- ◆ **Retention Time**
- ◆ **Scan Range** displays the front and end of the peak, defined by the **Peak Search Parameters**
- ◆ **Peaks** shows the scan at the peak apex
- ◆ **Peak Response** is the intensity of the peak
- ◆ **Peak Area**
- ◆ **% Area** is a ratio of the individual peak's response to the response of the largest peak
- ◆ **Hits Found** will always be blank

13.7.5.1.1 Add Peaks

Add Peaks will add an unidentified peak to the list in the **Peaks Found** window.

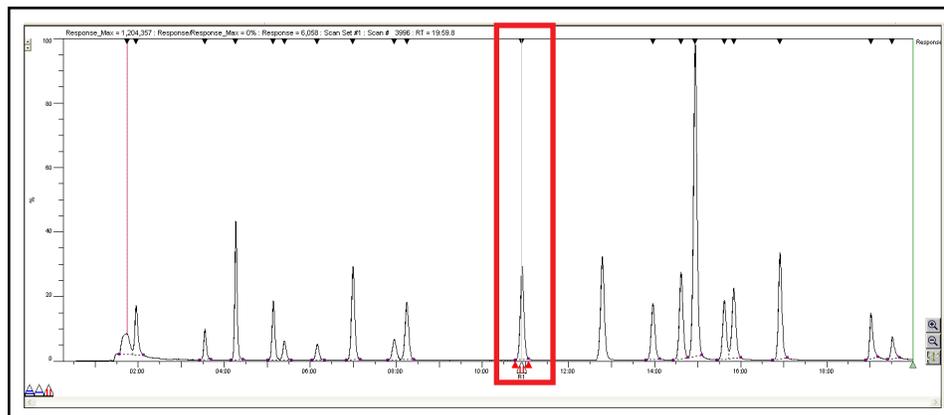
- 1 Use the **Range Tool** to select the location of the base points of the peak of interest. See steps 1-4 in section 13.10, [Range Tool](#), on page 13-34.
- 2 Once the red lines have been positioned, right-click in the chromatogram window. Select **Peaks >> Search for Peaks**.
- 3 Click **Add Peaks**. The peak will be added to the end of the peak list. (See [Figure 13-28](#).)

Figure 13-28 Add peaks



- 4 Click **Close**. The newly added peak and its base points will be displayed in the chromatogram. (See Figure 13-29.)

Figure 13-29 Added peak



13.7.5.1.2 Redo Peak Search

Redo Peak Search will repeat the peak search using updated **Peak Search Parameters**.

13.7.5.1.3 Peak Search Parameters

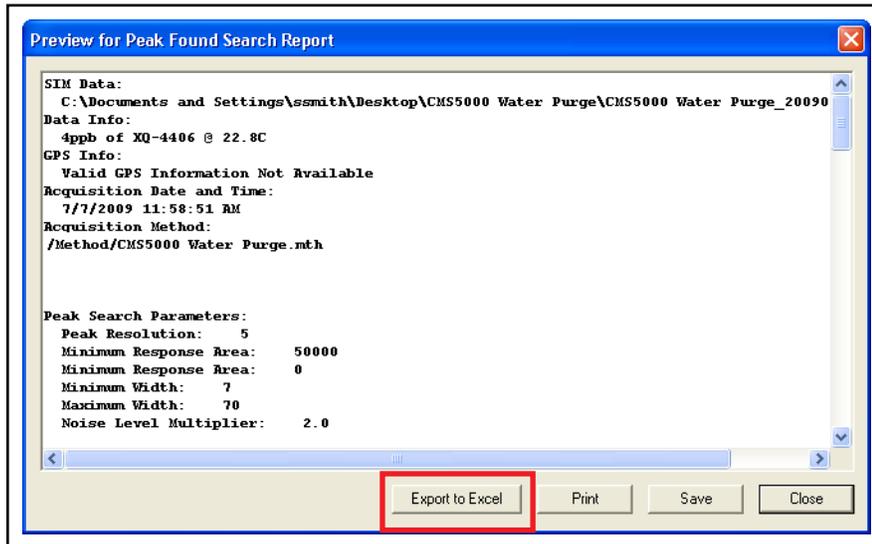
Peak Search Parameters behaves identically to **Change Search Parameters** on the **Peaks** submenu. See section 13.7.5.6, **Change Search Parameters**, on page 13-24.

13.7.5.1.4 Report Preview

Report Preview will reformat the **Peaks Found** window into an easy to read report. (See Figure 13-30.)

Once the preview is generated, click **Export to Excel** to send the report to Excel.

Figure 13-30 Report preview

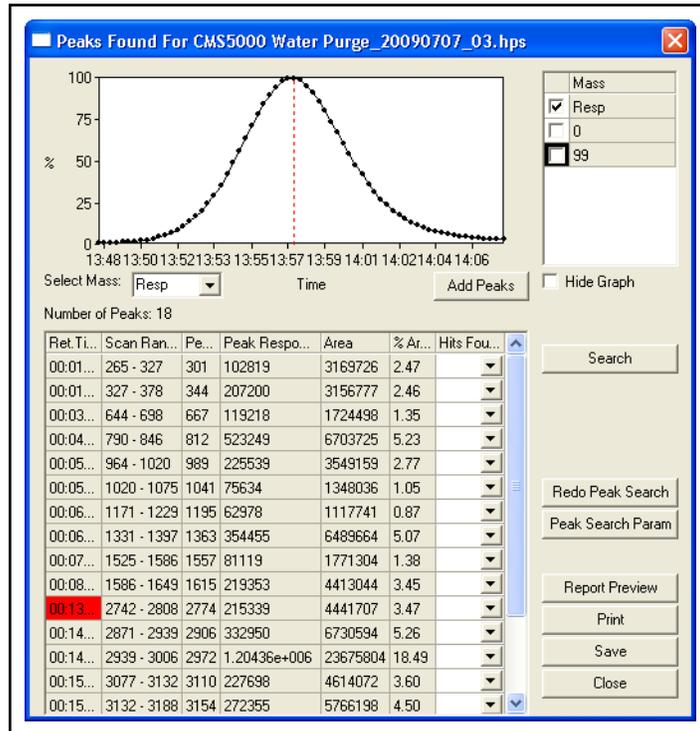


13.7.5.2 Show/Update Current Peaks

When the base points have been edited (see section 13.7.5.3, Edit Base Points, on page 13-21), **Show/Update Current Peaks** will recalculate the scan range, peak response, area and percent area utilizing the new base points.

- 1 Right-click in the chromatogram window. Select **Peaks >> Show/Update Current Peaks**. (Refer to Figure 13-25.)
- 2 The **Peaks Found** window with updated peak parameters is displayed. (See Figure 13-31.)

Figure 13-31 Show/update current peaks

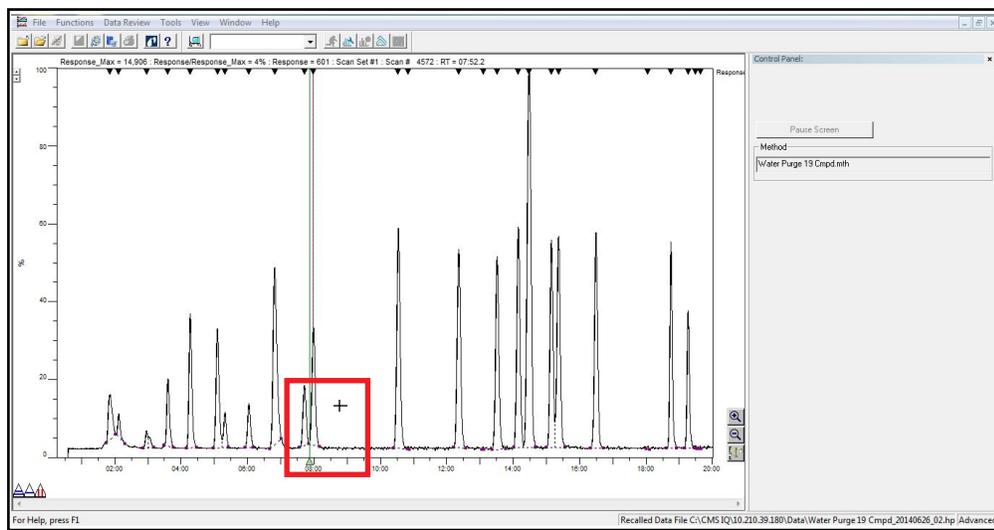


13.7.5.3 Edit Base Points

Edit Base Points will change the area of integration. Each purple dot on the chromatogram signifies a base point.

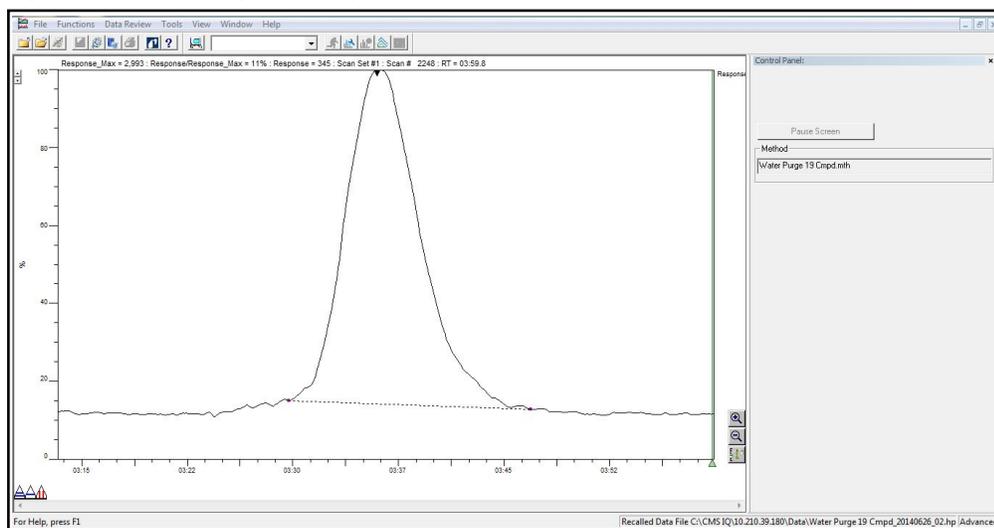
- 1 Perform the instructions in section 13.7.5.1, Search for Peaks, on page 13-16.
- 2 Right-click in the chromatogram window. Select **Peaks >> Edit Base Points**. Refer to Figure 13-25 on page 13-16.
- 3 The cursor appearance will change to a plus sign. (See Figure 13-32.)

Figure 13-32 Edit base peaks cursor



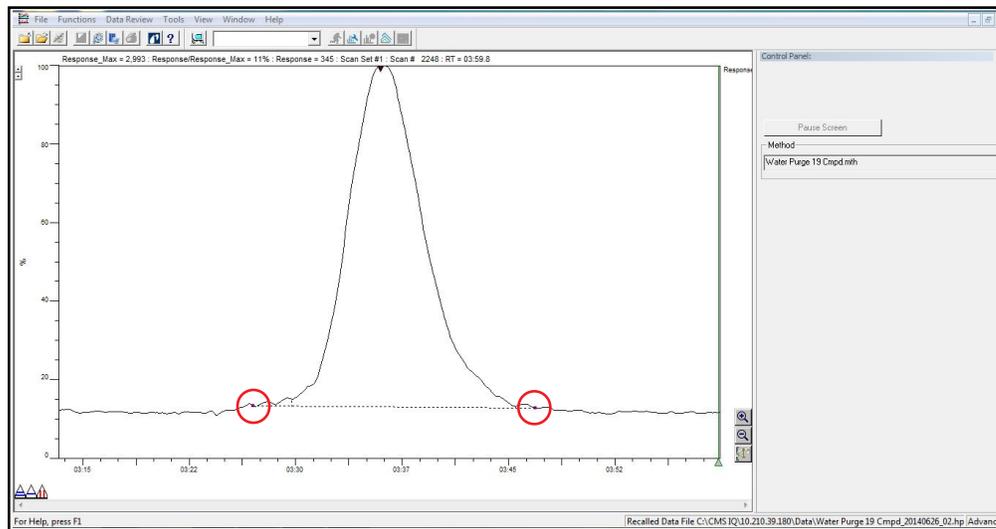
NOTE: For more accurate placement of the base point, zoom in on the desired peak. Refer to section 13.9, Using the Zoom Function, on page 13-29 for zoom instructions. (See Figure 13-33.)

Figure 13-33 Zooming in to edit points



- 4 Double-click the desired location for each base point. Each base point will relocate to the new position. (See Figure 13-34.)

Figure 13-34 Relocated base points



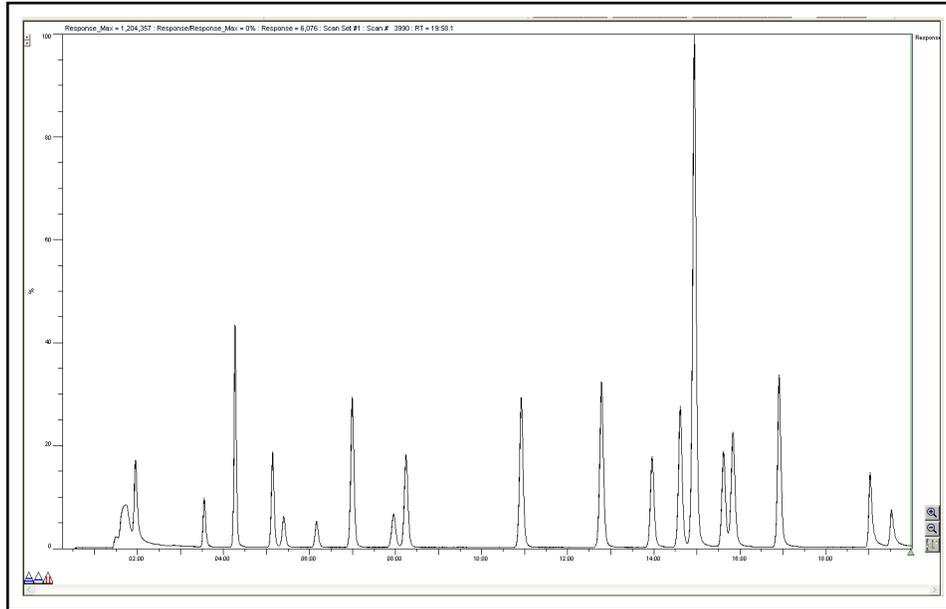
- 5 Verify the updated base points by opening **Show/Update Current Peaks**. Refer to section 13.7.5.2, Show/Update Current Peaks, on page 13-20. Alternately, select **Label the Peaks**, see section 13.7.5.5, Label the Peaks, on page 13-23 to view the updated peak area.

NOTE: To undo all manual changes to base points, click **Redo Peak Search** in the **Peaks Found** window. (Refer to Figure 13-31.)

13.7.5.4 Clear the Peaks

Clear the Peaks removes the peak identification arrows and base points from the graph. (See Figure 13-35.)

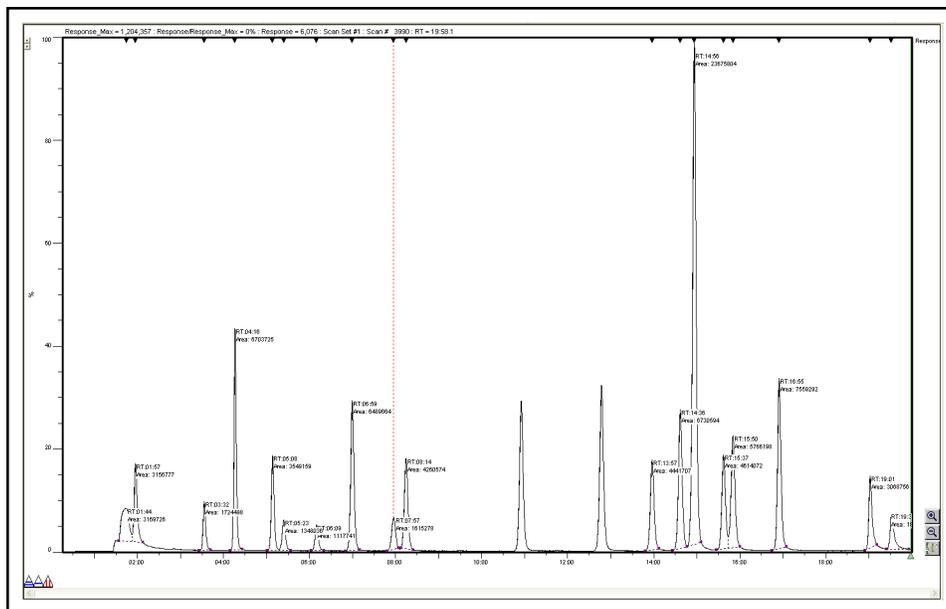
Figure 13-35 Clear the peaks



13.7.5.5 Label the Peaks

Label the Peaks displays the retention time and area of each peak. (See Figure 13-36.)

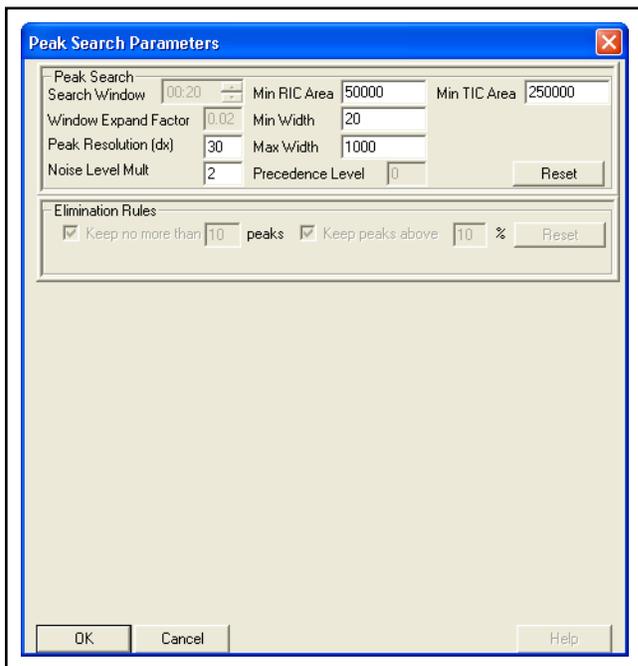
Figure 13-36 Label the peaks



13.7.5.6 Change Search Parameters

Change Search Parameters displays the **Peak Search Parameters** window and allows for modification of the peak resolution, noise level multiplier, minimum peak width for identification, maximum peak width for identification, minimum TIC and RIC (area). (See Figure 13-37.)

Figure 13-37 Peak Search Parameters window

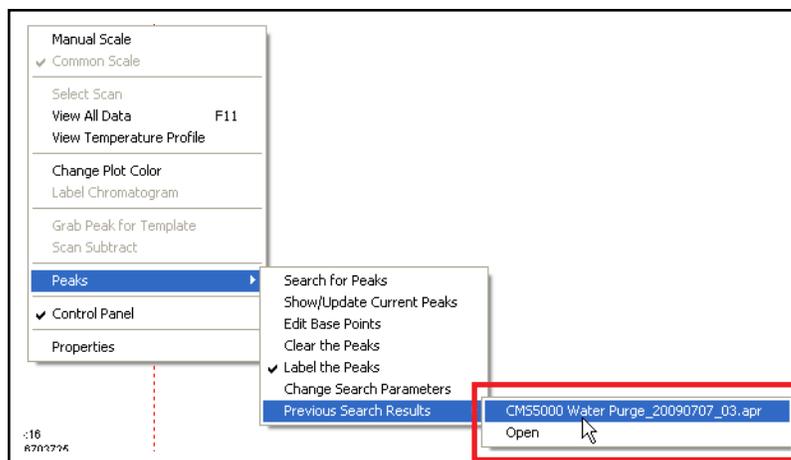


13.7.5.7 Previous Search Results

Previous Search Results accesses results from a previously saved search.

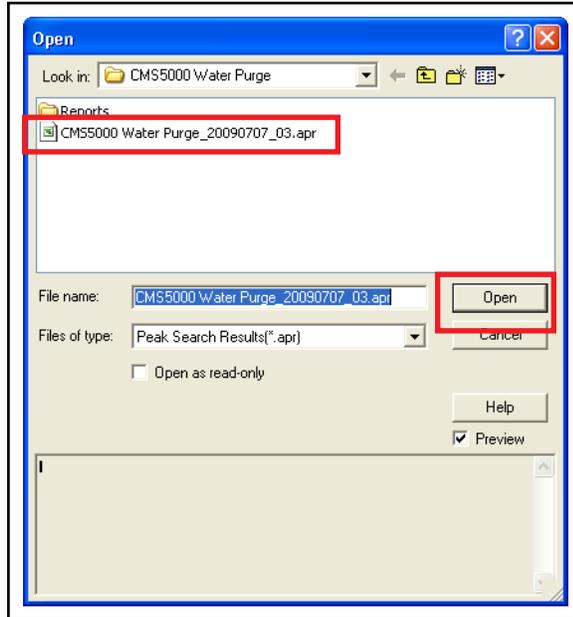
- 1 Right-click the in chromatogram window and select **Peaks >> Previous Search Results**. A new submenu will be displayed. (See Figure 13-38.)

Figure 13-38 Previous Search Results



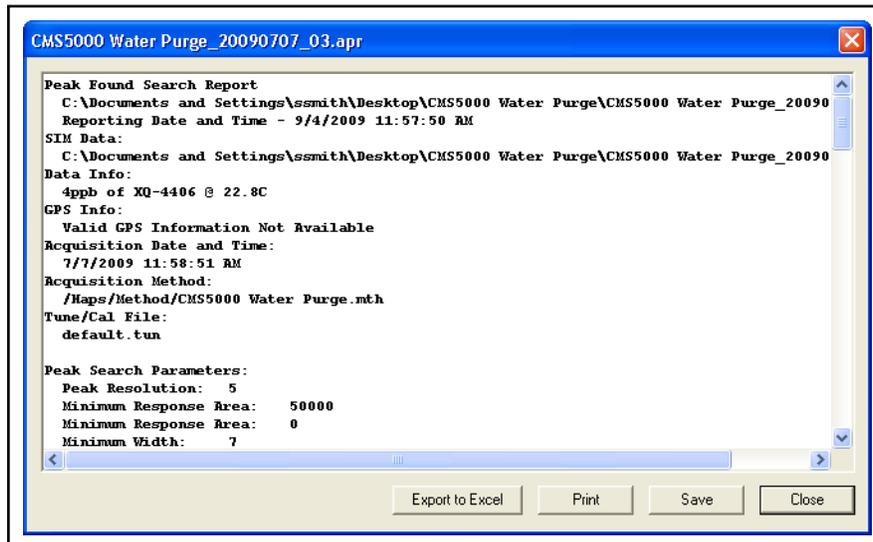
- 2 Recently saved searches are displayed. The last selection is **Open**.
- 3 From the submenu, select **Open** to display the **Open** window.
(See Figure 13-39.)

Figure 13-39 Open window



- 4 Select the desired file in the **Open** window and click **Open** to display the saved report. (See Figure 13-40.)

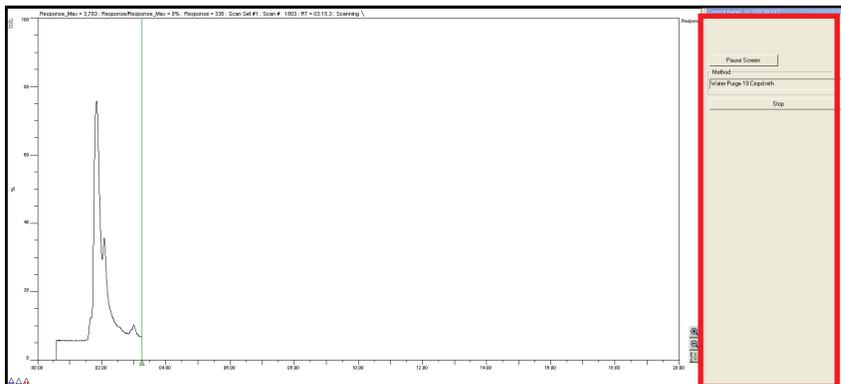
Figure 13-40 Saved report



13.7.6 Control Panel

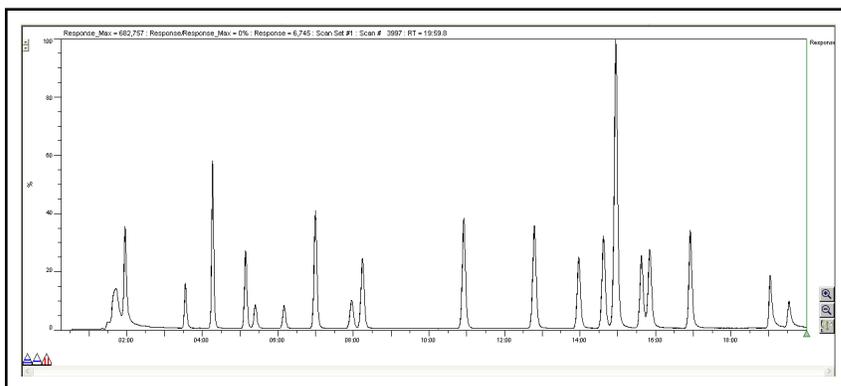
Select **Control Panel** to display the Control Panel on the **Data Review** window. (See Figure 13-41.) The Control Panel display is the default setting.

Figure 13-41 Window with control panel



Clear **Control Panel** to remove the Control Panel from the **Data Review** window. (See Figure 13-42.)

Figure 13-42 Window without control panel

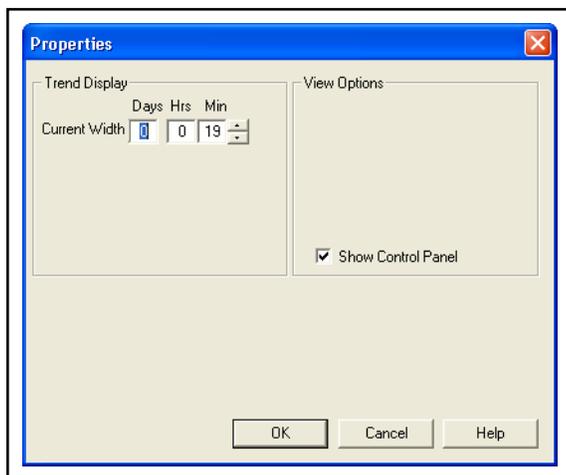


The **Control Panel** sidebar contains the name of the method used to create the data file. Click **Pause Screen** to temporarily cease data plotting on the computer. When the **Pause Screen** is clicked again, all collected data will be plotted and CMS IQ will continue to plot data in near real time. **Pause Screen** does not interrupt actual data collection. (Refer to Figure 13-41.)

13.7.7 Properties

Properties displays data review settings. On the top left hand side, the current width of the data file, in terms of time, is displayed. The **Show Control Panel** option is identical in function to the **Control Panel** option in the chromatogram window context menu. (See Figure 13-43.) Click **OK** to close **Properties** and save changes.

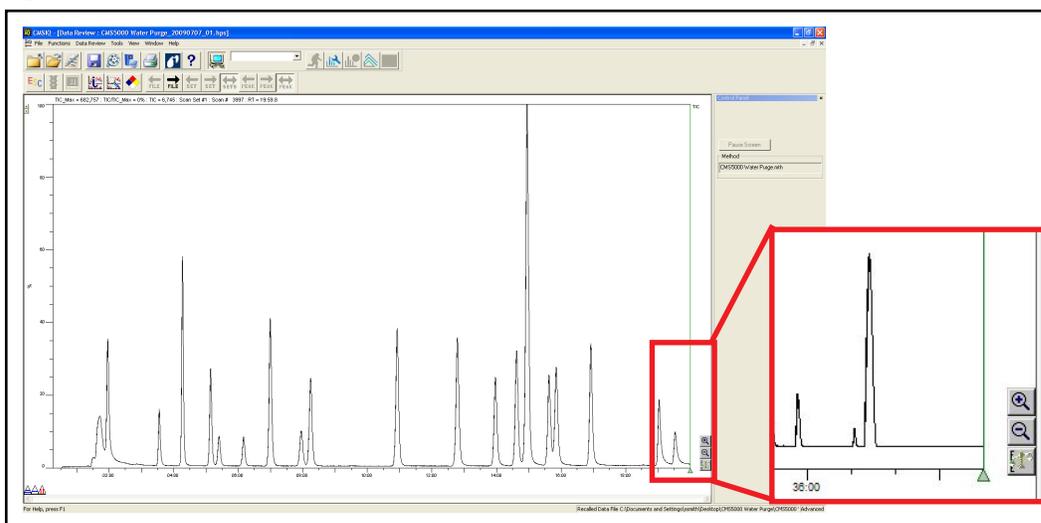
Figure 13-43 Properties window



13.8 How to Access the Scan Cursor

CMS5000 takes a data point every tenth of a second. The individual data points are referred to as scans. A specific scan is accessed using the **Scan Cursor** in the chromatogram window. The **Scan Cursor** is the green triangle with the vertical line located at the bottom right hand side of the window. (See Figure 13-44.) Moving the **Scan Cursor** to a specific scan will display the overall maximum Response, Response/Response Max (displayed as a percentage), scan Response, Scan #, and retention time of the scan.

Figure 13-44 Location of the Scan Cursor



The **Scan Cursor** can be moved to the desired location by:

- ◆ Clicking the Scan Cursor icon and dragging the icon to the scan of interest
- ◆ Double-clicking the left mouse button over the scan of interest
- ◆ Hovering the mouse over the vertical green line then clicking the left mouse button and dragging the **Scan Cursor** to the scan of interest
- ◆ Using the left and right arrow keys on the computer

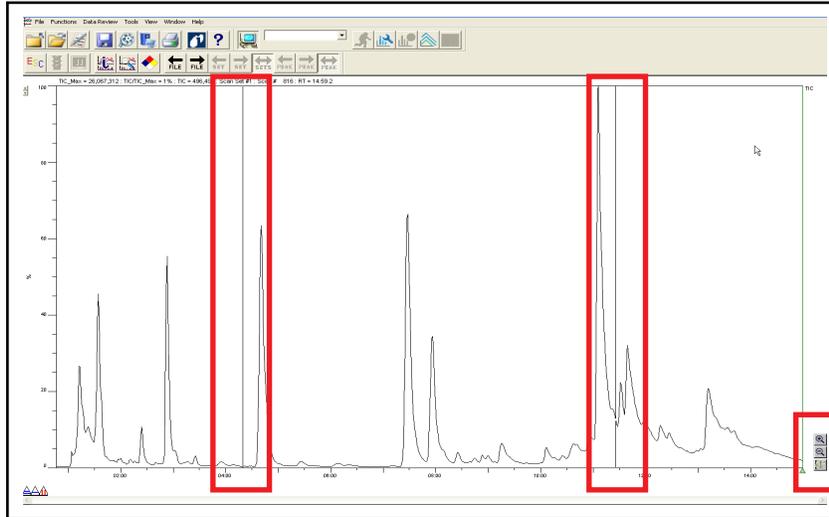
NOTE: To use the arrow keys first click in the chromatogram window to highlight it. A black outline will appear around the chromatogram.

13.9 Using the Zoom Function

The **Zoom** function expands the view of a particular section of the chromatogram. There are two ways to zoom in on a Chromatogram:

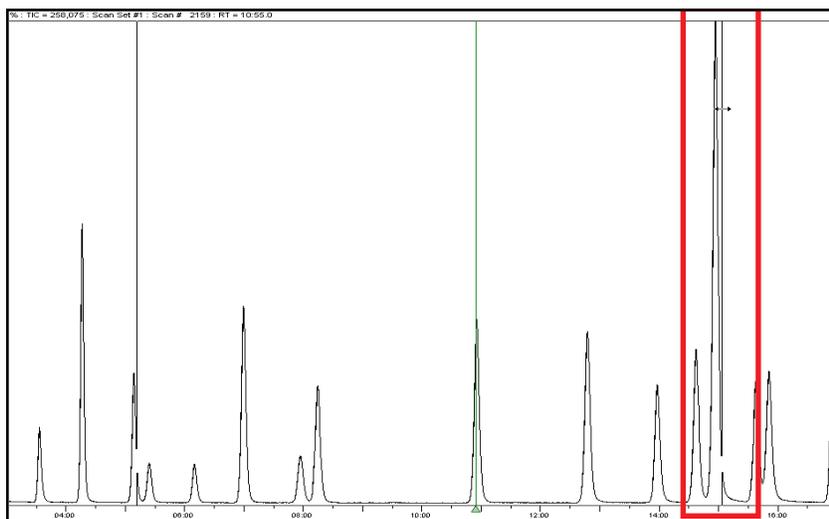
- 1 Click **Zoom In** .
- 2 Two vertical black lines will appear on the chromatogram. (See Figure 13-45.)

Figure 13-45 Zoom



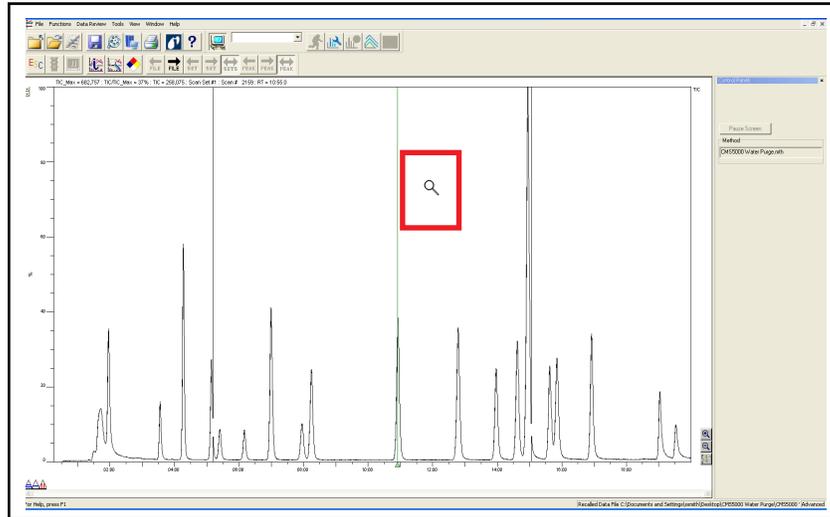
- 3 Hover the mouse over a vertical line and a double sided horizontal arrow will appear. Press and hold the left mouse button, drag the black vertical line to the desired position, and release. Repeat this process with the other vertical line. (See Figure 13-46.)

Figure 13-46 Selecting area to zoom



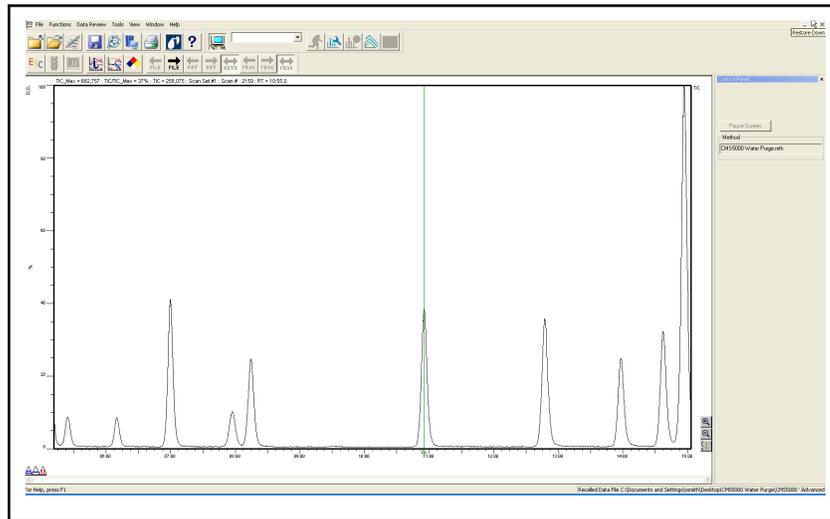
- 4 Move the cursor in between the two black vertical lines and a magnifying glass will be displayed. (See Figure 13-47.)

Figure 13-47 Magnifying glass



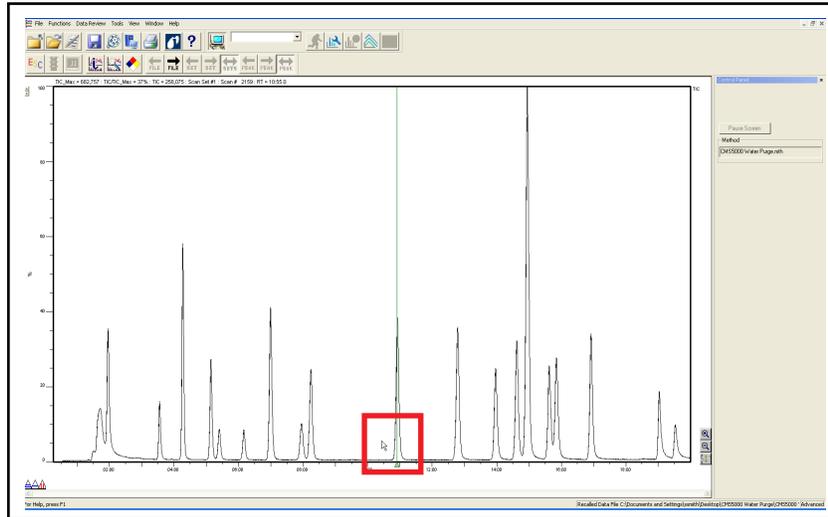
- 5 Click when the magnifying glass is displayed to zoom in on the selected area. (See Figure 13-48.)

Figure 13-48 Area zoom



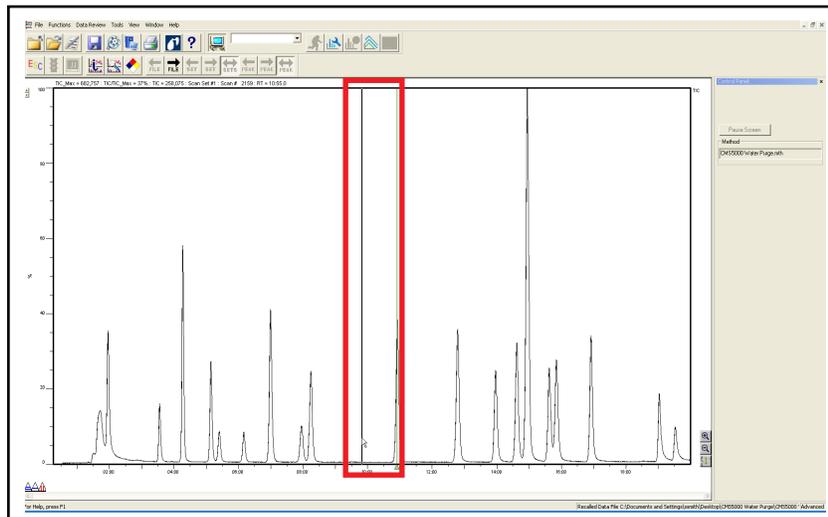
- 6 Alternately, press and hold the left mouse button at the desired starting point. (See Figure 13-49.)

Figure 13-49 Zoom start



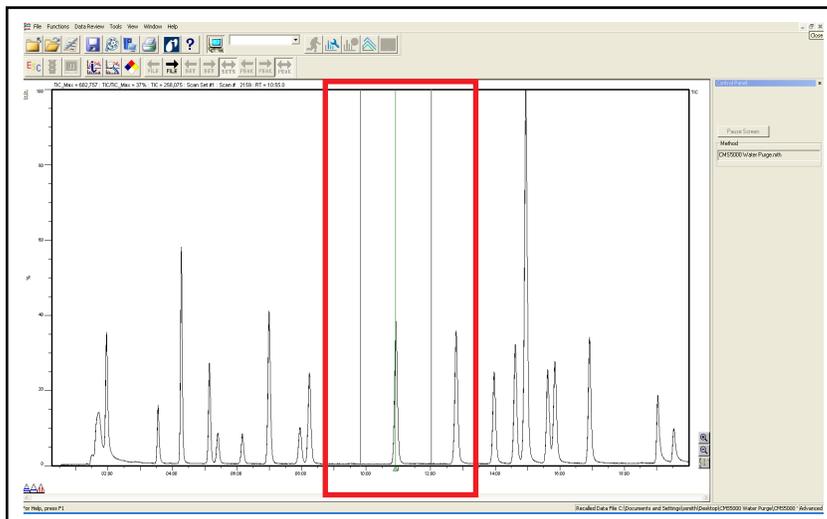
- 7 As the cursor is dragged, a vertical line will be displayed. (See Figure 13-50.)

Figure 13-50 Vertical line



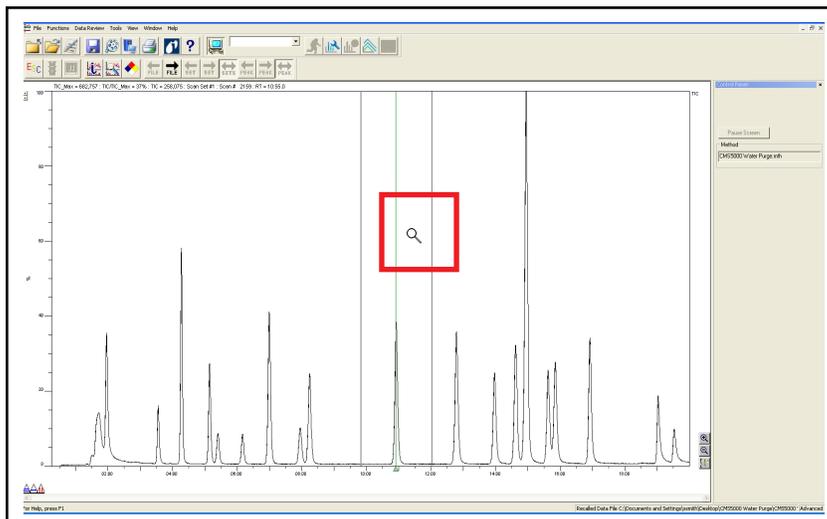
- 8 Drag the cursor to the desired zoom ending point and release the mouse button. (See Figure 13-51.)

Figure 13-51 Zoom end



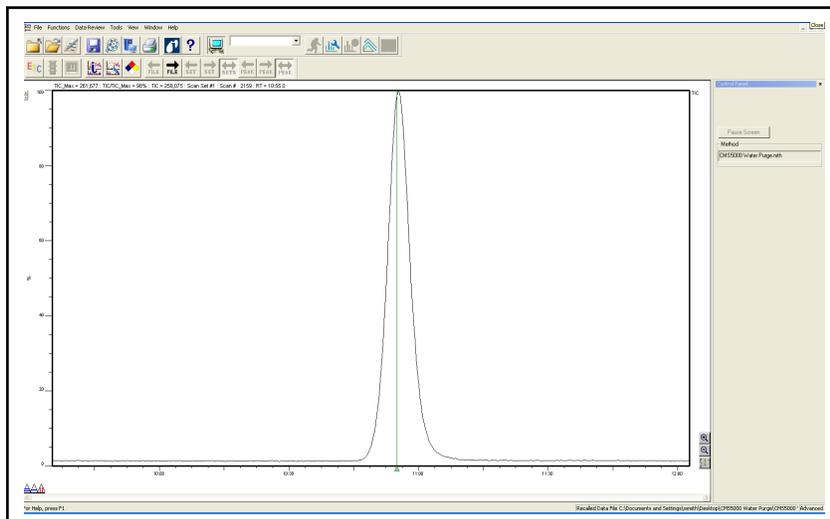
- 9 Move the cursor in between the two black vertical lines and a magnifying glass will be displayed. (See Figure 13-52.)

Figure 13-52 Magnifying glass



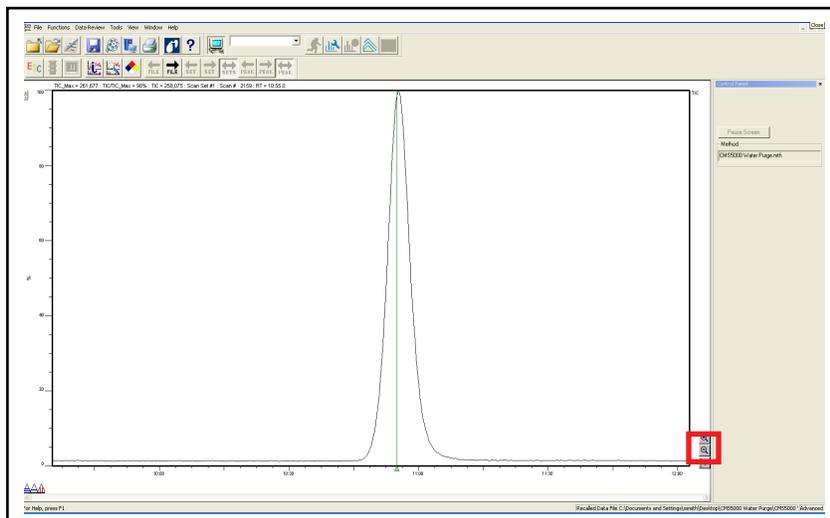
- Click when the magnifying glass is displayed to zoom in on the selected area. (See Figure 13-53.)

Figure 13-53 Area Zoom



- To return to the full chromatogram, click **Zoom Out** . (See Figure 13-54.) Alternately, press **F11** on the computer keyboard.

Figure 13-54 Zoom out

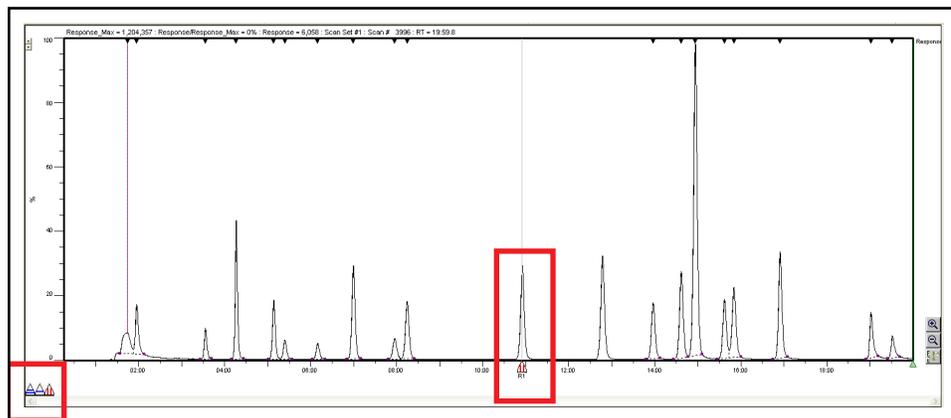


13.10 Range Tool

The **Range Tool**  is used to reintegrate peaks and adjust the scan range.

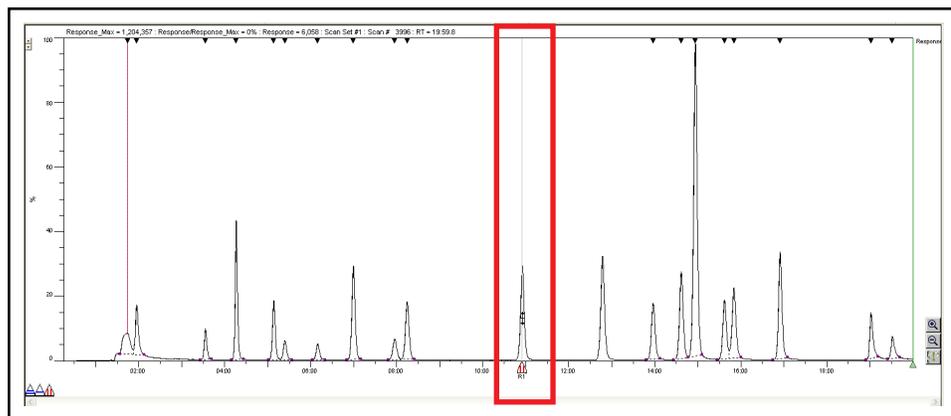
- 1 Use the **Range Tool** to determine the scan range. The **Range Tool** is a triangle with two red vertical lines which is located at the bottom left hand side of the window.
- 2 Click and drag the range tool underneath the x-axis until it is aligned with the desired peak apex. (See Figure 13-55.)

Figure 13-55 Positioning range tool



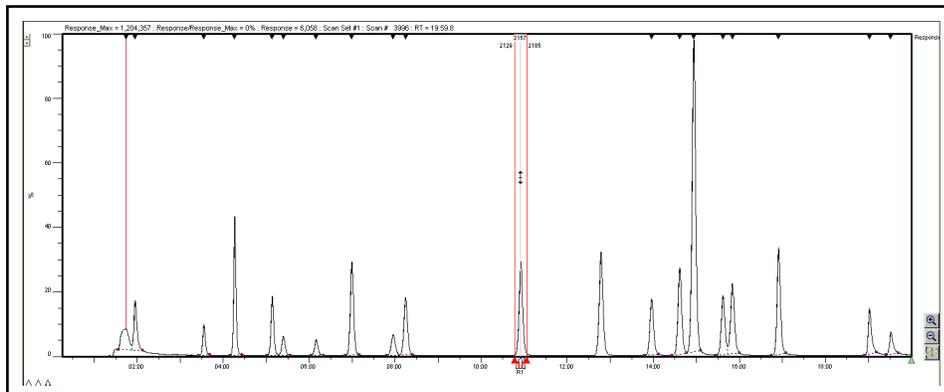
- 3 Position the cursor on the gray line that appears above the **Range Tool**. A double-sided horizontal arrow will appear. (See Figure 13-56.)

Figure 13-56 Range arrow



- 4 To set the scan range, press and hold the left mouse button, then drag up. Two red triangles at the bottom of the window with red vertical lines will be displayed. The red lines set the scan range limits. Release the left mouse button when the red lines cover the desired scan range. (See Figure 13-57)
 - ◆ Adjust the red lines by hovering the cursor over either red triangle and a double-sided horizontal arrow will appear. Press and hold the left mouse button to drag the red vertical line to the desired location.

Figure 13-57 Positioning the red lines



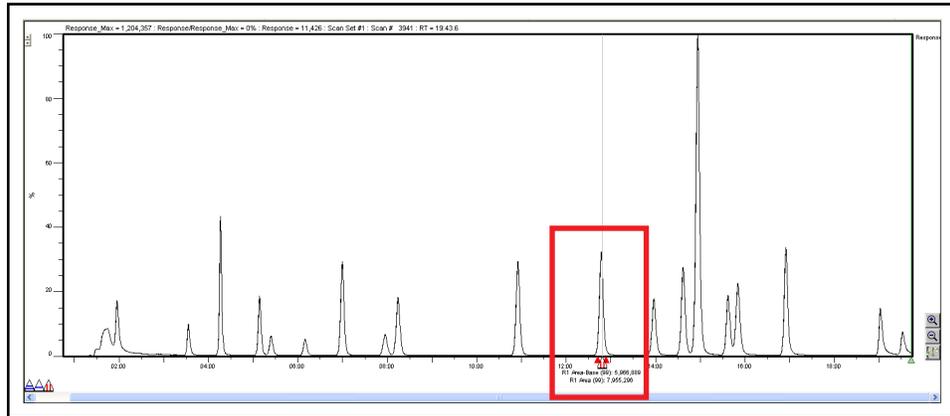
- 5 Right-click on the range tool to provide the following menu options. (See Figure 13-58.)

Figure 13-58 Range tool menu



- Remove** Removes the range cursor
- Remove All** Removes the range cursor, retention time, and area labels
- Show Integration** Displays the integration on the x-axis (See Figure 13-59.)

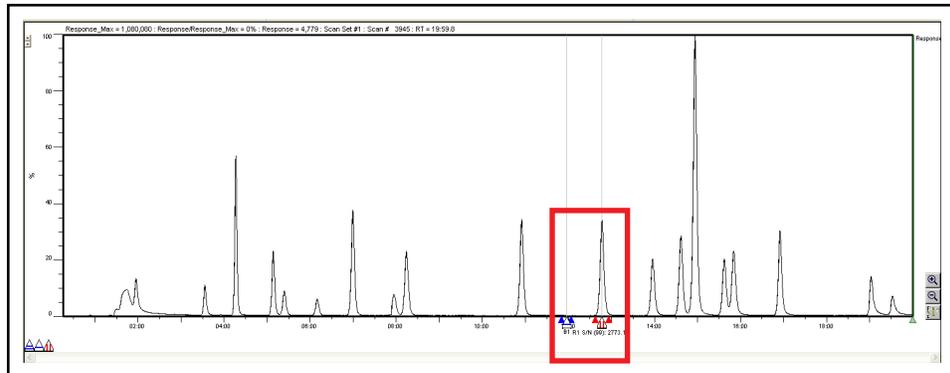
Figure 13-59 Show integration



Show Signal/Noise Shows the signal to noise ratio

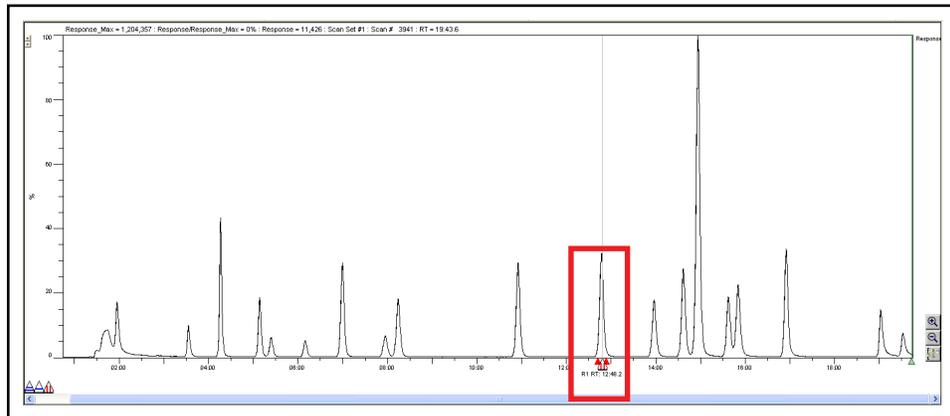
NOTE: A background must be selected before selecting **Show Signal/Noise**.
See section 13.10.1, **Background Tools**, on page 13-37.
(See Figure 13-60.)

Figure 13-60 Show signal to noise



Show Retention Time Displays the retention time on the x-axis
(See Figure 13-61.)

Figure 13-61 Show retention time

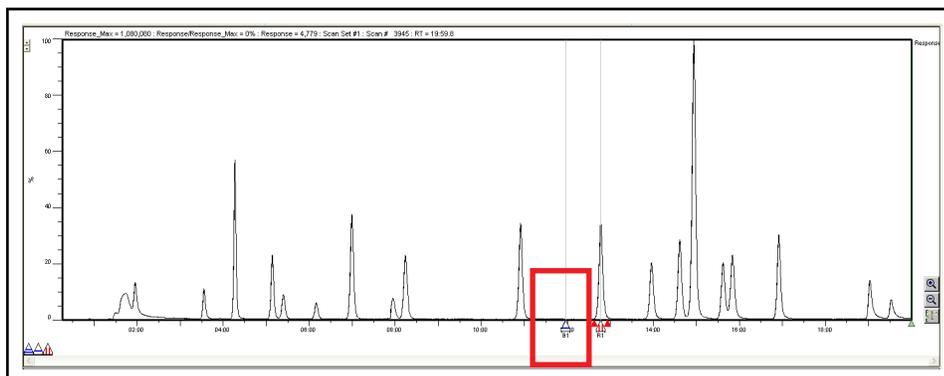


13.10.1 Background Tools

Background Tools  are used to calculate signal to noise parameters. Two separate background ranges can be selected from the chromatogram. To select a background, follow the instructions below.

- 1 Use **Background Tools** to determine the background range. **Background Tools** are located in the bottom left hand side of the window.
- 2 Press and hold the left mouse button, then drag one of the blue triangles to a baseline region preceding a peak. (See Figure 13-62.)

Figure 13-62 Positioning Background Tool

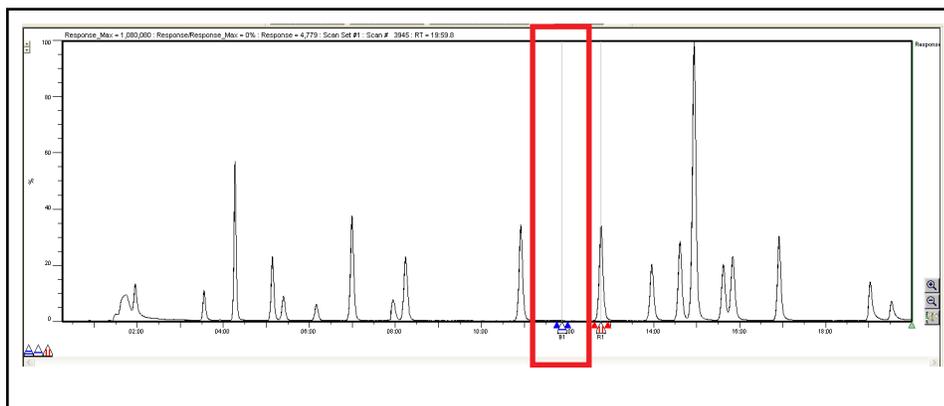


- 3 Position the cursor on the gray line that appears above the **Background Tool** and a double-sided horizontal arrow will appear.

To set the background range, press and hold the left mouse button, then drag up. Two blue triangles at the bottom of the window with blue vertical lines will be displayed. Release the left mouse button when the blue lines cover the desired background range. These blue lines set the background range limits.

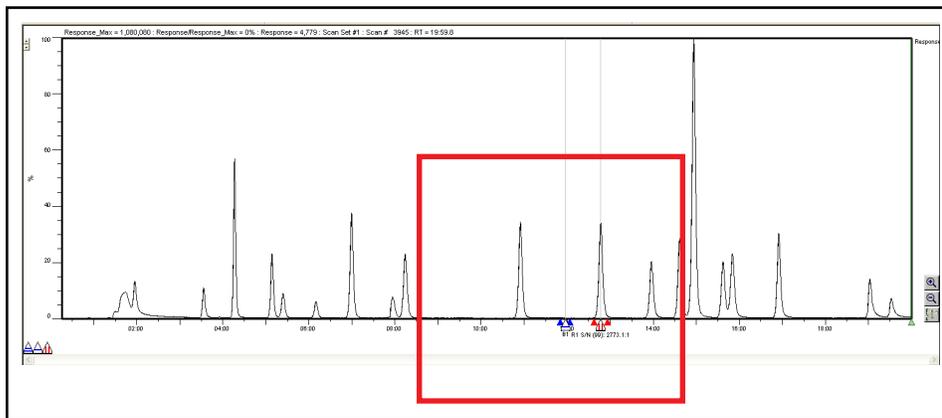
Adjust the blue lines by hovering the cursor over either blue triangle and a double-sided horizontal arrow will appear. Press and hold the left mouse button to drag the blue triangle and blue vertical line to the desired location. (See Figure 13-63.)

Figure 13-63 Positioning blue lines



- To display signal to noise values, click **Show Signal/Noise** in the **Range Tool** menu. (See Figure 13-64.)

Figure 13-64 Show signal/noise



- Right-click **Background Tool** to display the following menu. (See Figure 13-65.)

Figure 13-65 Background Tool Menu



- Remove** Removes the background cursor
- Show Integration** Same as Show Integration on the Range Tool. Refer to section 13.10, Range Tool, on page 13-34
- Show Retention Time** Same as Show Retention Time on the Range Tool. Refer to section 13.10, Range Tool, on page 13-34

Chapter 14

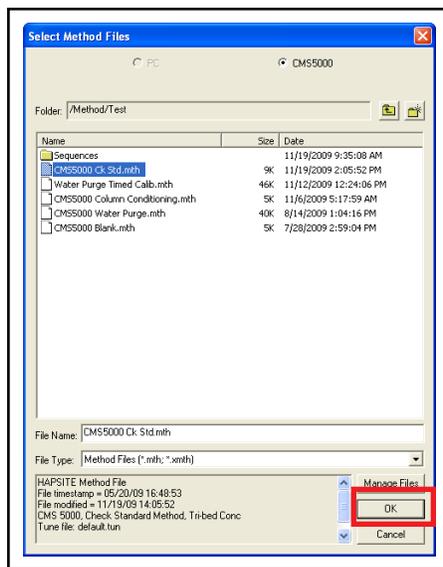
Run Method

14.1 Run Method Procedure

CMS5000 can be operated from a computer using CMS IQ. To run a method, use the following procedure.

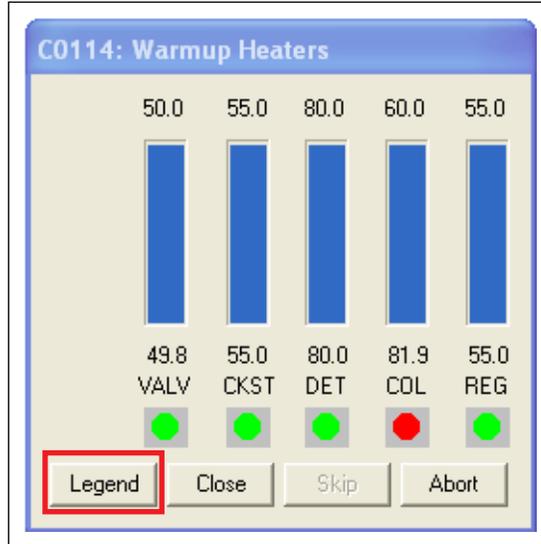
- 1 Double-click the **CMS IQ** icon  to open CMS IQ software.
- 2 Double-click the **Run Method** icon .
- 3 Select the desired method file (e.g., **Water Purge 19 Cmpd**) and click **OK**. (See Figure 14-1.)

Figure 14-1 Select method to run



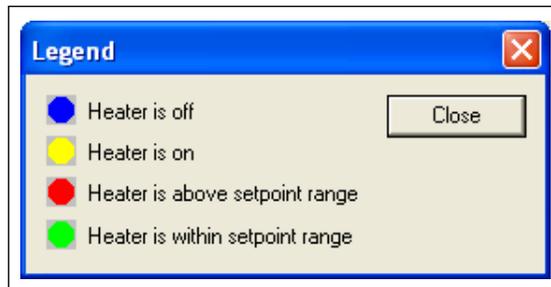
- 3a** The heated components of CMS5000 must reach their initial set points before the method will begin. The **Warmup Heaters** window will appear if the components are not within range. (See Figure 14-2.)

Figure 14-2 Heater status grid



NOTE: Click the **Legend** button to explain what the colors under each component represent. (See Figure 14-3.)

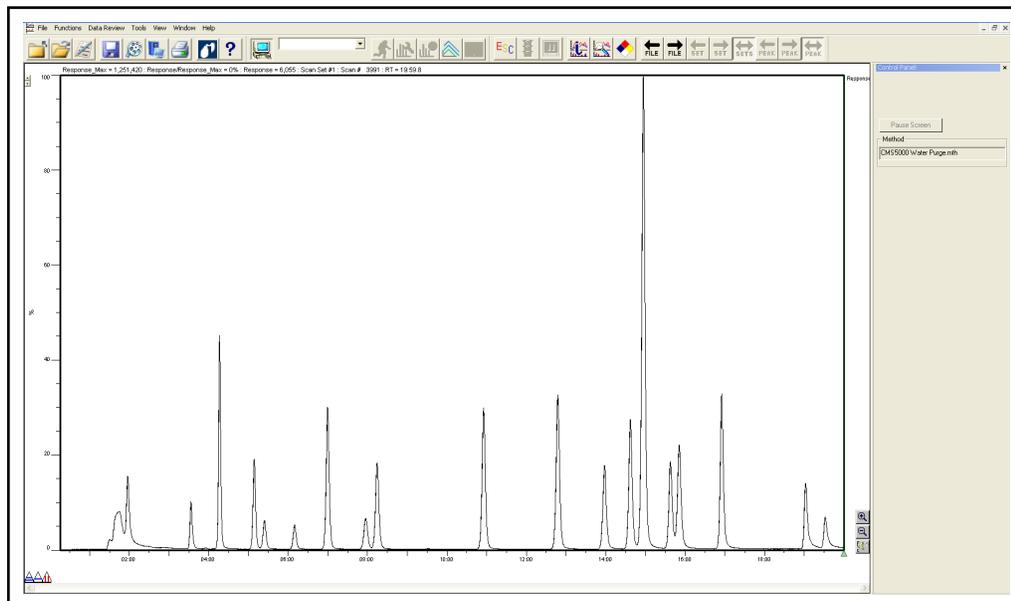
Figure 14-3 Legend



- 3b** When CMS5000 setpoints have been reached, the method will start running automatically.

- 4 Data will be displayed on the computer as the method is running. An example of a finished chromatogram is shown in Figure 14-4.

Figure 14-4 Example of finished sample run



Chapter 15

Chromatogram Overlay

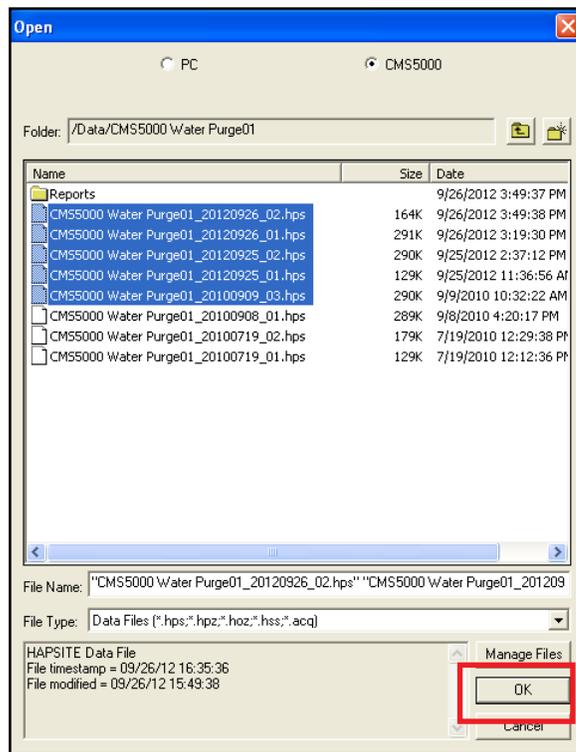
15.1 Introduction

Chromatogram Overlay allows multiple data files to be displayed in the same data review window.

15.2 Chromatogram Overlay

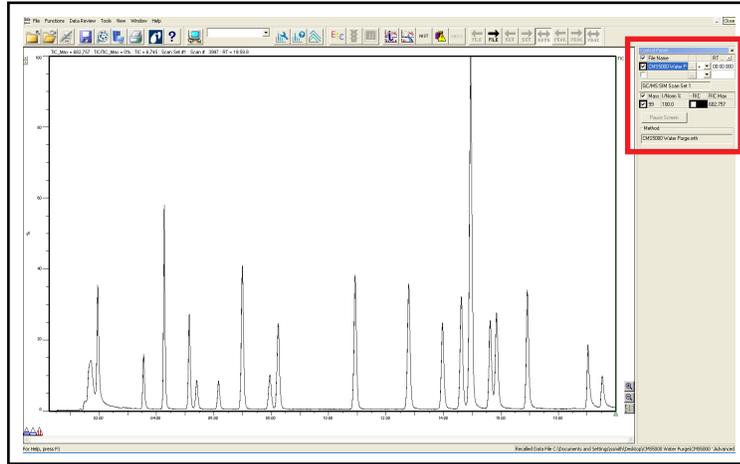
- 1 Click **Chromatogram Overlay** .
 - 2 Select one or more of the desired data files and click **Open**. (See Figure 15-1.)
- HINT:** Multiple data files can be selected by holding down the **Ctrl** key while clicking on additional data files. A range of data files can be selected by holding down the **Shift** key and selecting the first and last data file in the desired range.

Figure 15-1 Selecting data files



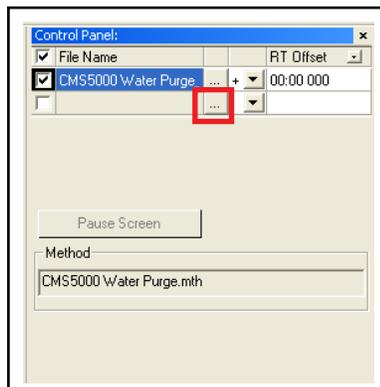
- The selected data file(s) are displayed in the **Data Review** window. The filename(s) will also be displayed under the **Filename** pane in the Control Panel. (See Figure 15-2.)

Figure 15-2 Data file in control panel



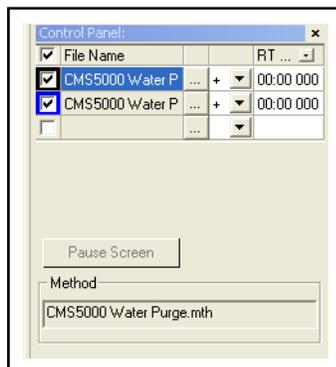
- Click **Browse (...)** in the row below the data file. (See Figure 15-3.)

Figure 15-3 Selecting another data file



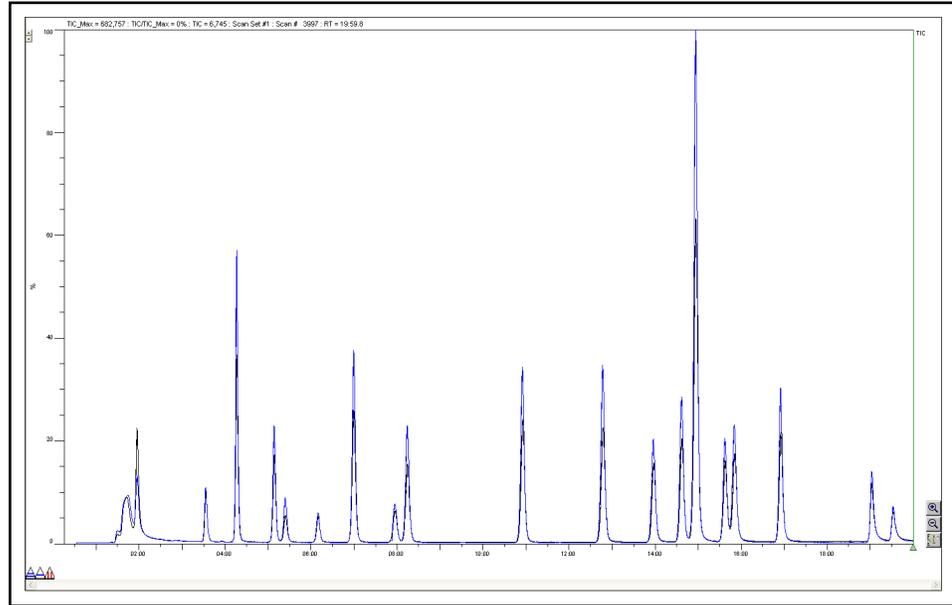
- Select one or more of the desired data files and click **Open**. The additional data file(s) will appear below. (See Figure 15-4.)

Figure 15-4 Second data file



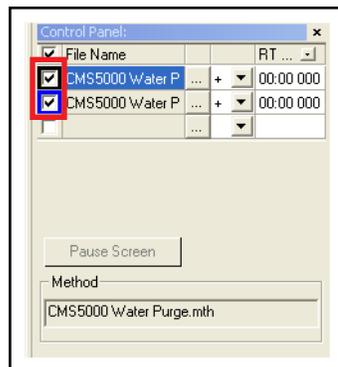
- 6 All selected chromatograms will appear in the **Data Review** window. Each data file displayed in the **Control Panel** will be plotted in the corresponding color of the checkbox located to the left of the file name. (See Figure 15-5.)

Figure 15-5 Chromatograms overlaid



- 7 To select or deselect data files to be plotted, select or clear the checkbox next to the file name in the **Control Panel**. (See Figure 15-6.)

Figure 15-6 Chromatogram selection

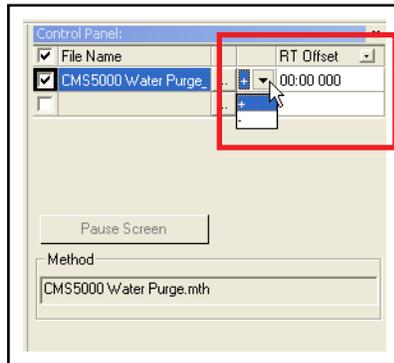


15.3 Retention Time Shift

The retention time of a specific compound may vary between data files. Shifting the retention times of one data file will align the peaks to allow for further comparison.

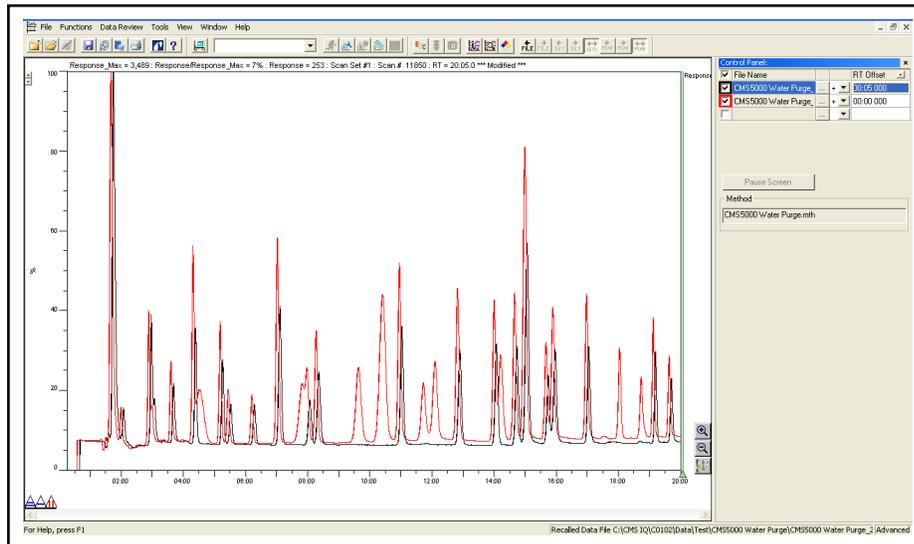
- 1 Follow steps 1-6 in section 15.2, Chromatogram Overlay, on page 15-1 to select the desired data files.
- 2 Shift the chromatogram by selecting **+** to shift the chromatogram forward, or **-** to shift the chromatogram backwards. Enter the desired amount of time under **RT Offset** for the chromatogram to shift. (See Figure 15-7.)

Figure 15-7 Shifting retention time



- 3 When the desired retention time shift has been entered, press **Enter**.
- 4 The shifted chromatogram will be displayed. (See Figure 15-8.)

Figure 15-8 Shifted chromatogram



15.4 Chromatogram Subtract

Chromatogram Subtract subtracts the peak area of one data file from the peak area of a second data file.

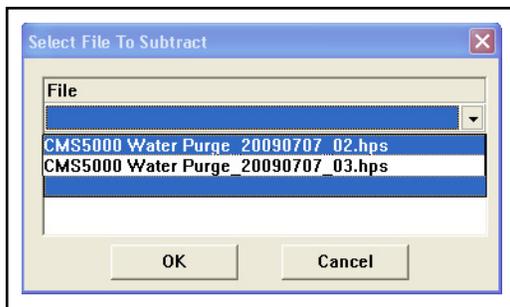
- 1 Follow steps 1-6 in section 15.2, Chromatogram Overlay, on page 15-1.
- 2 Right-click in the chromatogram and select **Select Chro To Subtract**. (See Figure 15-9.)

Figure 15-9 Select Chro To Subtract



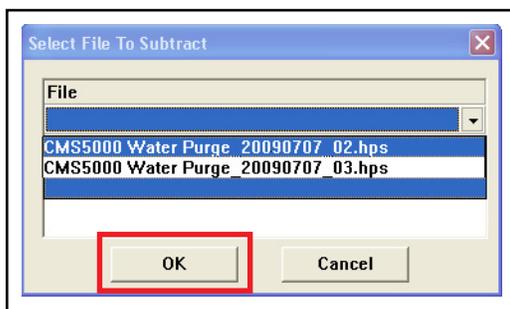
- 3 The **Select File To Subtract** window is displayed. (See Figure 15-10.)

Figure 15-10 Select File To Subtract window



- 4 Select the desired file to subtract in the shortcut menu. Click **OK**. (See Figure 15-11.)

Figure 15-11 Chromatogram selection



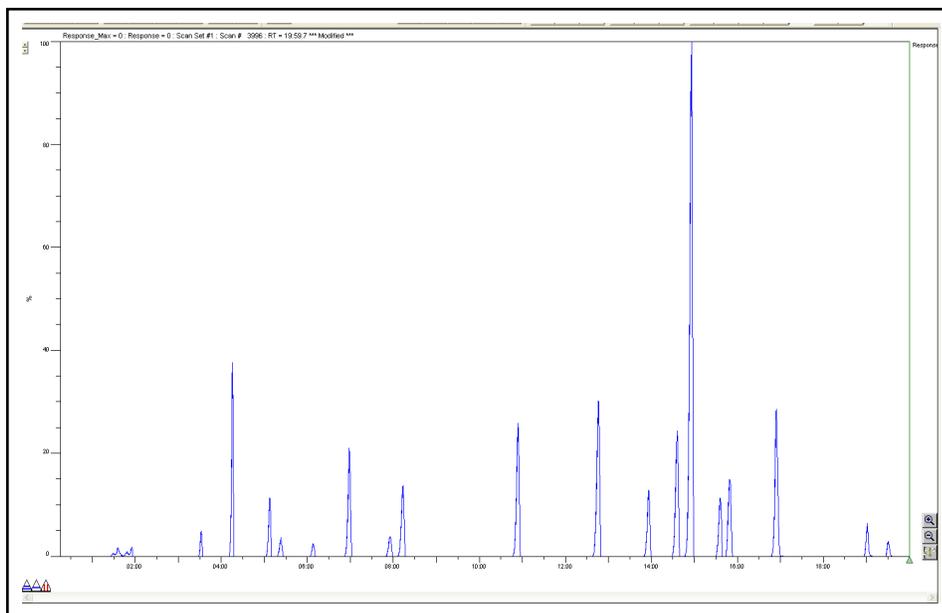
- 5 Right-click in the chromatogram and select **Chro Subtract**.
(See Figure 15-12.)

Figure 15-12 Chro Subtract



- 6 The selected data file is subtracted from the first data file. (See Figure 15-13.)

Figure 15-13 Subtracted chromatogram from Figure 15-5



Chapter 16

Method Editor

16.1 The Method Editor



CAUTION

Only trained personnel should edit or create methods. Changing parameters may adversely affect analytical data.

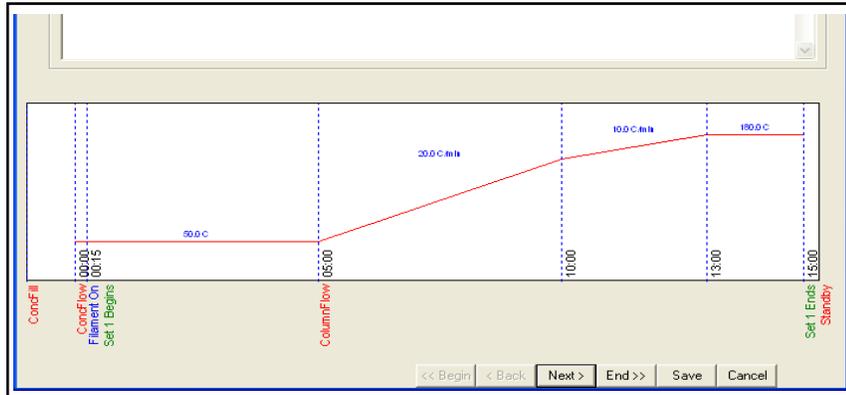
NOTE: Creating or editing methods is an **Advanced** user function. Refer to section 12.2.6.4.1, Changing Access Levels, on page 12-29.

Method Editor creates methods to identify and quantify volatile organic compounds. **Method Editor** is composed of the following screens:

| | |
|----------------------------------|--|
| Description | A description of the method |
| Startup | Selects the type of method to be created: Air, Water, or Ck Std Select Temperature settings |
| Inlet | Defines the temperatures, timing, inlet, and valve states |
| Scan Properties | Unavailable |
| Search | Designates the calibration library for the method. Also sets the Library Search Parameters |
| Data | Sets the Data File (.hps) component and specifies where the data will be stored. By default, the data file pathway uses the pathway of CMS5000IQ\data\method name\file name.file extension, e.g., C:\CMS5000IQ\data\Method01\filename.hps |
| Summary | Review and print the method parameters |

At the bottom of each screen of the **Method Editor**, the **Inlet States** and **Temperature** profile sequences are displayed. (See Figure 16-1.)

Figure 16-1 Method profile



Newly created methods start with a default set of **Inlet States** and a default **Temperature Profile**, which can be modified as required by the application.

16.2 Wizard Mode

Method Editor can be run in **Wizard Mode**, which moves through the method creation windows in a logical sequence and is recommended for new users. Adjustments can be made using the **<Back** and **Next >** buttons. Figure 16-2 shows the **Wizard Mode** navigation buttons.

Figure 16-2 Wizard mode method editor navigation buttons



All screens are available when **Wizard Mode** is not selected. Refer to section 12.2.5.3, Miscellaneous, on page 12-20 for instructions on selecting **Wizard Mode**.

NOTE: The **Method Editor** must be reopened to initiate the selected mode. (See Figure 16-3.)

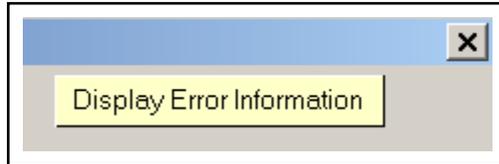
Figure 16-3 System properties miscellaneous tab wizard setting



All method parameters on each screen of the **Method Editor** are checked for synchronization and correctness. When a discrepancy occurs, **Method Editor** will highlight all questionable parameters and the **Display Error Information** button in yellow. (See Figure 16-4.)

NOTE: The **Method Editor** permits movement from screen to screen, even when errors are present.

Figure 16-4 Error information button



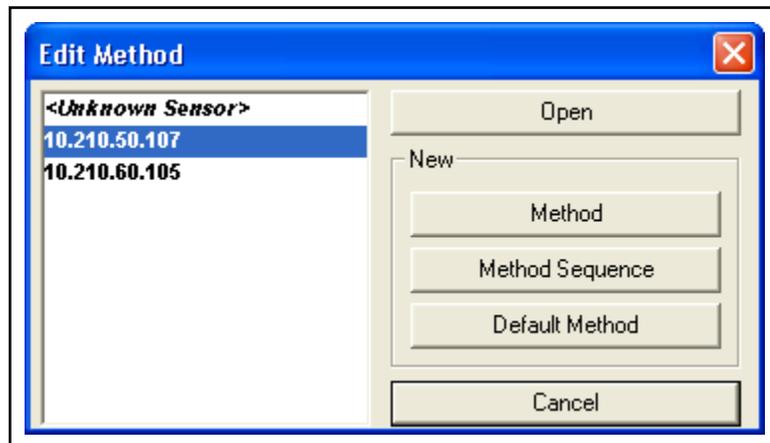
16.3 Accessing Method Editor



- 1 On the **System Setup** window, double-click **Method Editor**.
- 2 Select the CMS5000 name (CXXXX) or IP address associated with CMS5000 to which the method will be applied. (See Figure 16-5.)

NOTE: If only one CMS5000 is being used, it will be selected by default.

Figure 16-5 CMS5000 Selection



There are five options in **Method Editor**:

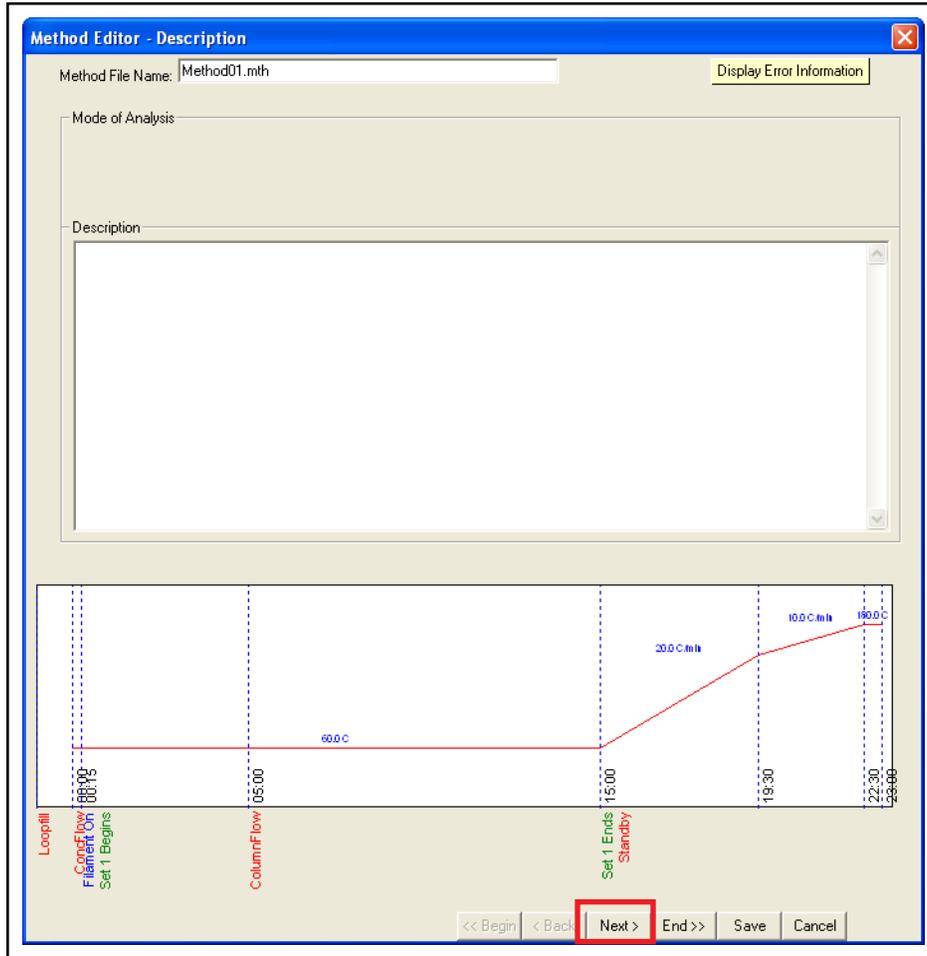
- Open** Opens an existing CMS5000 method for modification
- Method** Opens a blank method template to modify as necessary
- Method Sequence** Allows methods to be sequenced and run automatically
- Default Method** Selects a default method
- Cancel** Closes the Edit Method window

16.4 Description Screen

A description of the method and the method name are entered into the **Description** window. (See Figure 16-6.) To continue to the next section, click **Next >**.

NOTE: A method file ends with a file extension of *.mth.

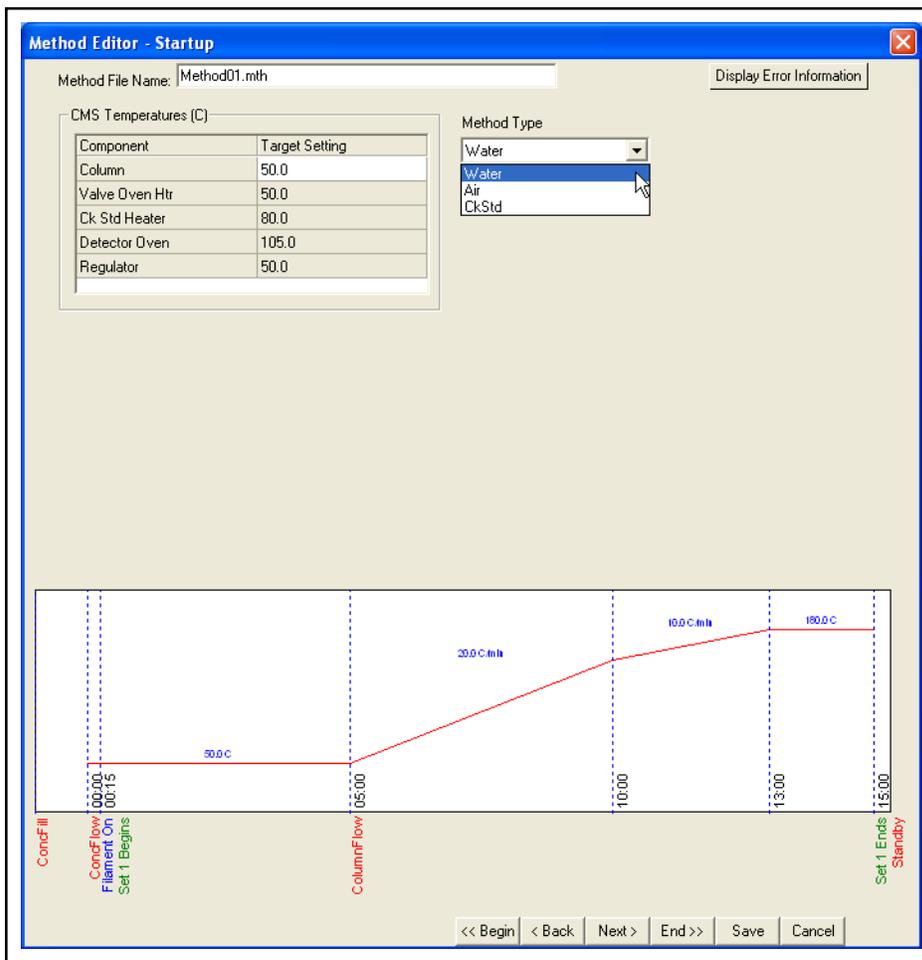
Figure 16-6 Method Editor - Description window



16.5 Startup

The **Startup** screen, shown in Figure 16-7, displays the initial settings for CMS5000 heaters. The initial temperature settings for the components described in section 16.5.1, CMS5000 Temperatures (°C), on page 16-6 are modified on this screen. The **Method Type (Air, Water, or Ck Std)** are selected on this screen.

Figure 16-7 Method Editor - Startup window



16.5.1 CMS5000 Temperatures (°C)

The following heated components must reach their set points before data acquisition can begin:

- Column** Initial target Column temperature for the method
- Valve Oven Htr** Target Valve Oven Heater temperature
- Ck Std Heater** Target Check Standard Heater temperature
- Detector Oven** Target Micro Argon Ionization Detector (MAID) temperature
- Regulator** Target Regulator temperature, which controls the column head pressure

16.5.2 Method Type Selection

- Water** Sets method parameters for water sampling
- Air** Sets method parameters for air sampling
- Ck Std** Sets method parameters for a Check Standard (toluene) method

NOTE: In the following sections, the **Method Type** is set to **Water**.

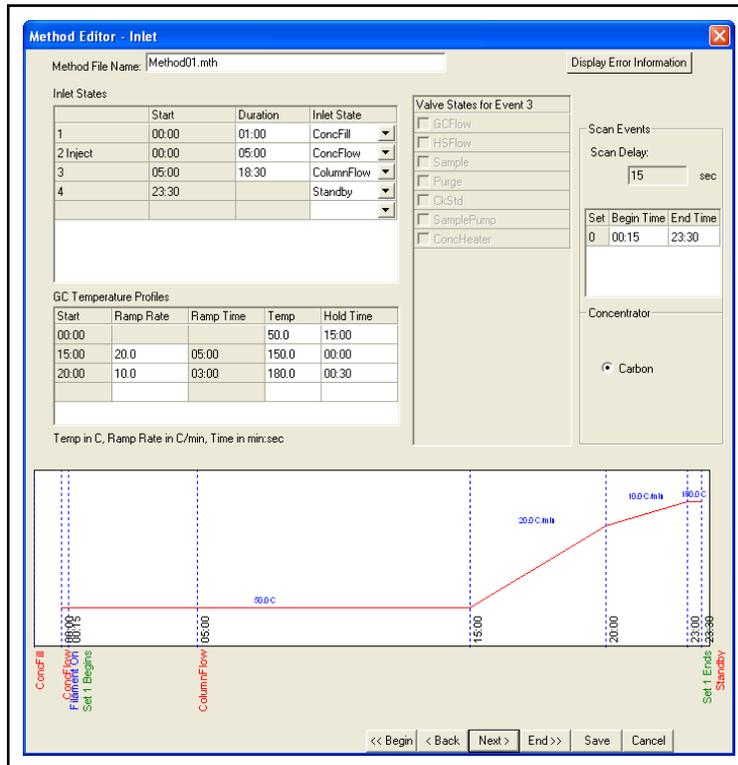
16.6 Inlet

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

NOTE: Adjusting settings on the **Inlet** screen may affect other method parameters and/or 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. (See Figure 16-8.)

Figure 16-8 Method Editor - Inlet window



16.6.1 Inlet States

Inlet States control CMS5000 valve settings for sampling, analysis, and purging. Figure 16-9 shows the grid used to program the inlet states.

Figure 16-9 Inlet States

| Inlet States | | | |
|--------------|-------|----------|-------------|
| | Start | Duration | Inlet State |
| 1 | 00:00 | 01:00 | ConcFill |
| 2 Inject | 00:00 | 05:00 | ConcFlow |
| 3 | 05:00 | 18:30 | ColumnFlow |
| 4 | 23:30 | | Standby |
| | | | |

| GC Temperature Profiles | | | | |
|-------------------------|-----------|-----------|-------|-----------|
| Start | Ramp Rate | Ramp Time | Temp | Hold Time |
| 00:00 | | | 50.0 | 15:00 |
| 15:00 | 20.0 | 05:00 | 150.0 | 00:00 |
| 20:00 | 10.0 | 03:00 | 180.0 | 00:30 |
| | | | | |

Temp in C, Ramp Rate in C/min, Time in min:sec

To edit the **Inlet State** grid, select an inlet state from the shortcut menu. (See Figure 16-10.)

Figure 16-10 Inlet State menu

| Water Method | Air Method | Ck Std Method | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|--|--------------|---------------|----------------|--|--|-------|----------|-------------|---|-------|-------|----------|----------|-------|-------|----------|---|-------|-------|------------|---|-------|--|---------|--|--------------|--|--|--|--|-------|----------|-------------|---|-------|-------|----------|---|-------|-------|--------------|---|-------|-------|-------------|---|-------|-------|--------|---|-------|-------|----------|----------|-------|-------|----------|---|-------|-------|----------|---|-------|-------|-------|--|--|--|---------|--|--------------|--|--|--|--|-------|----------|-------------|---|-------|-------|----------|----------|-------|-------|----------------|---|-------|-------|---------------|---|-------|--|-----------|--|--|--|--------|--|--|--|----------|--|--|--|------------|--|--|--|----------|--|--|--|----------|--|--|--|-------|--|--|--|---------|
| <table border="1"> <thead> <tr> <th colspan="4">Inlet States</th> </tr> <tr> <th></th> <th>Start</th> <th>Duration</th> <th>Inlet State</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>00:00</td> <td>01:00</td> <td>ConcFill</td> </tr> <tr> <td>2 Inject</td> <td>00:00</td> <td>05:00</td> <td>ConcFlow</td> </tr> <tr> <td>3</td> <td>05:00</td> <td>10:00</td> <td>ColumnFlow</td> </tr> <tr> <td>4</td> <td>15:00</td> <td></td> <td>Standby</td> </tr> </tbody> </table> | Inlet States | | | | | Start | Duration | Inlet State | 1 | 00:00 | 01:00 | ConcFill | 2 Inject | 00:00 | 05:00 | ConcFlow | 3 | 05:00 | 10:00 | ColumnFlow | 4 | 15:00 | | Standby | <table border="1"> <thead> <tr> <th colspan="4">Inlet States</th> </tr> <tr> <th></th> <th>Start</th> <th>Duration</th> <th>Inlet State</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>00:00</td> <td>00:05</td> <td>HSCreate</td> </tr> <tr> <td>2</td> <td>00:00</td> <td>00:30</td> <td>AirLinePurge</td> </tr> <tr> <td>3</td> <td>00:00</td> <td>01:00</td> <td>PreConcFill</td> </tr> <tr> <td>4</td> <td>00:00</td> <td>02:00</td> <td>Desorb</td> </tr> <tr> <td>5</td> <td>00:00</td> <td>00:08</td> <td>ConcFlow</td> </tr> <tr> <td>6 Inject</td> <td>00:00</td> <td>00:30</td> <td>DryPurge</td> </tr> <tr> <td>7</td> <td>00:30</td> <td>02:00</td> <td>HSCreate</td> </tr> <tr> <td>8</td> <td>02:30</td> <td>17:30</td> <td>Other</td> </tr> <tr> <td></td> <td></td> <td></td> <td>Standby</td> </tr> </tbody> </table> | Inlet States | | | | | Start | Duration | Inlet State | 1 | 00:00 | 00:05 | HSCreate | 2 | 00:00 | 00:30 | AirLinePurge | 3 | 00:00 | 01:00 | PreConcFill | 4 | 00:00 | 02:00 | Desorb | 5 | 00:00 | 00:08 | ConcFlow | 6 Inject | 00:00 | 00:30 | DryPurge | 7 | 00:30 | 02:00 | HSCreate | 8 | 02:30 | 17:30 | Other | | | | Standby | <table border="1"> <thead> <tr> <th colspan="4">Inlet States</th> </tr> <tr> <th></th> <th>Start</th> <th>Duration</th> <th>Inlet State</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>00:00</td> <td>01:00</td> <td>ConcFill</td> </tr> <tr> <td>2 Inject</td> <td>00:00</td> <td>05:00</td> <td>CkStdLinePurge</td> </tr> <tr> <td>3</td> <td>05:00</td> <td>10:00</td> <td>CkStdConcFill</td> </tr> <tr> <td>4</td> <td>15:00</td> <td></td> <td>PreDesorb</td> </tr> <tr> <td></td> <td></td> <td></td> <td>Desorb</td> </tr> <tr> <td></td> <td></td> <td></td> <td>ConcFlow</td> </tr> <tr> <td></td> <td></td> <td></td> <td>ColumnFlow</td> </tr> <tr> <td></td> <td></td> <td></td> <td>DryPurge</td> </tr> <tr> <td></td> <td></td> <td></td> <td>HSCreate</td> </tr> <tr> <td></td> <td></td> <td></td> <td>Other</td> </tr> <tr> <td></td> <td></td> <td></td> <td>Standby</td> </tr> </tbody> </table> | Inlet States | | | | | Start | Duration | Inlet State | 1 | 00:00 | 01:00 | ConcFill | 2 Inject | 00:00 | 05:00 | CkStdLinePurge | 3 | 05:00 | 10:00 | CkStdConcFill | 4 | 15:00 | | PreDesorb | | | | Desorb | | | | ConcFlow | | | | ColumnFlow | | | | DryPurge | | | | HSCreate | | | | Other | | | | Standby |
| Inlet States | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | Start | Duration | Inlet State | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 | 00:00 | 01:00 | ConcFill | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 Inject | 00:00 | 05:00 | ConcFlow | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | 05:00 | 10:00 | ColumnFlow | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | 15:00 | | Standby | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Inlet States | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | Start | Duration | Inlet State | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 | 00:00 | 00:05 | HSCreate | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | 00:00 | 00:30 | AirLinePurge | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | 00:00 | 01:00 | PreConcFill | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | 00:00 | 02:00 | Desorb | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | 00:00 | 00:08 | ConcFlow | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 Inject | 00:00 | 00:30 | DryPurge | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | 00:30 | 02:00 | HSCreate | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | 02:30 | 17:30 | Other | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | Standby | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Inlet States | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | Start | Duration | Inlet State | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 | 00:00 | 01:00 | ConcFill | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 Inject | 00:00 | 05:00 | CkStdLinePurge | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | 05:00 | 10:00 | CkStdConcFill | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | 15:00 | | PreDesorb | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | Desorb | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | ConcFlow | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | ColumnFlow | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | DryPurge | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | HSCreate | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | Other | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | Standby | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

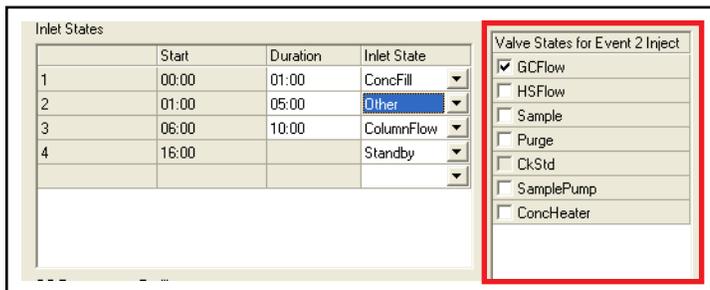
AirLinePurge Directs the sample through the air sample pathway and out the exhaust vent. The sample does not travel through the concentrator

NOTE: The sample cannot be the check standard.

| | |
|---------------------------------|---|
| LinePurge | Directs the water headspace sample through the air sample pathway and out the exhaust vent; the water purge is on in this state. The sample does not travel through the concentrator NOTE: The sample cannot be the check standard. |
| CkStdLinePurge | Directs the check standard out the exhaust vent, bypassing the GC column |
| AirConcFill | Directs air sample onto the concentrator |
| ConcFill | Directs water headspace sample onto the concentrator |
| CkStdConcFill | Directs the check standard onto the concentrator, when the water purge is on |
| PreDesorb | Begins the process of heat desorption of the analytes adsorbed on the concentrator prior to introduction onto the GC column |
| Desorb | Completes the heat desorption of analytes off the concentrator and onto the GC column |
| ConcFlow | Directs the desorbed sample from the concentrator onto the GC column |
| ColumnFlow | Directs the carrier gas flow directly through the GC column and is selected after ConcFlow to carry the sample completely through the GC column |
| DryPurge | Directs carrier gas through the concentrator to remove excess moisture and is used after ConcFill or CkStdConcFill |
| HSCreate | Bubbles carrier gas into the water sample to create the headspace. For water methods only |
| Other | Activates the Valve States menu to create a custom GC inlet state and is often used for GC troubleshooting. These options are described below (See Figure 16-11 .) |
| GCFlow | Directs carrier gas through the GC |
| HSFlow | Directs carrier gas into the headspace. For water methods only |
| Sample | Directs carrier gas across the concentrator |

- Purge** Directs carrier gas through the purge tube.
For water methods only
- Sample Pump** Turns on the sample pump
- ConcHeater** Turns on the concentrator heater

Figure 16-11 GC Valve states

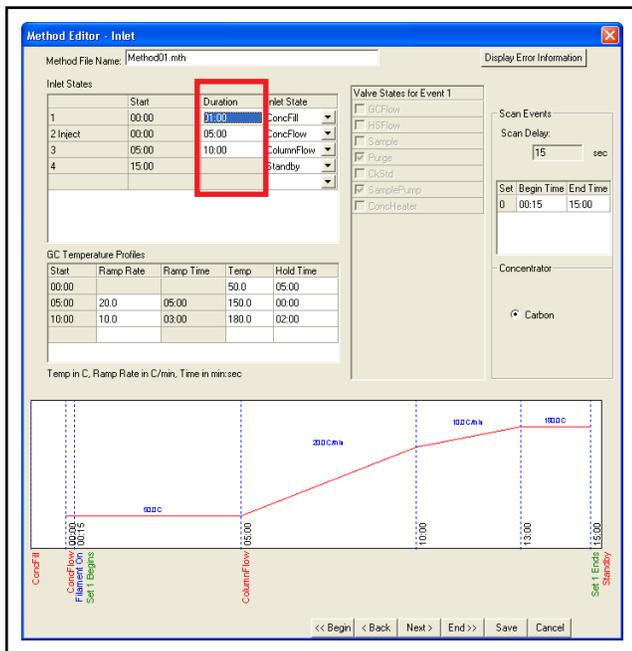


Standby Must be included in every method as the last state

After selecting the inlet state, enter the desired time period for the event in the **Duration** column. (See Figure 16-12.)

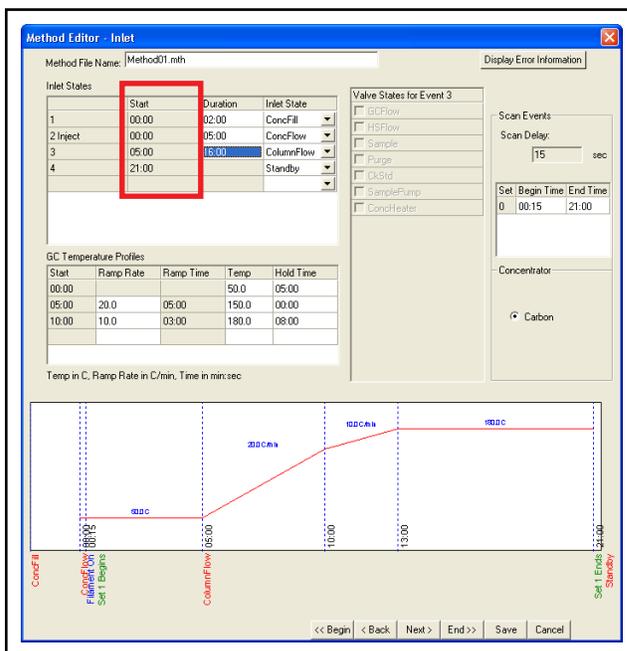
NOTE: The duration for PreDesorb and Desorb events cannot be changed.

Figure 16-12 Duration column



Upon entering the **Duration** settings, the **Start** time will be automatically calculated for the next **Inlet State(s)**. (See Figure 16-13.)

Figure 16-13 Start time recalculating



Inlet States can be deleted from the method. Highlight a cell in the desired row of the **Inlet States** table, and press **Delete** on the computer keyboard to remove the row.

Inlet States can be added to the method. Highlight a cell in the row below where the new **Inlet State** will be placed, and press **Insert** on the computer keyboard to insert a blank row. Add an Inlet State by selecting an inlet state from the shortcut menu. Refer to Figure 16-10 on page 16-8.

NOTE: If a row is selected while a blank row is present, pressing **Insert** will move the blank row to the selected row's position.

NOTE: Rows should not be inserted after the **Standby** event.

16.6.2 GC Temperature Profiles

GC Temperature Profiles specify the column temperature, ramp rate, and hold settings for the method. (See Figure 16-14.)

Figure 16-14 GC Temperature Profiles

| GC Temperature Profiles | | | | |
|-------------------------|-----------|-----------|-------|-----------|
| Start | Ramp Rate | Ramp Time | Temp | Hold Time |
| 00:00 | | | 50.0 | 05:00 |
| 05:00 | 20.0 | 05:00 | 150.0 | 00:00 |
| 10:00 | 10.0 | 03:00 | 180.0 | 02:00 |
| | | | | |

Temp in C, Ramp Rate in C/min, Time in min:sec

Adjustments to **Ramp Rate**, **Temp** (Temperature), and **Hold Time** columns will automatically update dependent parameters. For example, increasing the **Temp** will increase the **Ramp Time**; increasing the **Hold Time** will adjust the **Start** time of the next parameter. (See Figure 16-15.)

NOTE: A maximum of four rows is allowed in the profile.

Figure 16-15 Adjusting temperature profile

| GC Temperature Profiles | | | | |
|-------------------------|-----------|-----------|-------|-----------|
| Start | Ramp Rate | Ramp Time | Temp | Hold Time |
| 00:00 | | | 50.0 | 05:00 |
| 05:00 | 20.0 | 06:30 | 180.0 | 01:00 |
| 12:30 | 10.0 | 00:00 | 180.0 | 02:00 |
| | | | | |

Temp in C, Ramp Rate in C/min, Time in min:sec

16.6.3 Scan Events

- Scan Delay** Sets the baseline response. Data is not collected during this event
- Begin Time** Specifies the beginning of data collection
- End Time** Specifies the end of data collection
- Concentrator** Specifies the type of concentrator

Figure 16-16 Scan Events

Scan Events

Scan Delay: sec

| Set | Begin Time | End Time |
|-----|------------|----------|
| 1 | 00:15 | 20:00 |

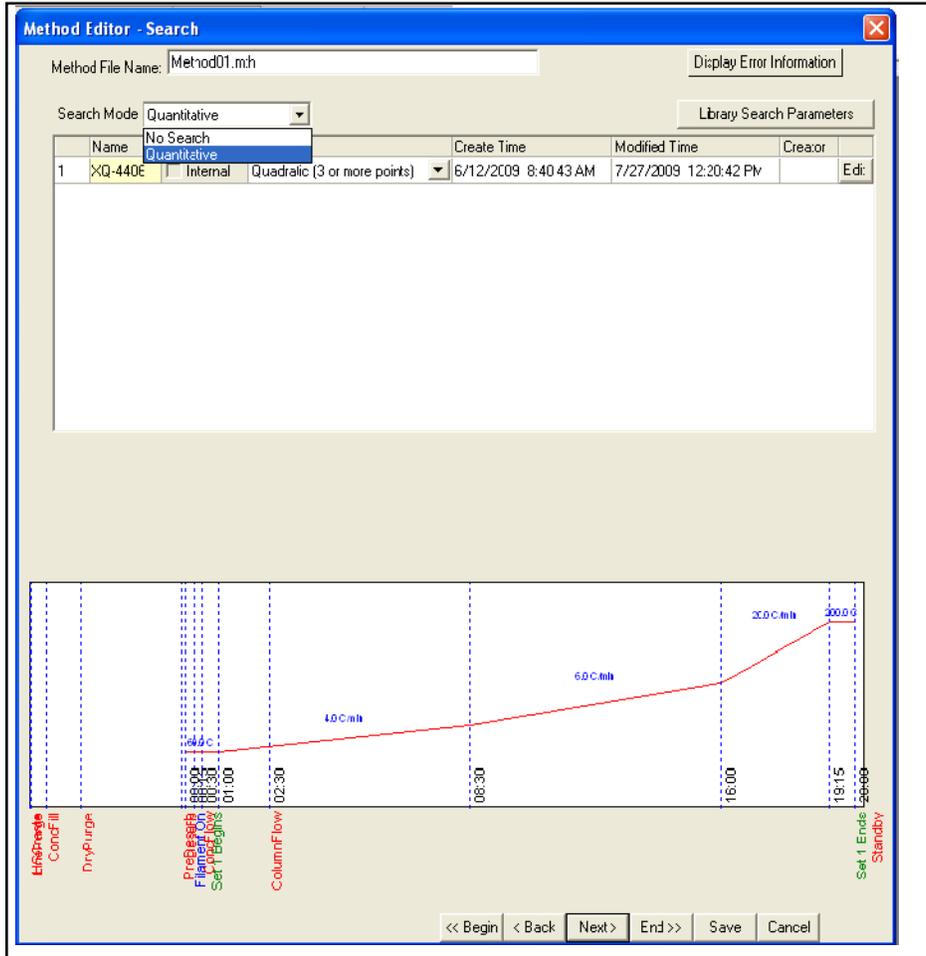
Concentrator

Carbon

16.7 Search

The **Search** window allows parameters to be set to qualify and quantify data. (See Figure 16-17.) To quantify data, a calibration library must be created. See Chapter 17, Calibration for instructions on creating a calibration library.

Figure 16-17 Method Editor - Search window



There are two choices in the **Search Mode** shortcut menu:

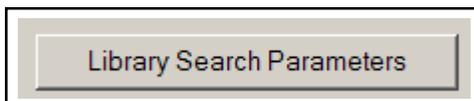
- No Search** A library search will not be conducted and a report will not be displayed on the front panel at the end of a run. If there is no library present, this is the only option available
- Quantitative** Generates a Quantitative (Quant) report at the end of a run by referencing the designated library

16.7.1 Setting Up a Quantitative Search

Once a calibration library has been created (see Chapter 17, Calibration), **Library Search Parameters** will be activated. (See Figure 16-18.)

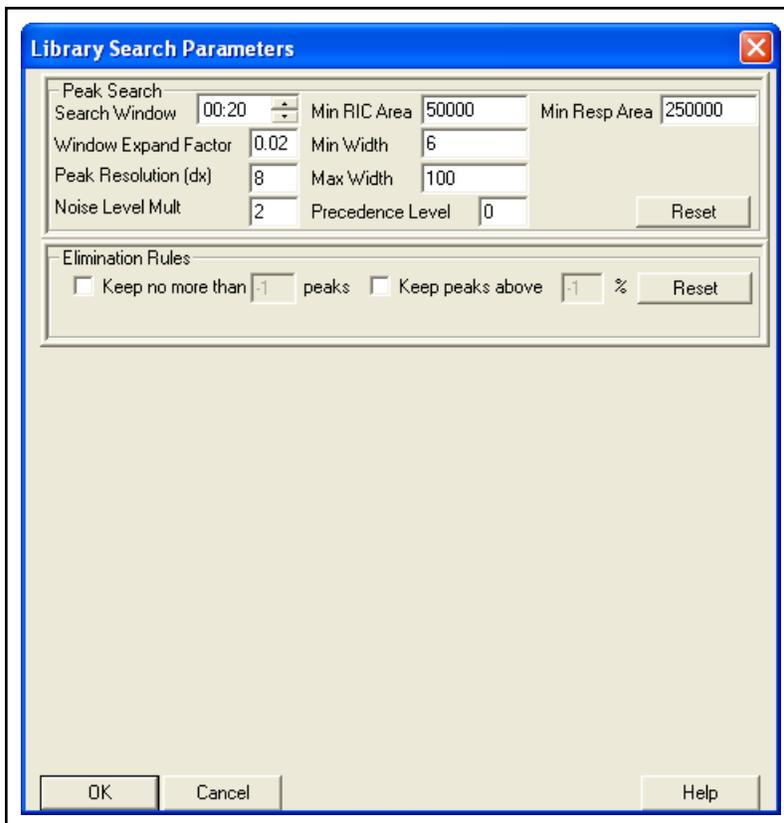
Library Search Parameters sets the peak identification criteria of the library compounds as well as the unknown analytes.

Figure 16-18 Library Search Parameters button



Click **Library Search Parameters** to display the peak identification criteria of the library. (See Figure 16-19.)

Figure 16-19 Library Search Parameters window



The **Peak Search** pane contains the parameters used in distinguishing a peak from the baseline. The five options most useful for adjusting the **Peak Search** are:

- Search Window** Defines the acceptable retention time range for a peak. The default value is 10 seconds. When using the default value, a given analyte will identify a peak within five seconds on either side of the expected retention time of the analyte
- Peak Resolution** This number indicates the minimum number of scans between two peaks. It is used to determine whether a peak should be split into two or considered as one
- Window Expand Factor** Increases the Search Window throughout a run based on retention time. The default value is 0.01. If using the default value, an analyte with a retention time of ten minutes (600 seconds) would add 6 seconds to either side of the Search Window (600 seconds times 0.01), resulting in a total addition of 12 seconds to the Search Window value above. When using the default 10 second Search Window, the Window Expand Factor would increase this value to 22 seconds total at a 10 minute retention time.
- Min Width** Minimum number of scans per peak. The default value is 20 scans, equivalent to a peak width of 2 seconds. Any peak with fewer scans than this value will be disregarded. Decreasing this number will instruct the software to accept peaks that are less broad than the default parameters allow
- NOTE:** In some cases, Min Width may be set too low. Setting a higher Min Width may be more effective at distinguishing peaks.
- Max Width** Maximum number of scans per peak. The default value is 250 scans, equivalent to a peak width of 25 seconds. Any peaks that have more scans than this value will be disregarded by the software. Increasing this number will instruct the software to accept peaks that are more broad than the default parameters allow

Min Resp Area The Min Resp Area is the minimum area under a peak. The default value is 2500. Any peaks that have a smaller area will be disregarded by the software. Decreasing this number will instruct the software to accept peaks that are smaller than the default parameters allow

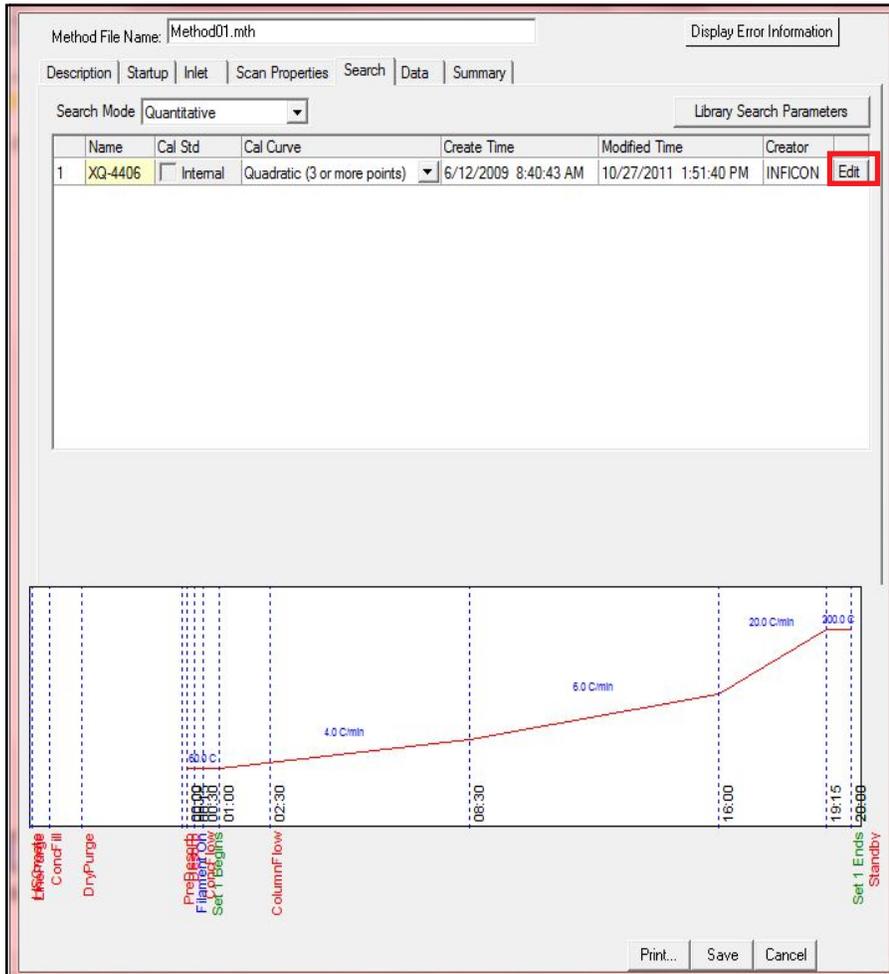
Precedence Level When compared to the compound-specific precedence level, it determines which search parameters to use - the global parameters specified in [Figure 16-19](#) or the compound-specific parameters. As a general rule, leaving this set to 0 allows one to use specific search parameters for individual compounds

Parameters **Min RIC Area**, **Noise Level Mult** and **Elimination Rules** are unavailable.

16.7.2 Compound Specific Search Parameters

The **Library Search Parameters** function is used to set the global search parameters for the library. Individual **Search Parameters** for specific compounds can also be set. To view the compounds in the library select **Edit**. (See Figure 16-20.)

Figure 16-20 Edit



Highlight the desired compound (in this example, Chloroform) and select the **Search Parameters** tab. (See Figure 16-21.)

Figure 16-21 Search Parameter tab

The screenshot shows a dialog box titled "Library Analyte List - XQ-4406". It contains a table of analytes and a detailed view for "Chloroform".

| Name | CAS# | RT Time | Standard | Conc. |
|--------------------------|------|-----------|----------|-------|
| Methylene Chloride | | 03:33.000 | Analyte | |
| trans-1,2-dichloroethene | | 04:14.199 | Analyte | |
| cis-1,2-dichloroethene | | 05:05.700 | Analyte | |
| Chloroform | | 05:20.600 | Analyte | |
| 1,2-dichloroethane | | 06:05.600 | Analyte | |

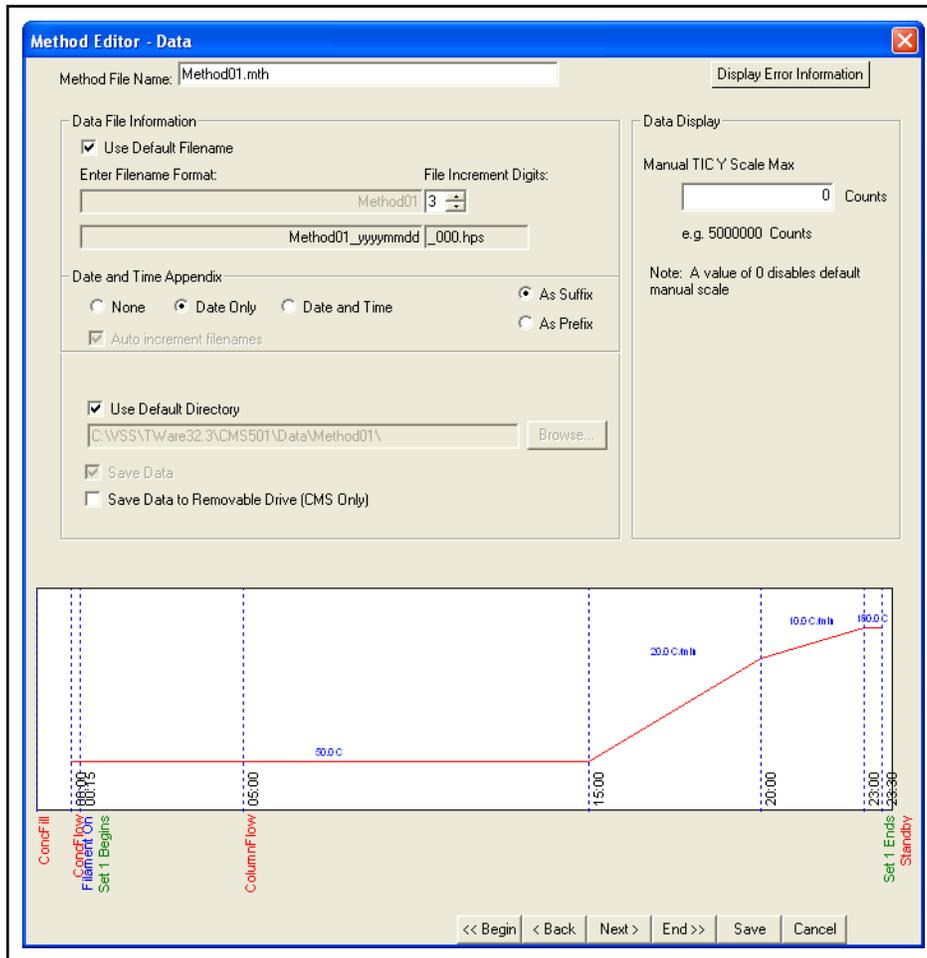
Below the table, the "Chloroform" section is expanded to show the "Search Parameters" tab. The "Precedence Level" is set to 1, which is highlighted with a red box. Other parameters include Search Window Size (00:30), Window Expand Factor (0.05), Peak Resolution (5), Noise Level Mult (2), Minimum Area (50000), Minimum Width (7), Maximum Width (70), and Template/Calibration Files.

Adjust the **Search Parameters**. In order for the compound specific **Search Parameters** to override the **Library Search Parameters** the **Precedence Level** must be set at a higher number. For example, if the **Library Search Parameters** are set at the default **Precedence Level** of 0, the compound specific **Search Parameters** must have the **Precedence Level** set at 1. (See Figure 16-21.)

16.8 Data

The **Data** screen allows for customization of the file name and storage location of the data files for the method. (See Figure 16-22.)

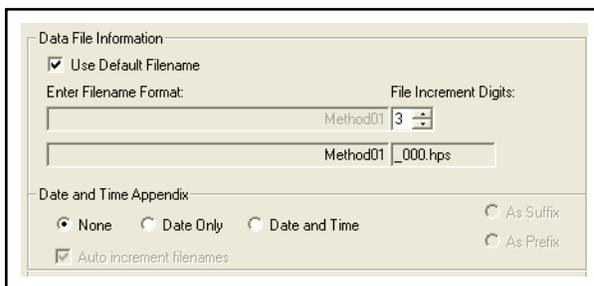
Figure 16-22 Method Editor - Data window



16.8.1 Data File Information

Use Default Filename When selected, the method will use a default format for the data file name. The default file name is a combination of the method file name, the date, and the sample run number (See Figure 16-23.)

Figure 16-23 Data File Information pane



File Increment Digits Used to set the number of digits appended to the data file name. By default, File Increment Digits are set to three

16.8.2 Date and Time Appendix

The **Date and Time Appendix** can be used to add the date and time to the data file.

NOTE: The date and time will correspond to the start of the method.

None. When selected, the date and time will not be added to the file name (See Figure 16-24.)

Figure 16-24 Date and Time Appendix - None Selected



Date Only. When selected the date will be added to the file name (See Figure 16-25.)

Figure 16-25 Date and Time Appendix - Date Selected



Date and Time When selected, both the date and time will be added to the data file name (See Figure 16-26.)

Figure 16-26 Date and Time Appendix - Date and Time Selected

As Suffix When **Date Only** or **Date and Time** is selected, the date and time are added to the end of the filename (See Figure 16-27.)

Figure 16-27 As Suffix

As Prefix When **Date Only** or **Date and Time** is selected, the date and time are added to the beginning of the filename (See Figure 16-28.)

Figure 16-28 As Prefix

Auto increment filenames Determines whether data files will have numbers appended to the end of the file name. By default a number is appended to ensure data files have unique file names. When **Date and Time** is selected, data files will always have unique files names and appending numbers to the data file becomes optional (See Figure 16-29.)

Figure 16-29 Auto increment filenames deselected

The screenshot shows a configuration window with the following elements:

- Use Default Filename
- Enter Filename Format: File Increment Digits:
- Date and Time Appendix:
 - None
 - Date Only
 - Date and Time
 - As Suffix
 - As Prefix
- Auto increment filenames

16.8.2.1 Date and Time Format

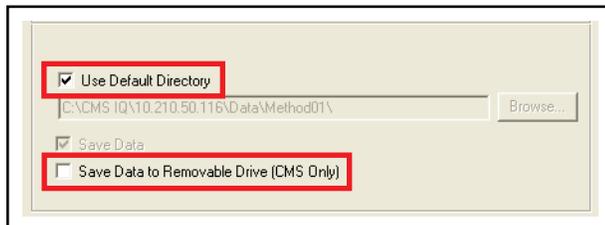
yyyy year
mm month
dd day
hh hour
mm minute
ss second

16.8.3 Use Default Directory

When **Use Default Directory** is selected, all data files will be saved in the default directory. To specify a different path, clear the **Use Default Directory** checkbox and type the desired file pathway. (See Figure 16-30.)

If **Save Data to Removable Drive** is selected, data will be saved to a removable drive (such as a USB drive). If the checkbox is cleared, data will be saved directly to the CMS5000 hard drive.

Figure 16-30 Use Default Directory

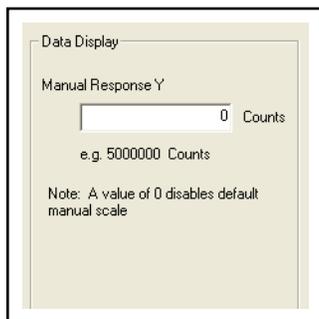


16.8.4 Data Display

Manual Response Y is used to enter a count number, which will scale the Y-axis or intensity of the chromatogram.

NOTE: If 0 is entered in the **Counts** box, the response will automatically scale to the peak with the largest count. (See Figure 16-31.)

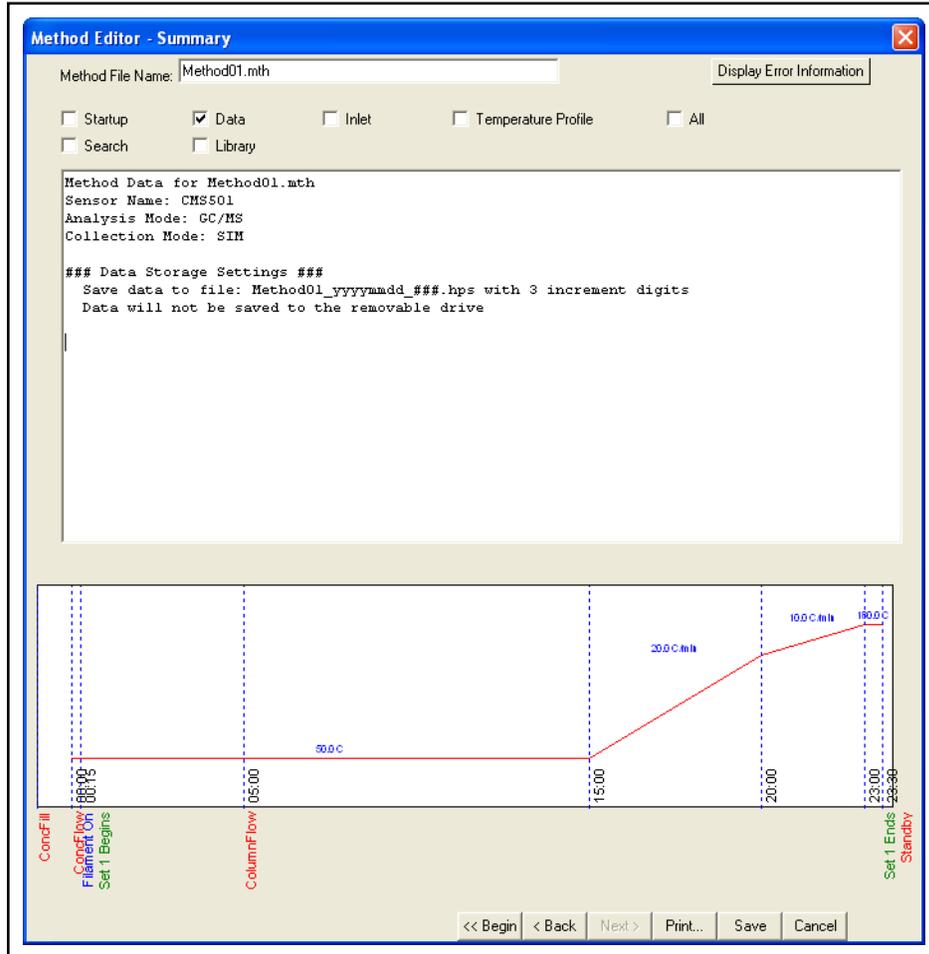
Figure 16-31 Data Display



16.9 Summary Screen

The **Summary** screen provides options to select desired components to display in the method text report. Method settings can be reviewed on the screen before the method is saved. (See Figure 16-32.)

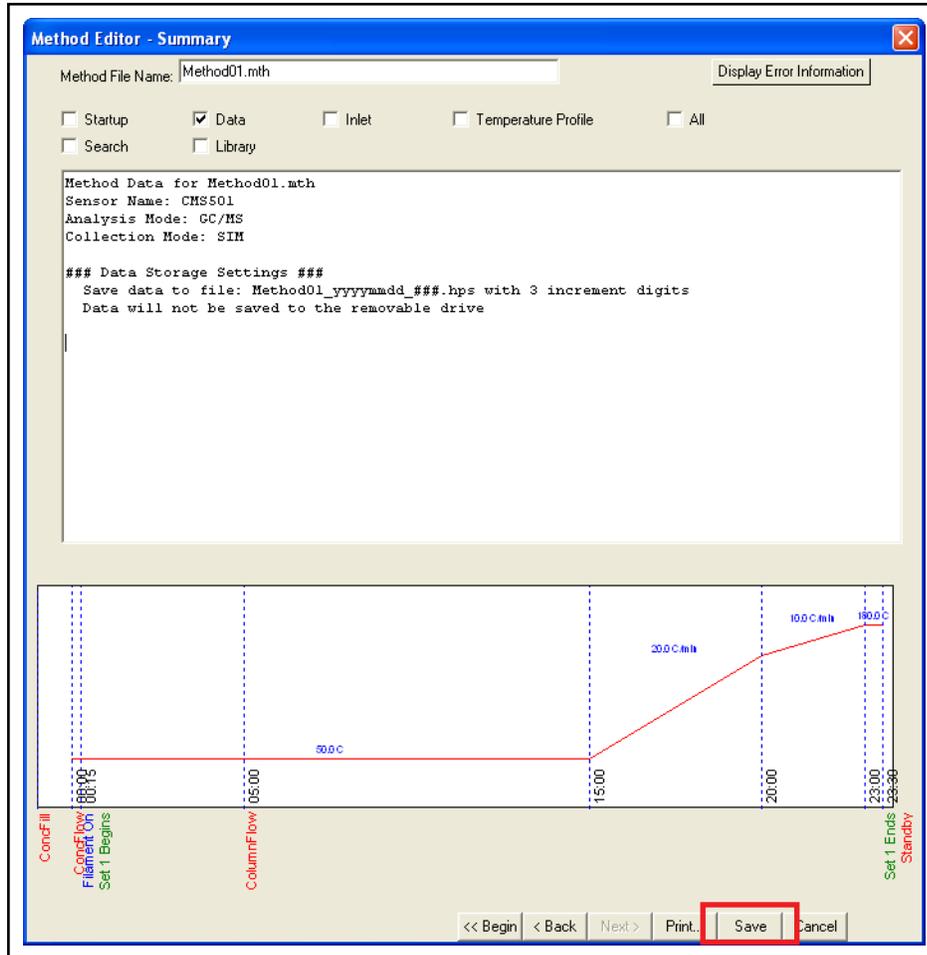
Figure 16-32 Method Editor - Summary window



16.10 Saving a Method

- 1 To save a newly created method, click **Save**. (See Figure 16-33.)

Figure 16-33 Method Editor - Summary window

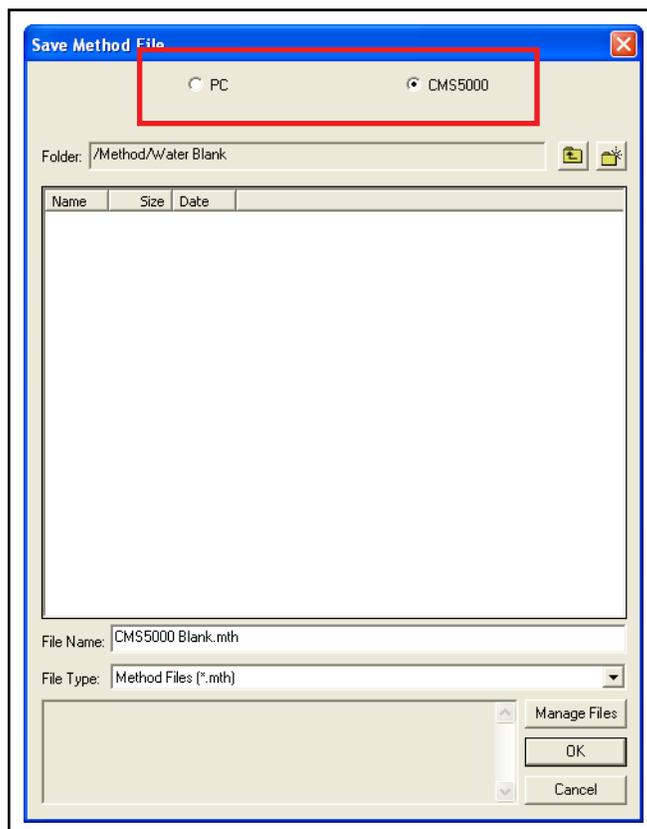


- The **Save Method File** window will display. (See Figure 16-34.) The method can be saved either to the computer or CMS5000. Select **PC** or **CMS5000** to determine where the method should be saved.

NOTE: When the computer is communicating with CMS5000, CMS5000 is the default location to save a method file.

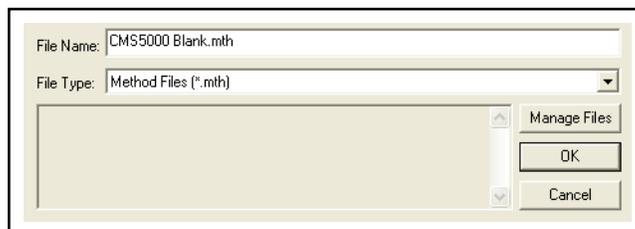
NOTE: Method files can be saved on CMS5000 only if CMS5000 is communicating with the computer. Refer to [Chapter 4, Setting Up Computer Communication](#) for information on connecting the computer and CMS5000.

Figure 16-34 Save Method File window



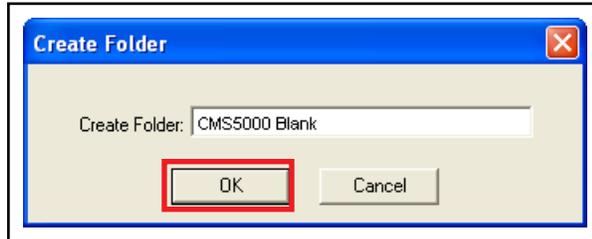
- In the **File Name** box, enter the new method file name. (See Figure 16-35.)

Figure 16-35 Entering a new method file name



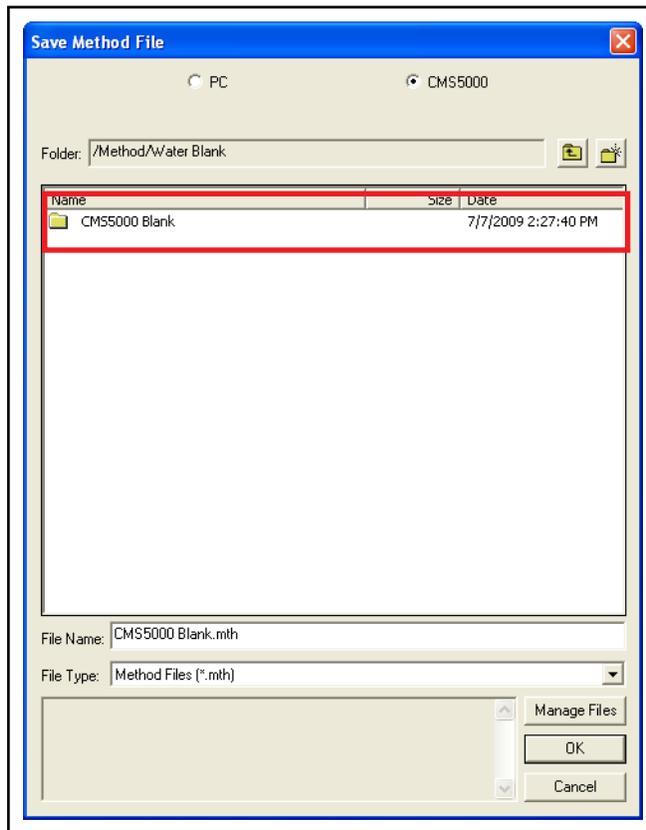
- 4 The method file may be saved in the CMS5000 method directory.
- 5 To create a new folder, click **Create Folder**  and enter the name of the new folder. Click **OK**. (See Figure 16-36.)

Figure 16-36 Create new folder



- 6 Double-click the new folder to save the data file to this location. (See Figure 16-37.)

Figure 16-37 Double-click folder



NOTE: Saving the new method file with the original name will overwrite (replace) the method that was used as the template.

Chapter 17

Calibration

17.1 Introduction To Calibration

CMS5000 identifies compounds based on the retention time of peaks in a chromatogram and determines concentration based on the area of the peak. Chemical standards with different known concentrations are analyzed to create an equation used to calculate the concentration of unknown samples based on peak area. Creating this equation is known as *calibration* and the equation is known as the *calibration curve*.

Calibration data is stored in the method *library*. The library contains the compound name, calibration curve, and retention time for every compound in the method. In water methods, the water beta factor (coefficient) and water temperature are also present to adjust for the partition coefficient of each compound. See [section 17.7, Water Beta](#) for more information.

Methods must be calibrated prior to analyzing unknown samples. Since the detector response will drift over time, the method will require periodic recalibration. CMS5000 contains preloaded, default factory methods, including a check standard method.

17.2 Method Development



CAUTION

Only trained personnel should create methods.

Creating a new method requires experimentally determining the retention time of every compound of interest. This requires running known standards of individual compounds. Once the retention time of every compound is known, a method library can be created. See [section 17.6, Using the Calibrate Function](#), on page 17-20.

HINT: Multiple compounds can be run at once if the elution order is known. Elution order can be determined using the retention index of compounds, found in reference literature.

Method parameters may need to be changed during development. Refer to [Chapter 16, Method Editor](#).

17.3 Check Standard

CMS5000 contains an internal permeation tube which releases toluene at a consistent rate. A check standard method uses the toluene as an internal standard to monitor detector drift.

When the **CkStd Autocal** is active, the results of an analytical method will be adjusted based on detector drift.

The check standard and analytical method must be recalibrated when the **CkStd Multiplier** reaches its **Min** or **Max** value. Refer to section 12.6.8.3, *Enable CkStd Autocal*, on page 12-65.

NOTE: The **Check Standard** should always be recalibrated before calibrating an analytical method.

17.4 Calibrating the Check Standard

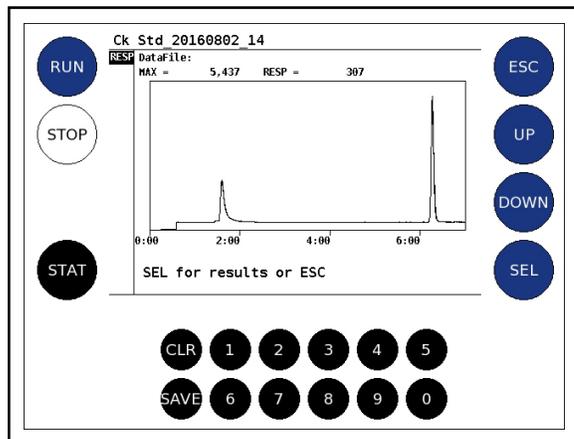
- 1 Run the check standard method *Ck Std.mth* until a stable toluene response has been observed on at least three consecutive runs. Refer to [Chapter 8, Basic Operation](#) for information on running a method. The check standard draws a sample from the internal toluene permeation tube.

NOTE: A stable response is defined as three consecutive runs where the **Relative Standard Deviation Percentage** or **RSD%** (*Standard Deviation* divided by *Average* times 100) of the toluene peak area is less than 2%. Multiple runs of the check standard method may be required to obtain a stable toluene response.

NOTE: When CMS5000 is initially set up, or after prolonged periods of time when CMS5000 is powered off or is not being purged with argon, the MAID detector must be equilibrated by leaving CMS5000 powered on with sufficient argon flow for a period of at least 24 up to 48 hours.

- The check standard run will look similar to the chromatogram shown in Figure 17-1.

Figure 17-1 Complete check standard method run



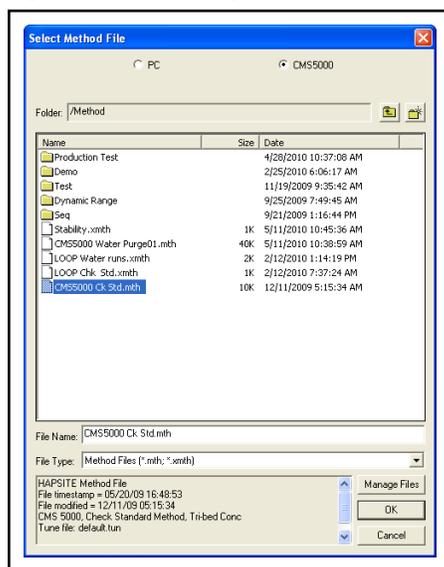
- Double-click  to open CMS IQ.



- Click **Calibrate** .

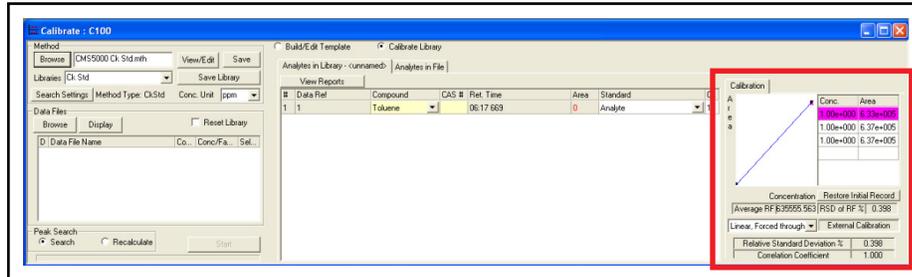
- Double-click on the desired method to open. (See Figure 17-2.)

Figure 17-2 Selecting method for calibration



- 6 The **Calibrate** window is displayed. The current calibration data is shown in the **Calibration** tab. (See Figure 17-3.)

Figure 17-3 Calibrate window



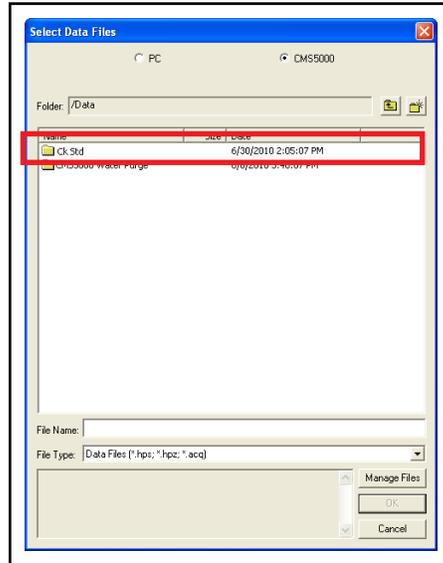
- 7 Click **Browse** in the **Data Files** pane to select the desired data files. (See Figure 17-4.)

Figure 17-4 Data file Browse button



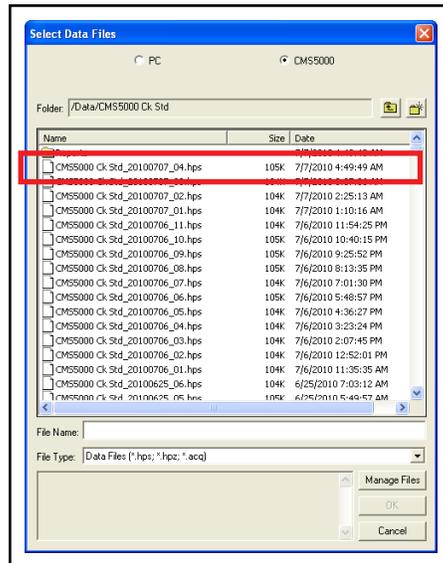
- The **Select Data Files** window will be displayed. Double click on the Check Standard method folder. (See Figure 17-5.)

Figure 17-5 Selecting method data folder



- Select the most recent data file. (See Figure 17-6.)

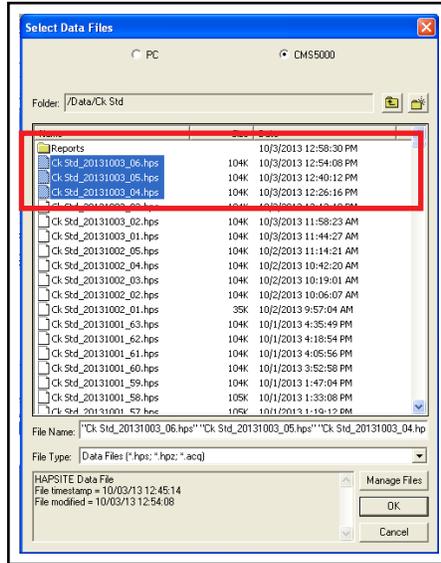
Figure 17-6 Selecting a data file



- Hold down the **Shift** key on the computer and select the third data file to select the three most recent data files. (See Figure 17-7.)

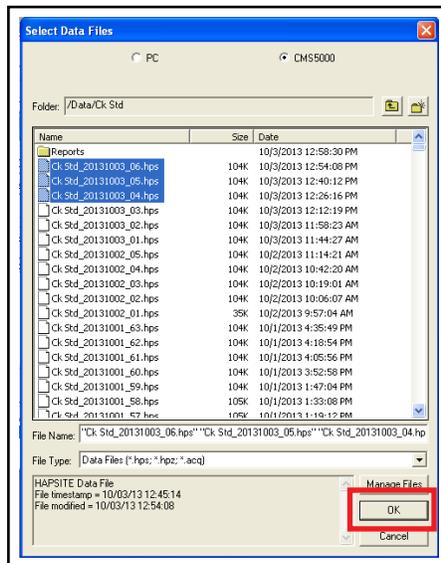
NOTE: To load data files one at a time, skip Step 10.

Figure 17-7 Selecting multiple data files



- Click **OK** to load the selected data files. (See Figure 17-8.)

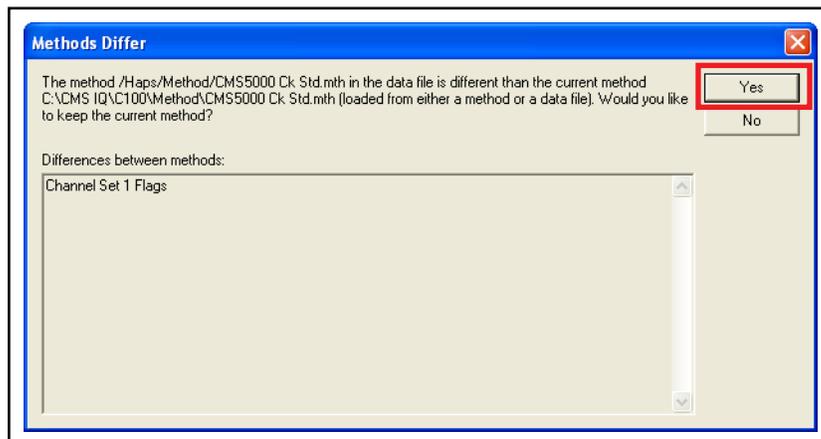
Figure 17-8 Load selected data files



- 12** The **Methods Differ** message is displayed. This window is normal and does not indicate an error. A separate message will display for each selected data file. Click **Yes** to verify that the data file should be used for calibration. (See Figure 17-9.)

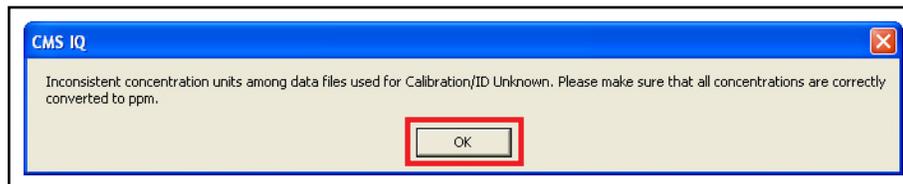
NOTE: If **No** is clicked, the selected data files will load into a blank library.

Figure 17-9 Methods Differ message



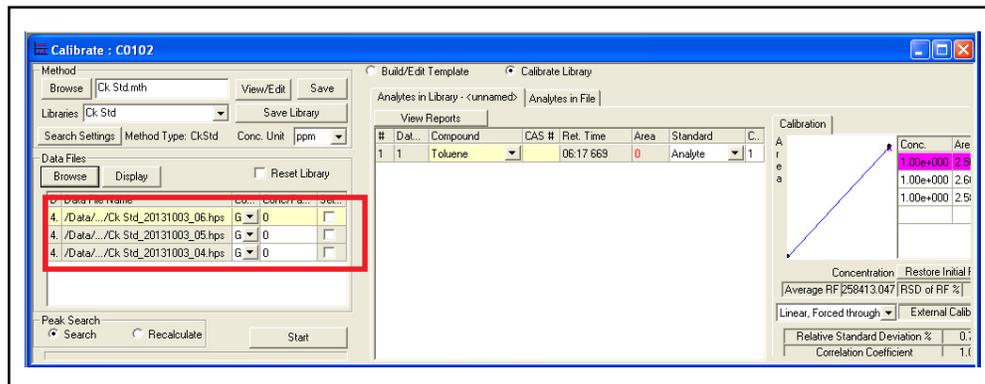
- 13** A message is displayed stating that the units between the data files are inconsistent. (See Figure 17-10.) This message will be displayed unless a concentration was pre-designated in the **Data File Information** window, and it uses the same units as the method. Click **OK**. Refer to section 13.5, Data File Information Window, on page 13-6 for more information.

Figure 17-10 Inconsistent data files message



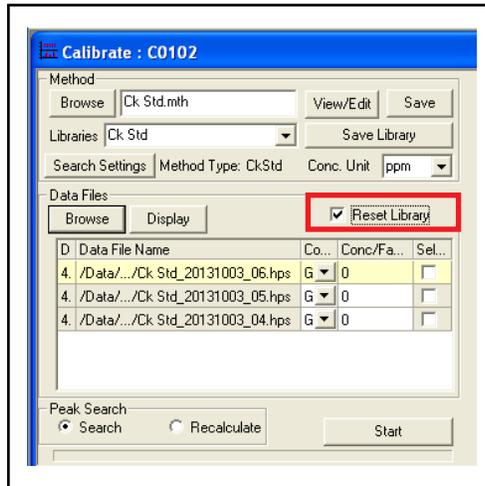
- 14** The selected data file(s) will be displayed in the **Data Files** list. (See Figure 17-11.)

Figure 17-11 Data Files list



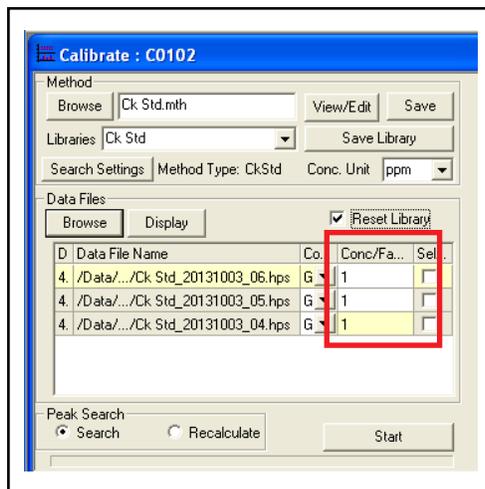
- 15 If necessary, repeat Step 7 through Step 14 until the three most recent data files are displayed in the **Data Files** list.
- 16 Select **Reset Library** to remove the current data in the **Calibration** tab. (See Figure 17-12.)

Figure 17-12 Reset Library checkbox



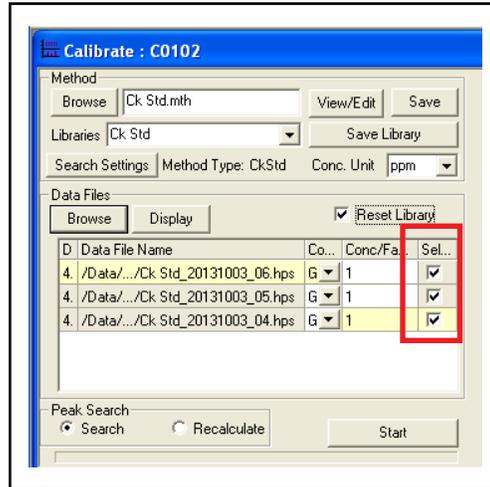
- 17 In each **Conc/Factor** box, type the value of 1. (See Figure 17-13.)

Figure 17-13 Conc/Factor column



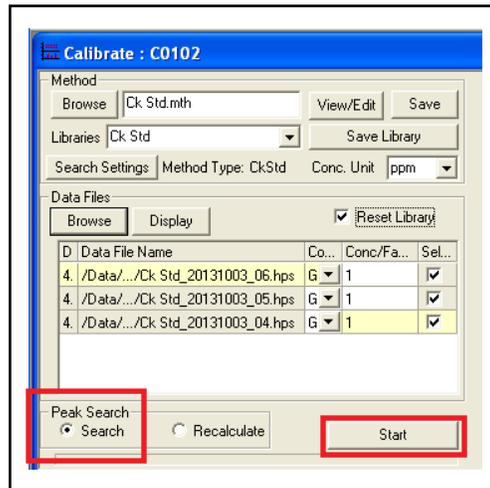
- 18 Select the **Select** checkbox for each data file to be included in the calibration. (See Figure 17-14.)

Figure 17-14 Select checkbox



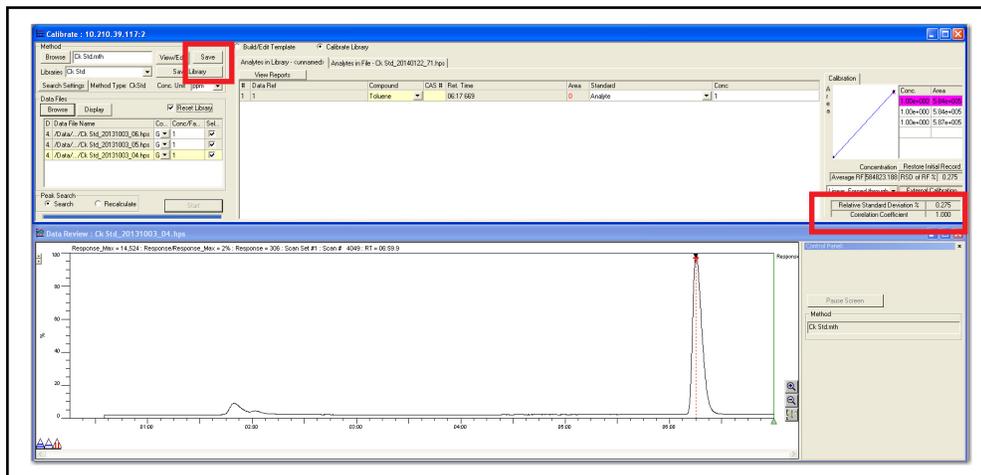
- 19 In the **Peak Search** pane, verify **Search** is selected. (See Figure 17-15.)
- 20 Click **Start** to initiate the calibration.

Figure 17-15 Selecting Search option and starting calibration



- 21** Ensure the **Relative Standard Deviation Percent (%RSD)** of the calibration is less than 2%. Click **Save** to save the method. (See Figure 17-16.)

Figure 17-16 Analytes in File tab



- 22** The check standard calibration is now complete.

NOTE: If the %RSD is greater than 2%, repeat the process starting with Step 1 in section 17.4, Calibrating the Check Standard.

17.5 Calibrating the Analytical Method

CMS5000 Water and Air methods require calibration at initial startup. Perform subsequent calibrations as necessary.

Standards of a known concentration must be analyzed on CMS5000 to create a calibration curve for analysis of unknown samples. Recommended methods for preparing chemical standards are described below.

NOTE: The method for creating standards will differ for water or air methods.

17.5.1 Multiple Standards vs Multiple Calibration Methods

A calibration curve requires at least four standards to be run. Two approaches can be used:

- ◆ Prepare four or more standards of varying concentration. Using multiple standards can reduce the risk of systematic error, but is more time consuming
- ◆ Prepare one standard and create four or more methods that vary the sample collection time. Using multiple calibration methods allows for simpler calibration, but it will mask errors in standard preparation

**WARNING**

Use appropriate Personal Protection Equipment (PPE) when handling chemicals. Refer to the MSDS of the standard(s) being used.

17.5.2 Water Standards

Standards for water analysis must be prepared in water to account for the partition coefficient of each compound. Purchased chemical standards are often prepared in methanol and will typically require dilution.

Figure 17-17 Optional calibration vessel



- 1 Using high purity water, fill the calibration vessel to the level of the etched mark or fill with 2 L of high purity water. When filled to the mark, the vessel will contain 2L of water. (Refer to Figure 17-17.)

NOTE: For best results, the water temperature of the calibration standards needs to be uniform and stable.

- 2 Calculate the volume of chemical standard to dilute into the water. The volume of standard needed is equal to the desired final concentration times the final volume, divided by the concentration of the chemical standard. (See equation [1].)

$$\text{Volume of Chemical Standard} = \frac{\text{Final Concentration} \times \text{Final Volume}}{\text{Concentration of Chemical Standard}} \quad [1]$$

- 2a** Most calibration standards require less than 500 uL of chemical standard. In these situations, the volume of the chemical standard can be ignored and the equation is simplified. (See equation [2].)

$$\text{Volume of Chemical Standard} = \frac{\text{Final Concentration} \times \text{Volume of Water}}{\text{Concentration of Chemical Standard}} \quad [2]$$

NOTE: Ensure all units used in the calculation are consistent.

- 2b** For example, if a 2,000 ppm (2,000,000 ppb) chemical standard is being used to create a 10 ppb calibration standard, then 10 uL of the chemical standard will be added to 2L (2,000,000 uL) of water. (See equation [3].)

$$\text{Volume of Chemical Standard in uL} = \frac{10 \text{ ppb} \times 2,000,000 \text{ uL}}{2,000,000 \text{ ppb}} \quad [3]$$

- 3** Using an appropriately sized syringe, draw up the required volume of chemical standard.
- 4** Using a stirring rod, gently stir the water in the calibration vessel until a vortex has formed. Do not allow the water to spill out of the vessel. (See Figure 17-18.)

Figure 17-18 Stirring vessel to form vortex



- 5 Remove the stirring rod. Immediately immerse the syringe needle at least one inch below the surface of the water and inject the chemical standard. (See Figure 17-19.)

Figure 17-19 Injecting chemical standard



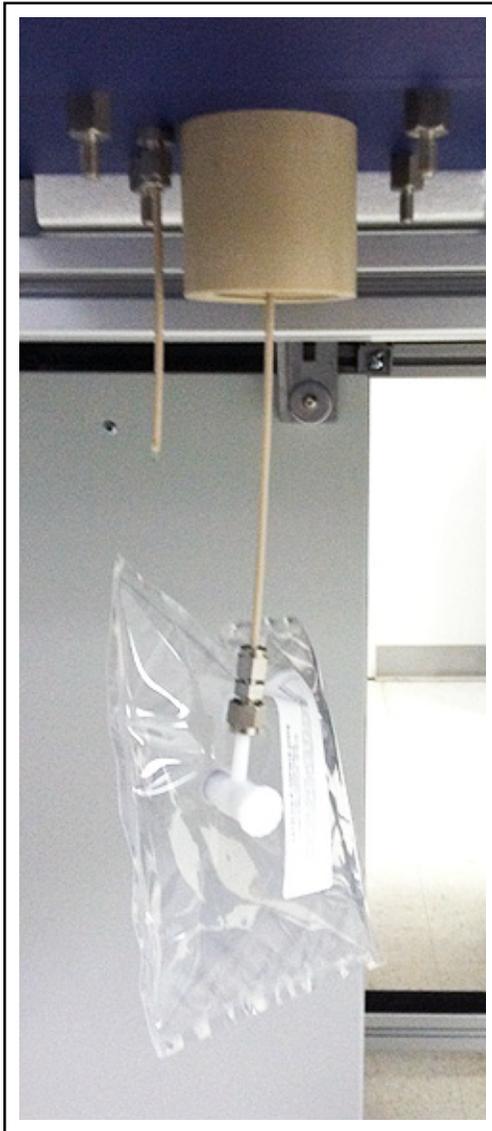
- 6 Remove the syringe and place the stirring rod back into the vessel. Continue to stir gently for another ten seconds, remove the stirring rod.
- 7 Attach the calibration vessel to the instrument. Refer to section 3.6, Attaching the Water Sampling Vessel, on page 3-7.
- 8 Proceed to section 17.5.4, Running Standards, on page 17-19.

17.5.3 Air Standards

Air chemical standards are typically supplied in compressed gas cylinders. Air standards must be sampled at atmospheric pressure on CMS5000. The chemical standard can be brought to atmospheric pressure in two ways:

- ♦ Fill a Tedlar[®] bag with the compressed standard and attach it to the CMS5000 air port using the air sample adapter (PN 935-752-G1) (See [Figure 17-20.](#))
- ♦ Connect the standard or a gas dilution system onto an in-line sampling system installed on the CMS5000 ports. Refer to [section 3.8.2, In-line Air Sampling](#), on page 3-12

Figure 17-20 Tedlar bag calibration



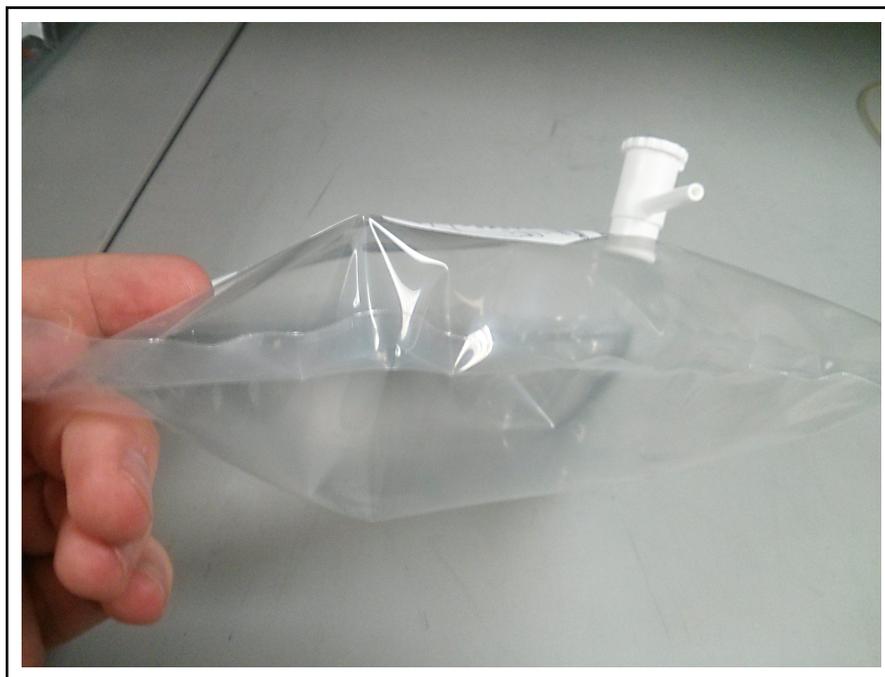
17.5.3.1 Directly Filling Tedlar Bag

If diluting standards is unnecessary, a Tedlar bag can be filled directly from a compressed gas cylinder standard.

NOTE: Alternatively, a gas cylinder can be connected to an in-line sampling system.

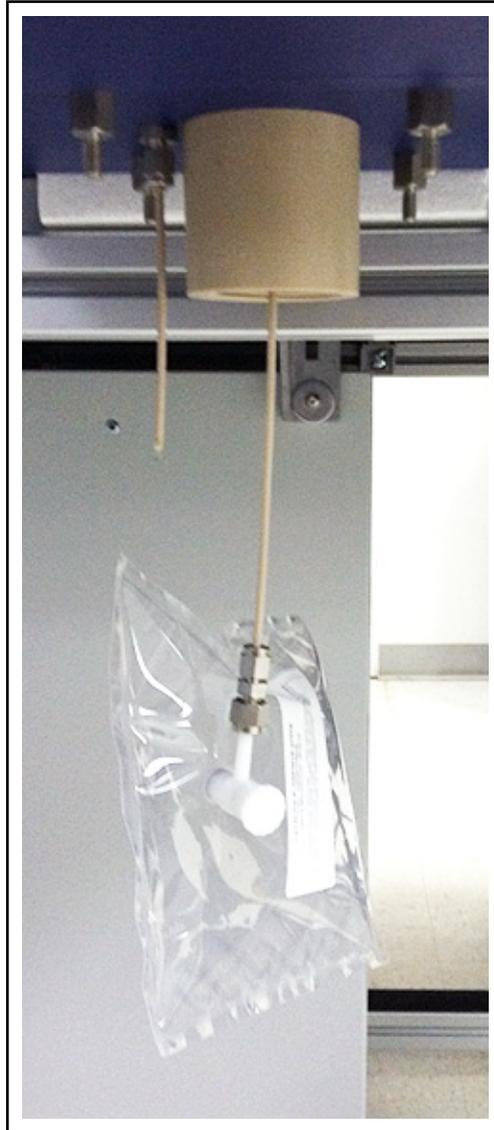
- 1 Attach the appropriate regulator to the gas cylinder.
- 2 Attach a clean, empty 1L Tedlar bag (PN 070-1686) to the gas cylinder.
- 3 Fill the Tedlar bag with the standard gas. Avoid filling the bag more than 80% of its maximum volume. (See Figure 17-21.)

Figure 17-21 Inflated Tedlar bag



- 4 Connect the Tedlar bag to the air sample adapter and finger-tighten the nut until the Tedlar bag is firmly in place. (See Figure 17-22.)

Figure 17-22 Air sample adapter



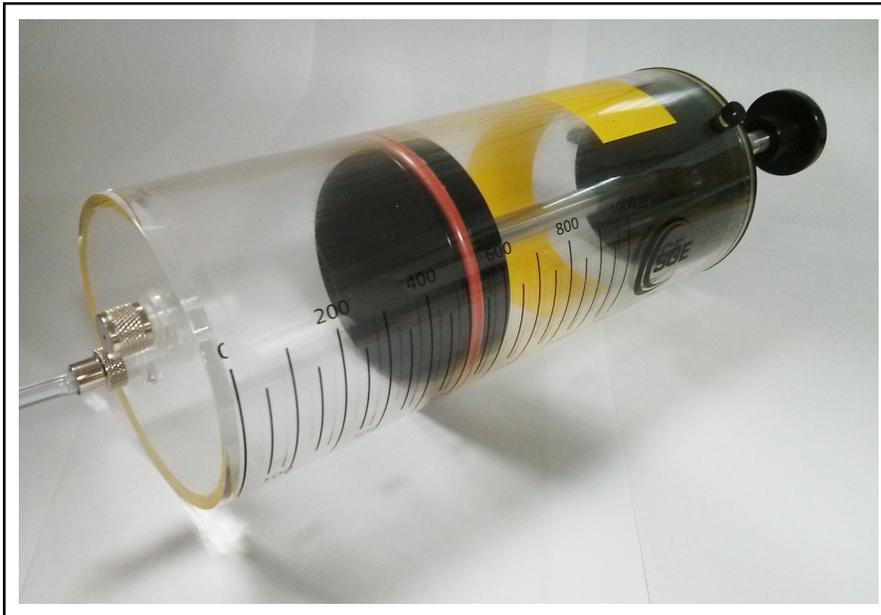
- 5 Connect the air sample adapter to the instrument and open the Tedlar bag. Refer to section 3.8.2, In-line Air Sampling, on page 3-12.

17.5.3.2 Diluting Gas Samples

If multiple calibration standards with different concentrations are required, or the concentration of the gas standard cylinder is not within the desired calibration range, gas samples will require dilution. A source of VOC free gas (zero air, nitrogen, argon, etc.) and the appropriate volume gas syringe are necessary for diluting gas standards. A 25 mL, 50 mL, or 1 L gas syringe may be required depending on the dilution. (See Figure 17-23.)

NOTE: Alternatively, an automatic gas dilution system may be used.

Figure 17-23 One L gas syringe



- 1** Calculate the volume of chemical standard to dilute into VOC free gas. The volume of standard needed is equal to the desired final concentration times the final volume, divided by the concentration of the chemical standard. (See equation [4].)

$$\text{Volume of Chemical Standard} = \frac{\text{Final Concentration} \times \text{Final Volume}}{\text{Concentration of Chemical Standard}} \quad [4]$$

- 1a** The final volume is typically 1 L, so the equation can be simplified. (See equation [5].)

$$\text{Volume of Chemical Standard} = \frac{\text{Final Concentration} \times 1000 \text{ mL}}{\text{Concentration of Chemical Standard}} \quad [5]$$

NOTE: Ensure all units in the calculation are consistent.

- 1b** For example, if a 10 ppm (10,000 ppb) chemical standard is being used to create a 50 ppb calibration standard, then 5 mL of the chemical standard will need to be added to the final volume of 1 L (1000 mL) of air. (See equation [6].)

$$\text{Volume of Chemical Standard} = \frac{50 \text{ ppb} \times 1000 \text{ mL}}{10,000 \text{ ppb}} \quad [6]$$

- 2** Calculate the volume of VOC free gas needed for the dilution. The volume is equal to 1000 mL minus the volume of the chemical standard.
(See [equation \[7\]](#).)

$$\text{Volume of VOC Free Gas} = 1000 \text{ mL} - \text{Volume of Chemical Standard} \quad [7]$$

- 2a** For example, if 5 mL of chemical standard needs to be added to the final volume of 1L, 995 mL of VOC free gas will be needed. (See [equation \[8\]](#).)

$$\text{Volume of VOC Free Gas} = 1000 \text{ mL} - 5 \text{ mL} \quad [8]$$

- 3** Use appropriately sized gas syringe(s) to draw up the calculated volume of VOC free gas.
 - 3a** The 1 L syringe is graduated to measure gas in multiples of 50 mL. If the required volume of VOC free gas is not a multiple of 50 mL, use the 1 L syringe to draw up the closest multiple of 50 mL, rounded down.
 - 3b** Use a smaller syringe with smaller graduation to obtain the remaining volume.
 - 3c** For example, if 995 mL of VOC free gas is needed, draw up 950 mL of gas in the 1 L syringe and 45 mL in a 50 mL syringe.
- 4** Connect the 1 L syringe to the Tedlar bag.
- 5** Follow the instructions on the Tedlar bag to open the valve and inject the VOC free gas.
- 6** Follow the instructions on the Tedlar bag to close the valve and remove the 1 L syringe.
 - 6a** If more than one syringe is needed for VOC free gas, repeat [Step 4](#) through [Step 6](#) with the additional syringe(s).
- 7** Connect the appropriate gas syringe to the chemical standard cylinder.
- 8** Fill the syringe with the calculated volume of chemical standard.
- 9** Connect the syringe to the Tedlar bag.
- 10** Follow the instructions on the Tedlar bag to open the valve and inject the chemical standard.
- 11** Follow the instructions on the Tedlar bag to close the valve and remove the syringe.
- 12** Allow two minutes for the gas mixture to fully equilibrate.
- 13** Connect the Tedlar bag to the air sample adapter and finger-tighten the nut until Tedlar bag is firmly in place. Refer to [Figure 17-22](#) on [page 17-16](#).
- 14** Connect the air sample adapter to the instrument and open the Tedlar bag.
(Refer to [Step 13](#).)
- 15** Proceed to [section 17.5.4, Running Standards](#), on [page 17-19](#).

17.5.4 Running Standards

Once a calibration standard is prepared and connected to CMS5000, it must be analyzed. It is recommended to analyze calibration standards immediately after they are prepared.

NOTE: Calibration standards must be run within six hours of preparation to ensure sample integrity.

- 1 Select the desired method and run the calibration standard. Refer to 14.1, Run Method.

If desired, click **Data File Info** while the standard is running to enter the concentration and description of the standard. Refer to section 13.4, Data Review Toolbar, on page 13-5. See Figure 17-24.

NOTE: Once an analysis has completed, changes to **Data File Information** will only be saved to the computer.

Figure 17-24 Data File Information window

The screenshot shows the 'Data File Information' dialog box. The 'Data' field is 'C:\Documents and Settings\XPMUser\My Document\Water Purge 19 Cmpd_201'. The 'Method' is '\Haps\Method\Water Purge 19 Cmpd.mth'. The 'Start Time' is '11/18/2013 2:31:04 PM'. The 'GPS Info' is 'Valid GPS Information Not Available'. The 'Conc.' field is highlighted with a red box and contains 'Level: 3' and 'Unit: ppb'. The 'Description' field is also highlighted with a red box and contains '3 ppb 19 Cmpd Water Purge Calibration Standard'. The 'Internal Standard' field is empty, with a note 'No Internal Standard Compound'. The window has 'OK' and 'Cancel' buttons at the bottom.

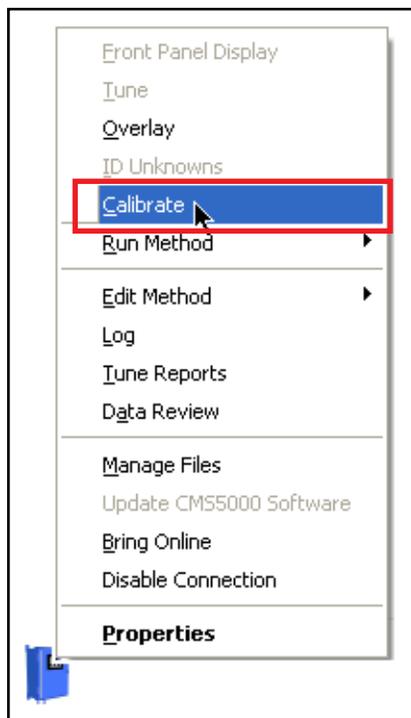
17.6 Using the Calibrate Function

The **Calibrate** function is used to build and calibrate chemical libraries.

- 1 When all standards have been analyzed, click the **Calibrate**  icon, located on the **Sensor** toolbar on the **System Setup** window.

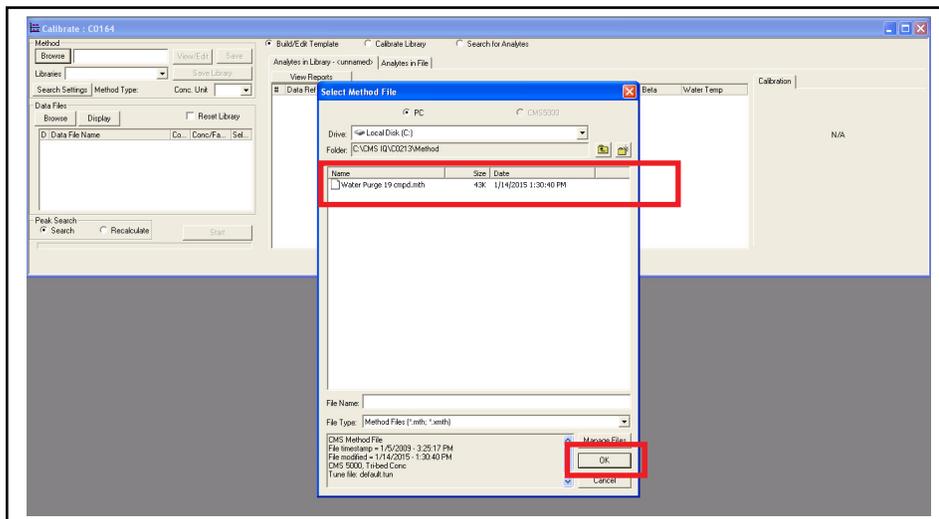
Alternately, right-click the **CMS5000** icon located on the **System Setup** window and click **Calibrate**. (See Figure 17-25.)

Figure 17-25 Alternate way of accessing Calibrate function



- 2 The following windows are displayed. Select the method used to run the standards. Click **OK**. (See Figure 17-26.)

Figure 17-26 Method file window in calibrate

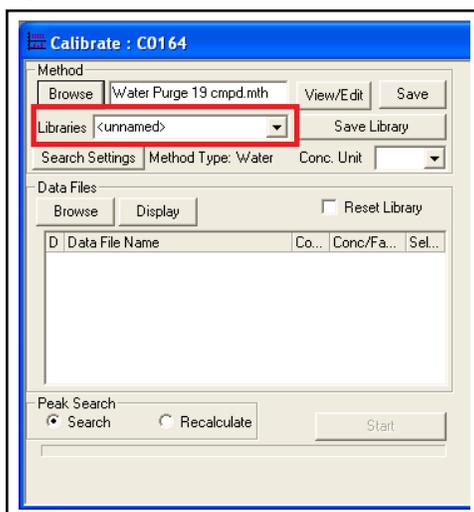


- 3 The method and library check boxes will populate. If the chemical library has already been created, skip to Step 16.

- ◆ If a library has been previously created for the desired method, the method name will be displayed in the library box
- ◆ If a library has not been created, the library box will display **<unnamed>** (See Figure 17-27.)

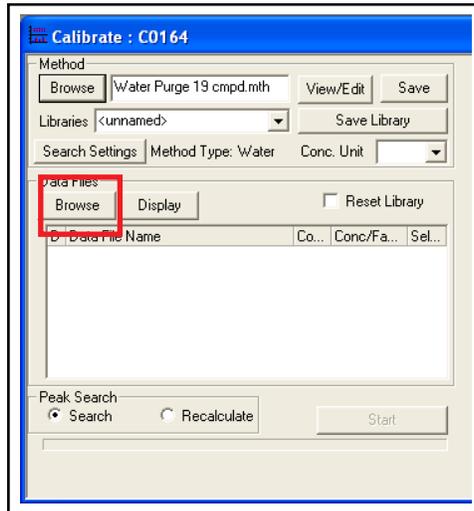
NOTE: If building a library, it can be named at the time it is saved. (See Step 14.)

Figure 17-27 Calibrate window



- 4 Click **Browse** in the **Data Files** pane. (See Figure 17-28.)

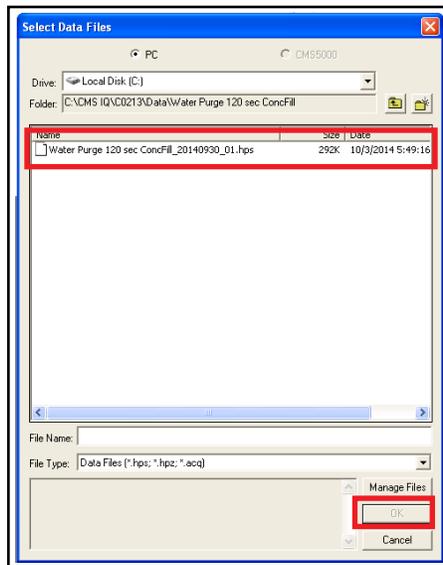
Figure 17-28 Browse data files



- 5 Select the data file of the standard with the highest concentration. Click **OK**. (See Figure 17-29.)

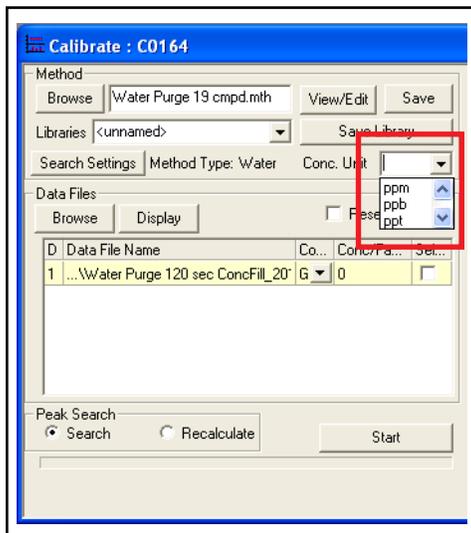
NOTE: The highest concentration standard is the best data file to use for creating a new library.

Figure 17-29 Selecting data file



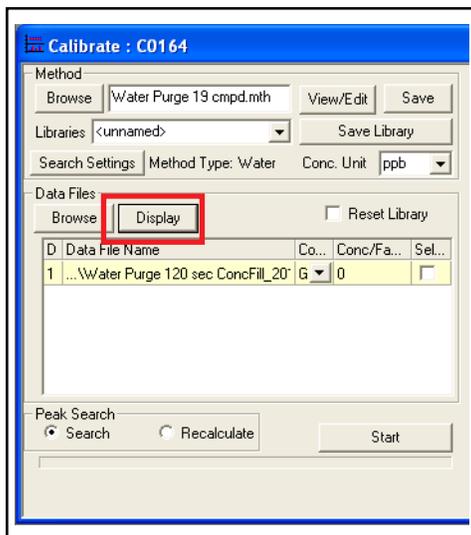
- 6 Type or select the concentration units from the **Conc. Unit** shortcut menu. (See Figure 17-30.)

Figure 17-30 Selecting concentration units



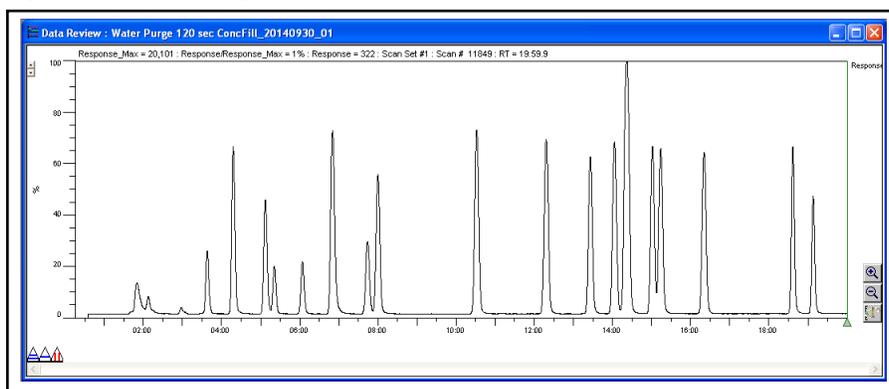
- 7 Click **Display** to display the chromatogram of the selected data file. (See Figure 17-31.)

Figure 17-31 Clicking display



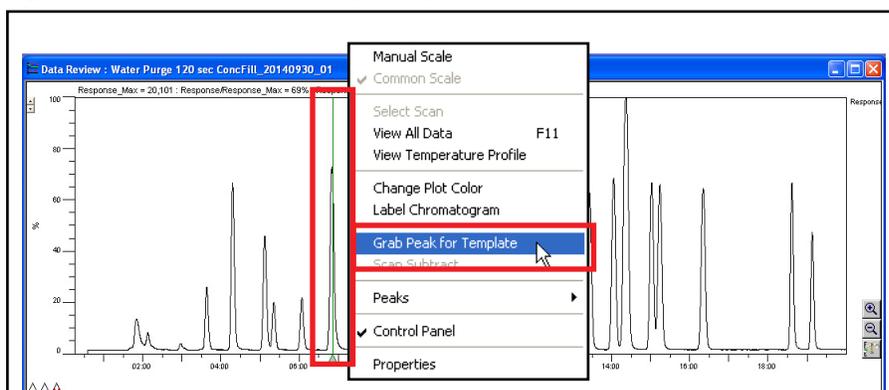
- 8 If the chemical library has not been created, each analyte must be selected from the chromatogram and manually added to the library template. To select a peak, refer to section 13.8, How to Access the Scan Cursor, on page 13-28. (See Figure 17-32.)

Figure 17-32 Selecting a peak



- 9 Once a peak is selected, right-click and click **Grab Peak for Template** to add an analyte to the library template. (See Figure 17-33.)

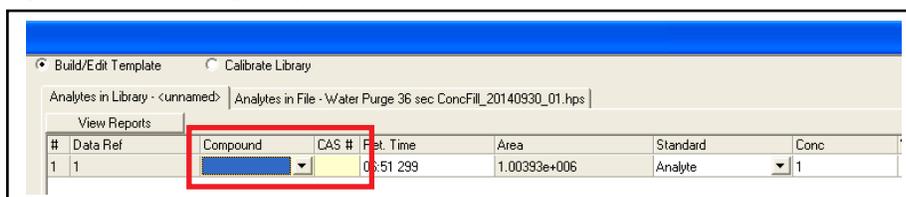
Figure 17-33 Grab Peak for Template option



- 10 The peak is added to the **Analytes in Library** table. Type the name of the analyte in the **Compound** box. (See Figure 17-34.) The compound which corresponds to a peak must be determined experimentally as part of the method development. Refer to section 17.2, Method Development, on page 17-1.

NOTE: If desired, type the Chemical Abstract Service (CAS) number in the **CAS #** box. (See Figure 17-34.)

Figure 17-34 Entering analyte name



- 11** The **Conc** box will be filled in with a value of 1 after the library is built in Step 18. (See Figure 17-35.) The **Conc** box is used when data files are in **Analyte** mode. See Step 18 through Step 21a.

Figure 17-35 Entering analyte concentration

| # | Ret. Time | Area | Standard | Conc | Water Beta | Water Temp |
|---|-----------|--------------|----------|------|------------|------------|
| 1 | 06:51 299 | 1.00393e+006 | Analyte | 1 | 4000 | 21.4 |

- 12** If the method is for water, a **Water Beta** and **Water Temp** box will display.
- ♦ **Water Beta** default value is 4000. See section 17.7, Water Beta, on page 17-36
 - ♦ **Water Temp** will be automatically set based on the temperature detected from the CMS5000 RTD thermometer (See Figure 17-36.)

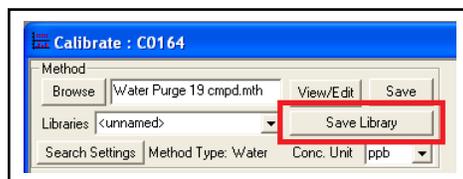
NOTE: Water Beta values are determined experimentally or derived from reference literature.

Figure 17-36 Water Beta value

| # | Ret. Time | Area | Standard | Conc | Water Beta | Water Temp |
|---|-----------|--------------|----------|------|------------|------------|
| 1 | 06:51 299 | 1.00393e+006 | Analyte | 1 | 4000 | 21.4 |

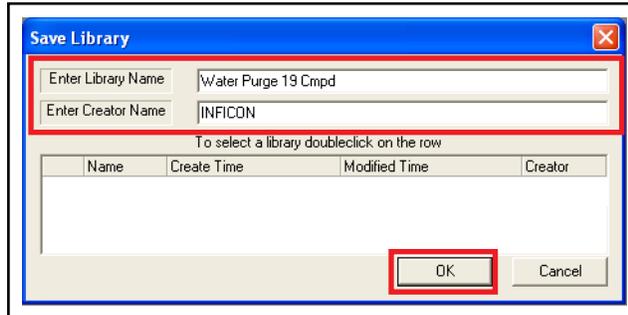
- 13** Repeat Step 8 through Step 12 for water methods or Step 8 through Step 11 for air methods to identify all remaining analytes.
- 14** To save the new library, click **Save Library** in the **Method** pane. (See Figure 17-37.)

Figure 17-37 Save Library button



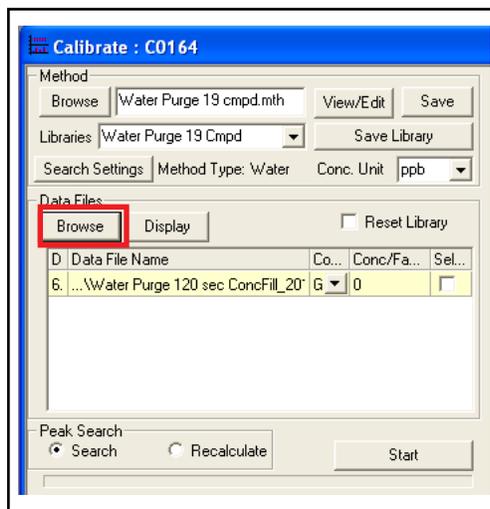
- 15 The Save Library window is displayed. (See Figure 17-38.)
 - 15a Type a name in the **Enter Library Name** box.
 - 15b Type a name in the **Enter Creator Name** box.
 - 15c Click **OK**.

Figure 17-38 Save library



- 16 To calibrate the library, click **Browse** in the **Data Files** pane. (See Figure 17-39.)

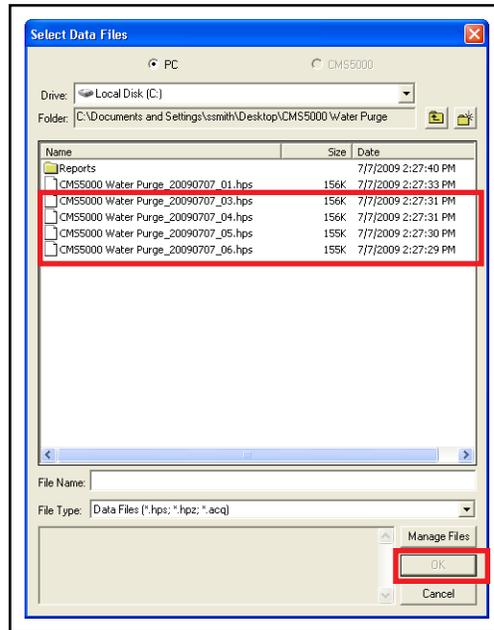
Figure 17-39 Browse



- 17 Select all the appropriate calibration data files. Data files are organized by method. Click **OK** to add them to the library. (See Figure 17-40.)

HINT: Multiple data files can be selected by holding down the **Ctrl** key while clicking on additional data files. Alternatively, a range of data files can be selected by holding down the **Shift** key and selecting the first and last data file in the desired range.

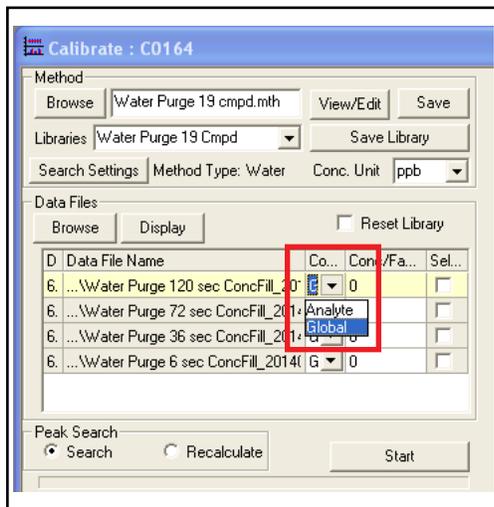
Figure 17-40 Select data files



18 The selected files will be displayed in the **Calibrate** window. The **Concentration Reference (Conc Ref)** box determines how the concentration of analytes is calculated. There are two options, **Global** and **Analyte**. (See Figure 17-41.)

- ◆ Select **Global** when the concentration of every compound in a data file is the same
- ◆ Select **Analyte** when the concentration of compounds in a data file differ

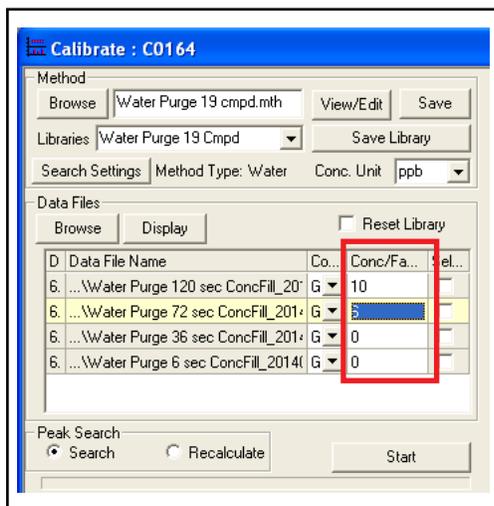
Figure 17-41 Selecting Concentration Reference



19 Type the concentration of the standard in the **Conc/Factor** column. (See Figure 17-42.)

NOTE: If compounds within a data file have varying concentrations, choose one compound to use as a reference.

Figure 17-42 Adding concentrations using the Global setting



- 20** When **Global** is selected, the method will ignore the number in the **Conc** column in the library. This column does not require further modification in order to calibrate the library. (See Figure 17-43.)

Figure 17-43 Concentration column using the Global setting

| # | Data Ref | Compound | CAS # | Ret. Time | Area | Standard | Conc | Water Beta | Water Temp |
|----|----------|--------------------|-----------|-----------|------|----------|------|------------|------------|
| 1 | 3 | Methylene Chl... | 03:33 000 | 0 | | Analyte | 1 | 400 | 0 |
| 2 | 7 | trans-1,2-dichl... | 04:14 199 | 0 | | Analyte | 1 | 400 | 0 |
| 3 | 7 | cis-1,2-dichlor... | 05:05 700 | 0 | | Analyte | 1 | 400 | 0 |
| 4 | 7 | Chloroform | 05:20 600 | 0 | | Analyte | 1 | 400 | 0 |
| 5 | 7 | 1,2-dichloroet... | 06:05 600 | 0 | | Analyte | 1 | 400 | 0 |
| 6 | 7 | Benzene | 06:54 799 | 0 | | Analyte | 1 | 400 | 0 |
| 7 | 7 | 1,2-dichloropr... | 07:51 299 | 0 | | Analyte | 1 | 400 | 0 |
| 8 | 7 | trichloroethene | 08:08 200 | 0 | | Analyte | 1 | 400 | 0 |
| 9 | 7 | Toluene | 10:31 700 | 0 | | Analyte | 1 | 400 | 0 |
| 10 | 7 | tetrachloroeth... | 12:18 900 | 0 | | Analyte | 1 | 400 | 0 |
| 11 | 7 | chlorobenzene | 13:27 299 | 0 | | Analyte | 1 | 400 | 0 |
| 12 | 7 | ethylbenzene | 14:03 000 | 0 | | Analyte | 1 | 400 | 0 |

- 21** If **Analyte** is selected, enter the ratio of each compound concentration, compared to the concentration of the reference compound selected in Step 19. For example, if benzene was chosen as a reference compound, leave 1 in the **Conc** column for benzene and type in the relative concentration of every other compound compared to benzene. (See Figure 17-44.)

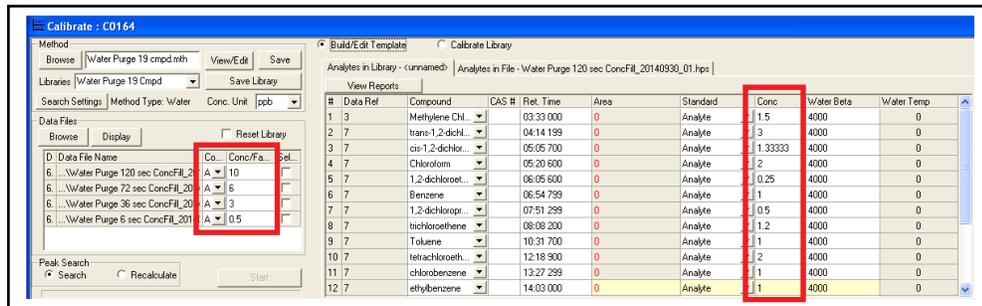
Figure 17-44 Entering concentrations using the Analyte setting

| # | Data Ref | Compound | CAS # | Ret. Time | Area | Standard | Conc | Water Beta | Water Temp |
|----|----------|--------------------|-----------|-----------|------|----------|---------|------------|------------|
| 1 | 3 | Methylene Chl... | 03:33 000 | 0 | | Analyte | 1.5 | 400 | 0 |
| 2 | 7 | trans-1,2-dichl... | 04:14 199 | 0 | | Analyte | 3 | 400 | 0 |
| 3 | 7 | cis-1,2-dichlor... | 05:05 700 | 0 | | Analyte | 1.33333 | 400 | 0 |
| 4 | 7 | Chloroform | 05:20 600 | 0 | | Analyte | 2 | 400 | 0 |
| 5 | 7 | 1,2-dichloroet... | 06:05 600 | 0 | | Analyte | 0.25 | 400 | 0 |
| 6 | 7 | Benzene | 06:54 799 | 0 | | Analyte | 1 | 400 | 0 |
| 7 | 7 | 1,2-dichloropr... | 07:51 299 | 0 | | Analyte | 0.5 | 400 | 0 |
| 8 | 7 | trichloroethene | 08:08 200 | 0 | | Analyte | 1.2 | 400 | 0 |
| 9 | 7 | Toluene | 10:31 700 | 0 | | Analyte | 1 | 400 | 0 |
| 10 | 7 | tetrachloroeth... | 12:18 900 | 0 | | Analyte | 2 | 400 | 0 |
| 11 | 7 | chlorobenzene | 13:27 299 | 0 | | Analyte | 1 | 400 | 0 |
| 12 | 7 | ethylbenzene | 14:03 000 | 0 | | Analyte | 1 | 400 | 0 |

- 21a** The number in the **Conc/Factor** column will be multiplied by the number in the **Conc** column to determine the concentration of every compound. (See Figure 17-45.)

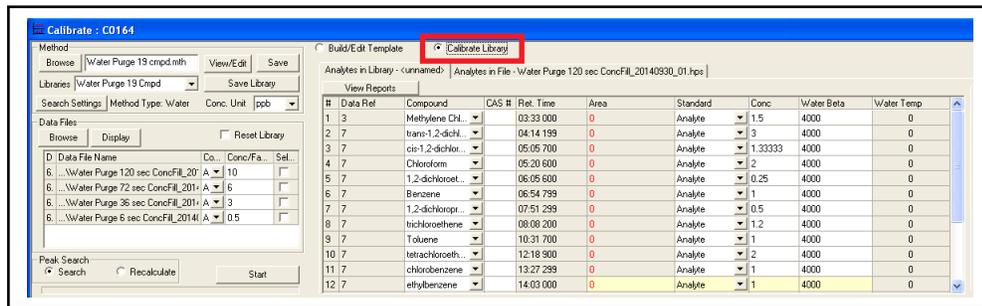
NOTE: For more details about Concentration Reference or Conc/Factor, see section 17.8, Glossary of Terms in the Calibrate Window, on page 17-37.

Figure 17-45 Conc/Factor



22 Select the **Calibrate Library** option. (See Figure 17-46.)

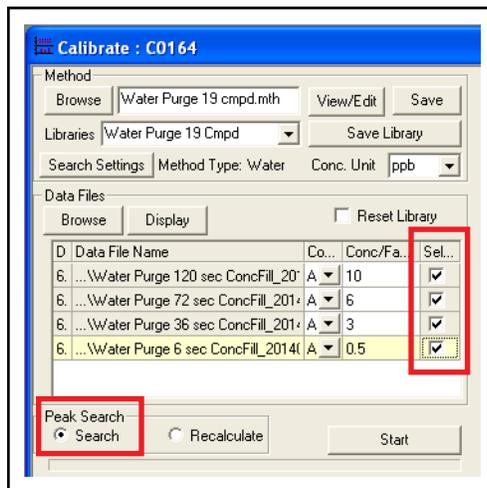
Figure 17-46 Calibrate Library option



23 In the **Peak Search** pane, select **Search**. (See Figure 17-47.)

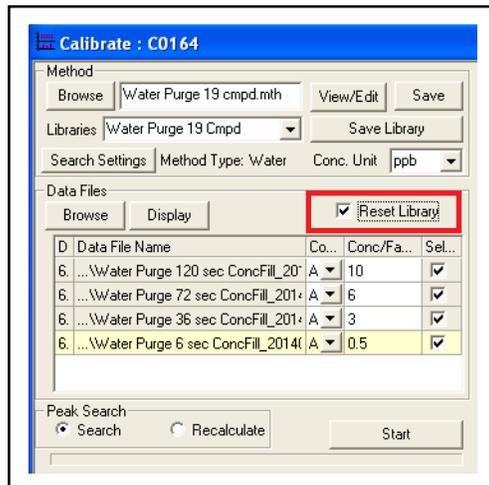
24 In the **Data Files** pane, select the **Select** checkbox for all data files.

Figure 17-47 Selected data files



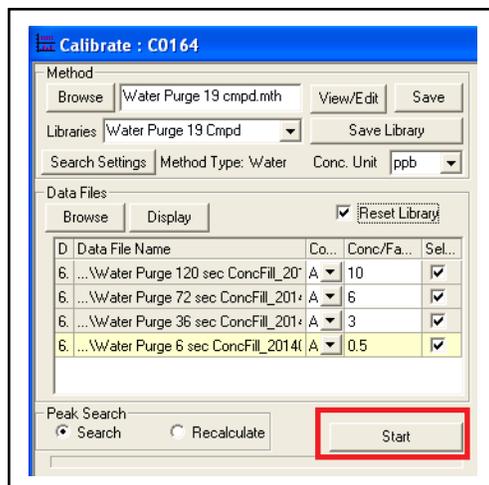
- 25 In the **Data Files** pane, select the **Reset Library** checkbox. (See Figure 17-48.)

Figure 17-48 Reset Library



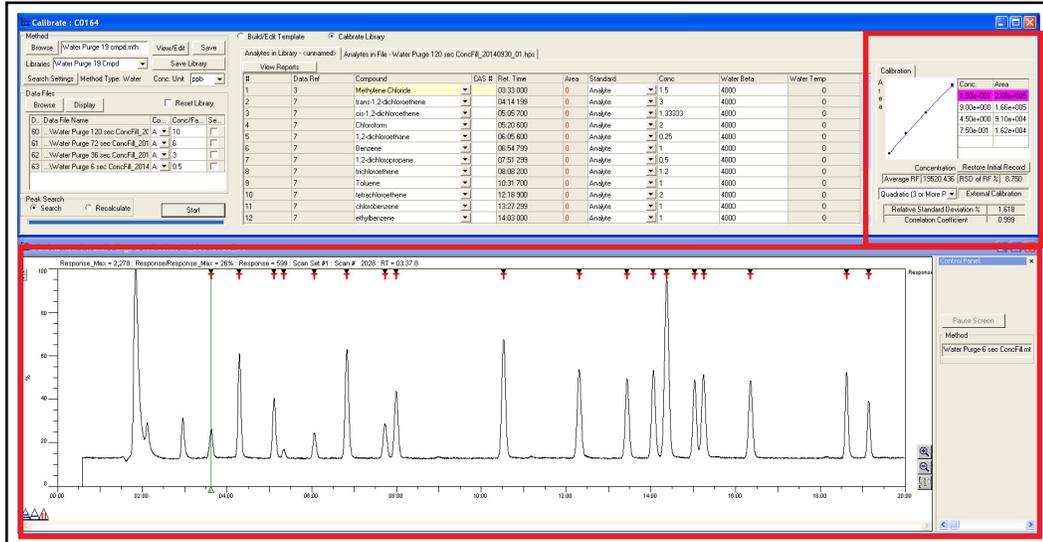
- 26 Click **Start** to calibrate the library. (See Figure 17-49.)

Figure 17-49 Start button



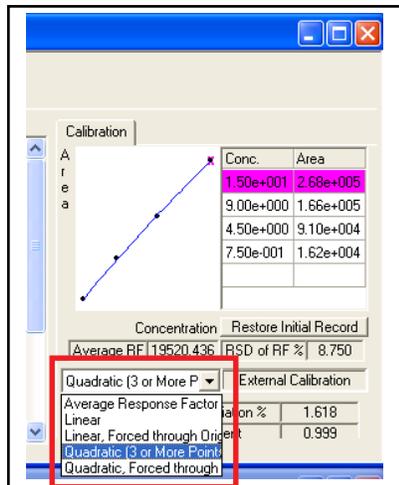
- 27 The method recalibrates using the new data files, displaying new curves in the **Calibration** tab, and shows a chromatogram from one of the data files. (See Figure 17-50.)

Figure 17-50 Method recalibrated



- 28 Select the appropriate curve fit for each analyte in the **Calibration** tab by selecting the desired fit in the shortcut menu. (See Figure 17-51.)

Figure 17-51 Curve fit

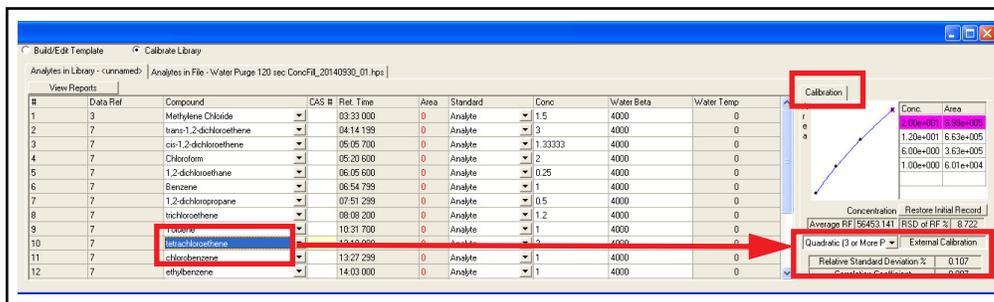


NOTE: Curve fit selection is based on the best fit of the data points.

- 29** In the **Calibration** window, click each analyte to verify the accuracy of each curve fit. Verify the calibration graph for each analyte is populated and does not contain outlying points. The Relative Standard Deviation Percent (%RSD) of each point should be less than 10%. (See Figure 17-52.) See Step 30 for information on outlying points.

NOTE: A minimum of four points are necessary to verify the accuracy of the curve.

Figure 17-52 Calibration curve

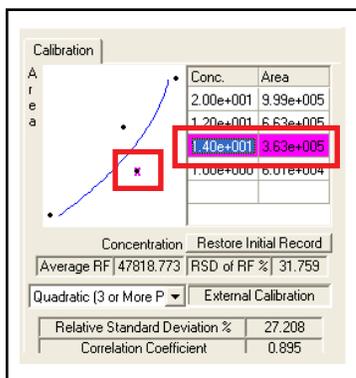


- 30** If an outlying point is found on a curve, the point may be deleted before being replaced. Click the corresponding concentration in the **Calibration** pane. This will highlight the row in pink. Press the **Delete** key on the computer to remove the point. (See Figure 17-53.)

NOTE: Outlying points should be discarded and the standard should be rerun.

NOTE: Click **Restore Initial Record** to restore the data points from the last time the library was saved.

Figure 17-53 Deleting an outlying point

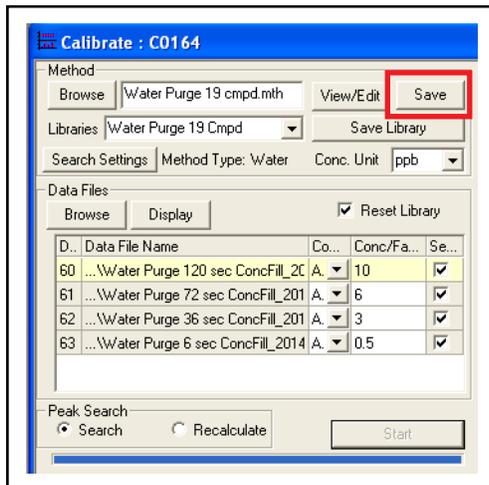


- 31** Calibration points from additional data files can be added to the curve(s) using the **Browse** button under **Data Files**. The method must be recalibrated to add additional points. Return to Step 16 if additional data files are necessary.

- 32** When the library calibration is complete, save the library. (Refer to Step 14 and Step 15.)

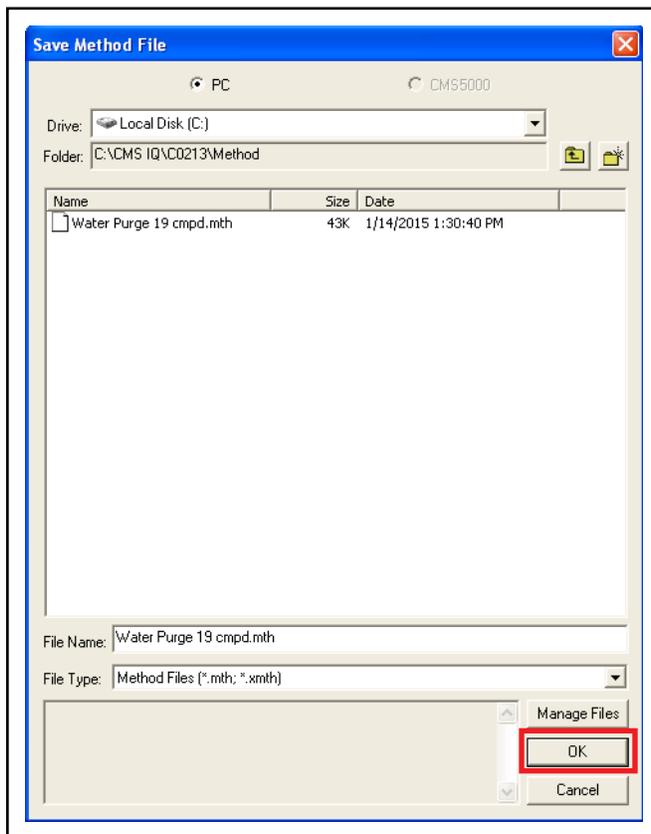
33 To save the method, click **Save** in the **Method** pane. (See Figure 17-54.)

Figure 17-54 Save method



34 Type a file name for the method. Click **OK**. (See Figure 17-55.) The library will now be incorporated into the method.

Figure 17-55 Save library to method

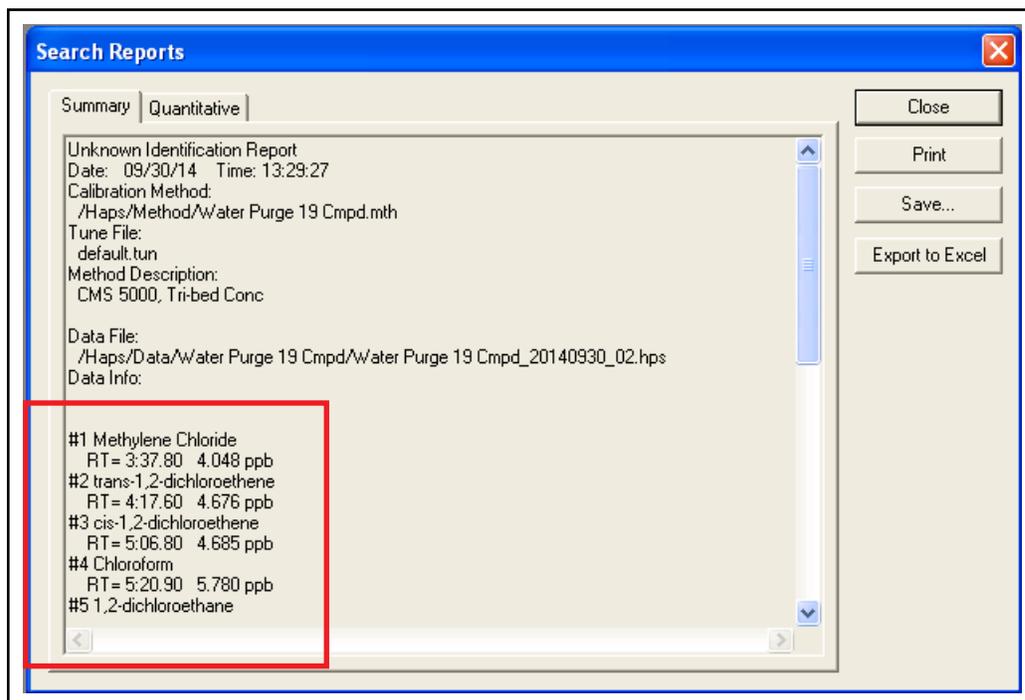


- 35 Once the method is saved, a verification standard must be run to confirm the calibration is accurate. Create a new chemical standard with a concentration somewhere between the highest and lowest concentration standards. Refer to section 17.5.2, *Water Standards*, on page 17-11 for preparing a water standard or section 17.5.3, *Air Standards*, on page 17-14 for preparing an air standard.
- 36 Run the verification standard with the newly calibrated method. Refer to section 17.5.4, *Running Standards*, on page 17-19.
- 37 Open the **Search Report** of the verification standard once the data file is created. Refer to section 13.6.1, *Access Reports*, on page 13-7 to open the **Search Report**.
- 38 Verify the concentration of every compound in the **Search Report** is within 30% of the verification standard's known concentration. If all compounds are within 30%, the verification standard has passed and the calibration is complete. (See Figure 17-56.)

If the verification standard does not pass, prepare a new verification standard and run again.

If the second verification standard does not pass, recalibrate the method. (Refer to section 17.5, *Calibrating the Analytical Method*, on page 17-10.)

Figure 17-56 Verification Standard Search Report



17.7 Water Beta

In water sampling, VOC's are separated from the water by *partitioning*, during the argon bubbling phase. Refer to section 1.1, Introduction, on page 1-1 for details on partitioning.

The partition coefficient of a compound is affected by water temperature. The warmer the water, the lower the partition coefficient, and the more VOC's are extracted by CMS5000 during the purge and trap process.

If a sample is at a different temperature than the standards used during calibration, the change in the partition coefficient will reduce the accuracy of results. CMS5000 records the water temperature during sample collection. When **Water Adjustment** is enabled in CMS IQ, CMS5000 adjusts results to account for the difference in temperature. Refer to section 12.6.8.2, Enable Water Adjustment, on page 12-65 for enabling the **Water Adjustment**.

The adjusted concentration of a compound is calculated based on the difference between the calibration temperature and reading temperature. (See equation [9].)

$$C_{tc_i} = C_i \times e^{\beta_i \left(\frac{1}{T_m} - \frac{1}{T_c} \right)} \quad [9]$$

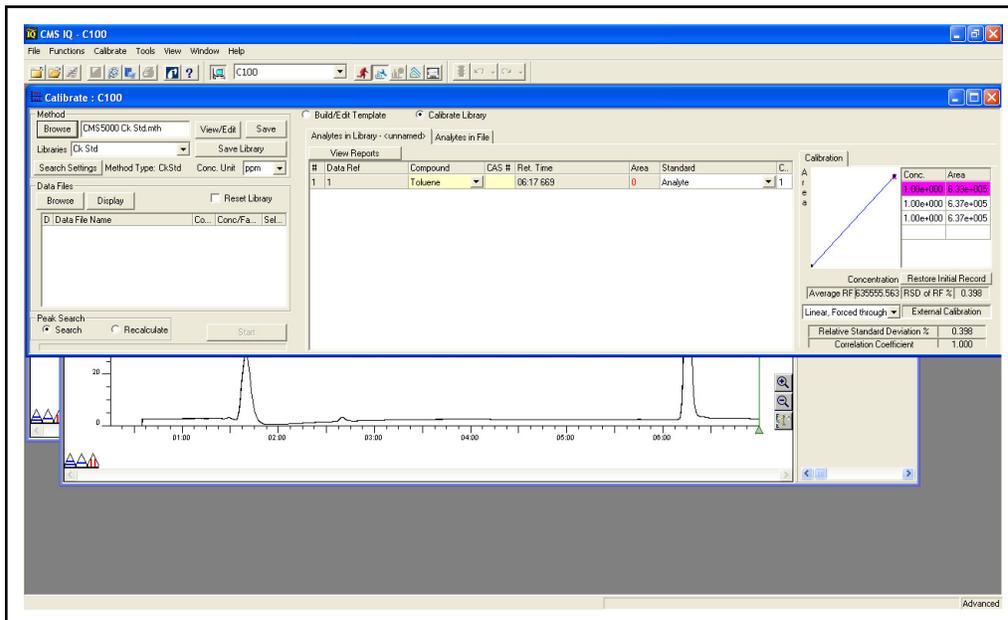
- ◆ C_{tc_i} is the adjusted compound concentration
- ◆ C_i is the initial compound concentration
- ◆ T_m is the temperature in kelvin during sample collection
- ◆ T_c is the temperature in kelvin during calibration
- ◆ β_i is the **Water Beta** value

A **Water Beta** value is assigned to each compound during method development to adjust for changes in water temperature.

The default value for the **Water Beta** is 4000. The **Water Beta** of individual compounds can be found in reference literature or can be determined experimentally.

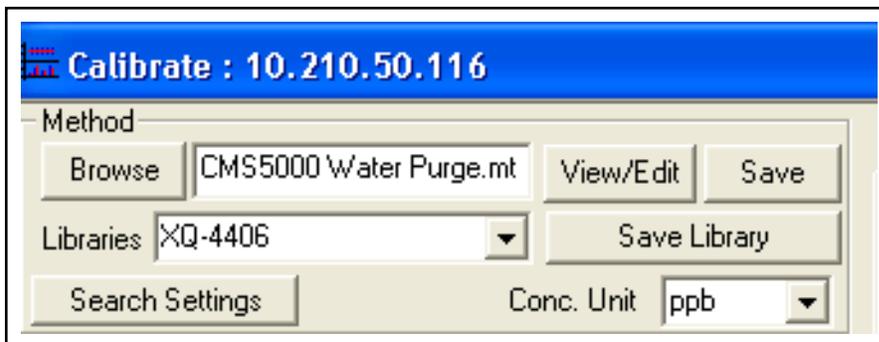
17.8 Glossary of Terms in the Calibrate Window

Figure 17-57 Calibrate window



17.8.1 Method

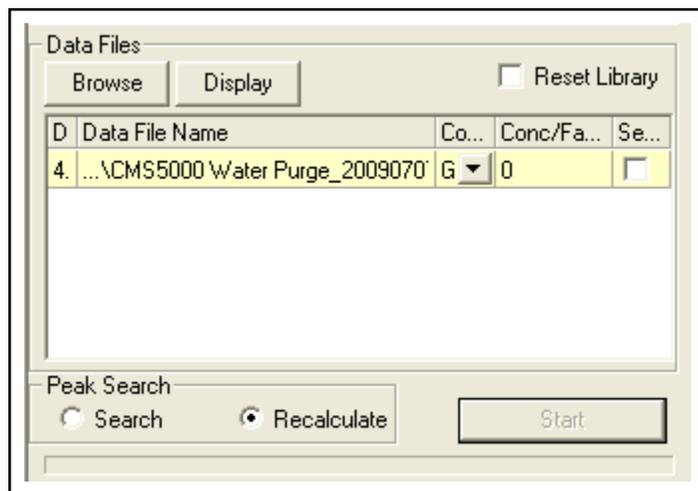
Figure 17-58 Method section



- Browse** Opens the Method Selection window
- View/Edit** Opens the Method Editor with the current method
- Save** Saves the current method
- Libraries** Displays the currently saved libraries
- Save Library** Opens the window to save the library
- Search Settings** Displays the Search Parameter settings
- Conc. Unit** Defines the concentration units

17.8.2 Data Files

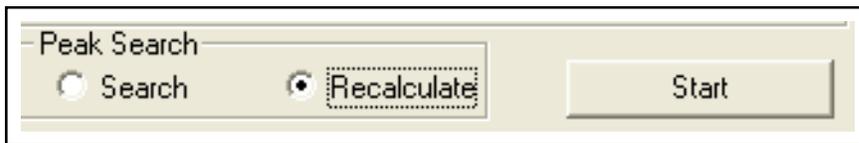
Figure 17-59 Data Files section



- Display** Displays the chromatogram for the selected data file
- Reset Library** When selected, will delete all previous data points in the library during calibration
- Browse** Selects the data files for building and calibrating the library
- Data Ref (D)**. Displays the data file reference number
- Data File Name** Displays the data file name and path
- Conc Ref (Co...)** Basis for calculating the concentration of data files. When **Global** is selected, the **Conc/Factor** column represents the concentration of all compounds. When **Analyte** is selected, the **Conc/Factor** column is multiplied by value in the **Conc** box of each analyte in the library. See [section 17.8.7, Calibrate Display](#), on page 17-41 for information on the **Conc** column in the library
- Conc/Factor (Conc/Fa...)** The concentration of the chemicals in the data file. The value is dependant on the **Conc Ref**. (Refer to [Step 18](#) through [Step 21a](#))
- Selection (Se...)**. When selected, the file will be processed when **Start** is selected

17.8.3 Peak Search Section

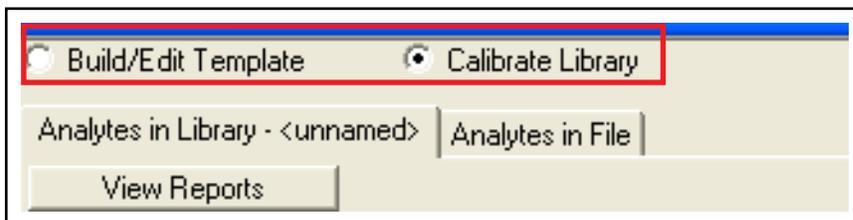
Figure 17-60 Peak Search section



- Search** Performs a peak search and calculates peak areas during calibration
- Recalculate** Recalculates the peak areas without performing a peak search during calibration. This is most useful after manual editing of peak baseline points
- Start** Initiates calibration

17.8.4 Calibrate Options

Figure 17-61 Template / Calibrate section



- Build/Edit Template** When selected, identifies analytes and retention times to build the calibration library template
- Calibrate Library** When selected, data files are processed to calibrate the library

17.8.5 Analytes

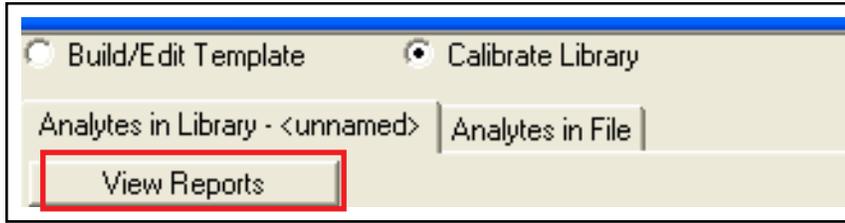
Figure 17-62 Analytes Tabs



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

17.8.6 View Reports

Figure 17-63 View Reports



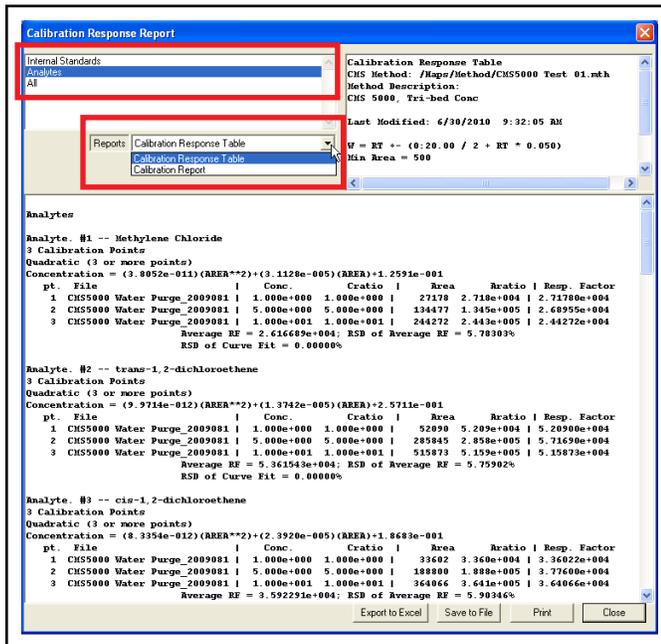
If View Reports is clicked, the following window and options are displayed. (Refer to Figure 17-63.)

NOTE: Select **Analytes** from the box at the top of the screen.

Calibration Response Table . . . Report that displays the response factor and curve statistics based on the selected curve type for each calibration standard

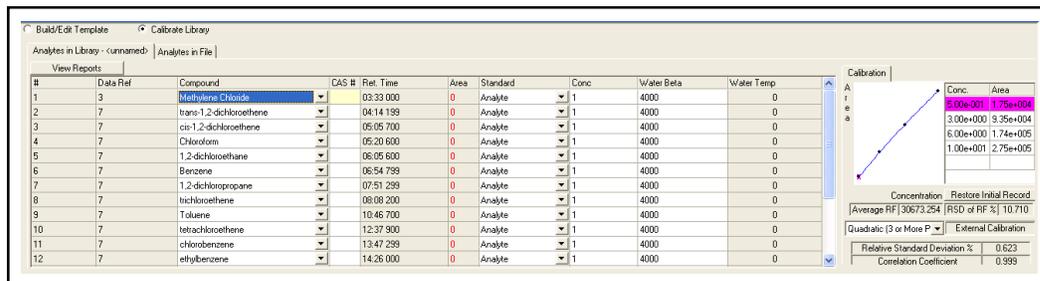
Calibration Report Report that displays the retention time, the area, and concentration of each calibration standard (See Figure 17-64.)

Figure 17-64 View Reports



17.8.7 Calibrate Display

Figure 17-65 Calibrate display



- #** The assigned analyte number in the library
- Data Ref** Displays the data file reference number of the data file used to add the peak to the library. Refer to [section 17.8.2, Data Files](#), on [page 17-38](#)
- Compound** Displays the analyte name that is assigned by the user
- CAS #** Chemical Abstracts Service number. This is a unique number assigned to each chemical that is accepted world-wide
NOTE: CAS# must be added by the user.
- Ret. Time** The retention time for the analyte
- Area** Displays the integrated analyte area
- Standard** Designates the compound as an analyte or an internal standard
NOTE: Analyte is typically selected, as most CMS5000 methods do not use internal standards.
- Conc.** Displays the concentration of the analyte relative to the other analytes
- Water Beta** Value used in concentration calculation that corrects for changes in water temperature. Refer to reference literature to obtain these values. For water methods only
- Water Temp** The temperature of the water being analyzed by CMS5000 at the time of calibration. For water methods only

Chapter A

Appendix

A.1 Modbus Protocol

The CMS ModBus server listens on TCP port 502.

All Strings are null terminated.

Timestamps are the number of seconds since midnight on 1/1/70 - UTC

Register Map -

0 : 699 - Analog Input Registers (read-only)

700 : 799 - Holding Register (read-write)

800 : 10000 - Analog Input Registers (read-only)

0: Status - 32 bit integer - 2 words

Bit 0 - restarting The system is restarting, rebooting or shutting down. When this bit is set, all other information on the modbus is invalid.

Bit 1 - method is running

Bit 2 - method is complete The method has finished its run, but hasn't exited yet (probably waiting for SEL).

Bit 3 - script is running

Bit 4 - script is sleeping between methods

Bit 5 - method is warming up

Bits 6-25 - undefined (all 0)

Bit 26 - system is waiting for user input

Bit 27 - Alarm

Bit 28 - Heater Timeout

Bit 29 - Argon Pressure Warning

Bit 30 - Argon Pressure Error

Bit 31 - System Error

6: Current Argon Pressure - float - 2 words

8: Current Water Temperature - float - 2 words

100: Current Method - 100 words - string

Return currently running method, empty string if no method is running

200: Current Script - 100 words - string

Return current script, empty string if no script is running

300: Current Message - 100 words

Return the status line from the bottom of the current screen. This is two parts separated by a | giving the left and right sides of the line.

400: Current Alarm Message - 100 words

700: Command - 100 words - command to execute Write a string to this field to execute a command on CMS5000. The string may be one of the following:

run "method" - run the specifies method. Method should be the full path and in quotes (e.g. run "/Method/Ck Std.mth")

abort - abort the current method

restart -

reboot -

shutdown - restart, reboot or shutdown the instrument

key keylist - simulate one or more key presses. Keylist may contain the following:

R - Run

P - Stop

H - Help

T - Stat

E - Escape

U - Up

D - Down

L - Select

0 1 2 3 4 5 6 7 8 9 - numbers 0-9

V - Save

C - Clear

sending the command "key EUL" would be the same as pressing the Escape, Up and Select keys one after the other.

Examples:

run "/Method/Ck Std.mth" - runs the method Ck Std.mth

key 4L1L1L- simulates pressing keys 4 SEL 1 SEL 1 SEL

reboot- reboots the system

800: Response - string - 100 words - response to last command

When a command is written to address 700, the response is set to "PENDING."

After the command has been processed by CMS5000, the response is set to either "OK" or "ERROR: error message"

Results Section:

The Results Section contains the results from the most recent run.

The sequence number is an arbitrary number that is incremented each time the results are updated. To make sure the results haven't changed while reading, read the sequence number first, read all of the results of interest, then read the sequence number again to make sure it is the same.

Address Field

1000 Sequence Number - 2 words

1002 Timestamp - 2 words - timestamp = time method started

1004 Number of Records - 1 word

1005 Flags - 1 word

Bit 0 - Alarm in records

1006 Argon Pressure = 2 words - float in kPa, -1.0 if not recorded

1008 Water Temperature - float in degrees C, -1.0 if not recorded

1010 Calibration Water Temperature - float in degrees C, -1.0 if not recorded

1100 Method Name - 100 words - name of method file - string

1200 DataFile Name - 100 words - name of data file - string

2000 Start of compound records.

Each records is 100 words. There can be up to 630 records (1000 - 64000).

Each record is a string with the following fields:

RECNO

CASNUM

Target name

Predicted RT

Actual RT

Area

Conc

No Adjust

Limit

Flags

The fields are separated by pipe characters ("|"). Any field that isn't being set by the current method is left empty.

A.2 Ethernet Integration

CMS5000 can be programmed to be integrated into the site's water monitoring system. The CMS5000API is a simple C/C++ programming interface that provides software programmers access to the CMS5000's basic control and status functions from within their applications. The CMS5000 API is not a stand-alone application; it is used by programmers to build their own applications.

CMS5000 API files:

CMS5000api.h (Header file)

CMS5000api.dll (Windows Dynamic Link Library)

CMS5000api.lib (Import library used to link to
CMS5000api.dll)

In addition to the CMS5000 API files, a sample application (CMS5000tester.exe) is provided that will start a method, get status as the method runs, then display some results when the method finishes. The source code for CMS5000tester.exe is provided along with a Microsoft VC++ project that can be used to build it.

A.2.1 CMS5000API.H

```
//-----
// CMS5000api.h provides an API for accessing a CMS5000's basic control and status functions.
//
// The following four lines of code (error checking omitted) show the proper steps for
// connecting to a CMS5000, starting a method, and then disconnecting.
//
// CMS5000_HANDLE CMS5000_handle;
//
// CMS5000_Connect( &CMS5000_handle, _T("10.1.1.1") );
//
// CMS5000_Run_Method( CMS5000_handle, _T("/Method/MyMethod.mth") );
//
// CMS5000_Disconnect( CMS5000_handle );
//
//-----

// The following ifdef block is the standard way of creating macros which make exporting
// from a DLL simpler. All files within the DLL are compiled with the CMS5000API_EXPORTS
// symbol defined on the command line. this symbol should not be defined on any project
// that uses the DLL. This way any other project whose source files include this file see
// CMS5000API_API functions as being imported from a DLL, whereas the DLL sees symbols
// defined with this macro as being exported.
#ifdef CMS5000API_EXPORTS
#define CMS5000API __declspec(dllexport)
#else
#define CMS5000API __declspec(dllimport)
#endif

#include "stdlib.h"

typedef void* CMS5000_HANDLE;

/*****
* Warnings Codes
*****/
#define CMS5000_WARN_NONE 0
#define CMS5000_WARN_GC_COLUMN_TEMPERATURE 1
#define CMS5000_WARN_VALVE_OVEN_TEMPERATURE 2
#define CMS5000_WARN_AI_DETECTOR_TEMPERATURE 3
#define CMS5000_WARN_CARD_CAGE_TEMPERATURE 4
#define CMS5000_WARN_WATER_TEMPERATURE 5
#define CMS5000_WARN_CK_STD_TEMPERATURE 6
#define CMS5000_WARN 9

/*****
* Method State may be one of the following:
*
* NONE - No method running
* WARMUP - Method is warming up
* WAITING - Method is waiting for RUN key to be pressed
* RUNNING - Method is running
* SEARCHING - Method has finished running, but is still searching
```

```

* COMPLETED - Method has completed and is waiting for user to press ESC
* FINISHED - Method has finished and is no longer active
*
*****/
#define CMS5000_MTHSTATE_NONE      0
#define CMS5000_MTHSTATE_WARMUP   1
#define CMS5000_MTHSTATE_START    2
#define CMS5000_MTHSTATE_WAITING  3
#define CMS5000_MTHSTATE_RUNNING  4
#define CMS5000_MTHSTATE_SEARCHING 5
#define CMS5000_MTHSTATE_COMPLETED 6
#define CMS5000_MTHSTATE_FINISHED 7

/*****
* Length Constants
*****/
#define METHOD_LENGTH      1024
#define FILE_NAME_LENGTH  1024
#define CASNUM_LENGTH     16
#define COMP_NAME_LENGTH  128
#define UNITS_LENGTH      16
#define PROMPT_MSG_LENGTH 2048

/*****
* Data Structures
*****/
typedef struct CMS5000API hw_status {
    float GCColumnTemp;
    float AIDetectorTemp;
    float GCBaoardTemp;
    float WaterTemp;
    float CkStdTemp;
    float RegulatorTemp;
    float InternalTemp;
    float ValveTemp;
    long  RESERVED1[8];
    float CarrierSupplyPressure;
    long  RESERVED2[15];
} HardwareStatus;

typedef struct CMS5000API sys_status {
    long  MethodState;
    long  WarningID;
    long  AnalyteAlarm; // check report file for specifics.
    long  ErrorFlag; // Fatal Error Exist. Check ErrorMessage.
    wchar_t ErrorMessage [PROMPT_MSG_LENGTH];
    long  RESERVED[29];
} SystemStatus;

typedef struct CMS5000API results_info {
    wchar_t MethodName [METHOD_LENGTH];
    
```

```

        wchar_t DataFileName [FILE_NAME_LENGTH];
        long SearchCount;
        long RESERVED[32];
    } ResultInfo;

typedef struct CMS5000API search_result {
    wchar_t CASNUM [CASNUM_LENGTH];
    wchar_t Compound [COMP_NAME_LENGTH];
    long Retention_Time;
    float Area;
    wchar_t Units [UNITS_LENGTH];
    float Concentration;
    float AlarmLevel;
    long RESERVED[345];
} SearchResult;

/*****
* Function Return Codes
* If function return is 0: No Error
* If function return is negative: CMS5000 error
* If function return is positive: Windows Error
*
*****/

#define RTN_NO_ERROR 0
#define RTN_CONNECTION_TIMED_OUT -1
#define RTN_CMD_INVALID_COMMAND_ARG -2
#define RTN_CMD_INVALID_METHOD_NAME -3
#define RTN_METHOD_NOT_FOUND -4
#define RTN_METHOD_ALREADY_RUNNING -5
#define RTN_COM_ERROR -6
#define RTN_ERROR -9

/*****
* CMS5000_Connect
*
* Connects to a CMS5000. Each Successful Connect must be paired with a Disconnect.
*
* Parameters
* CMS5000 : [OUT] Handle to a CMS5000
* CMS5000_ip_address : [ IN] IP address of CMS5000 you wish to connect to
*
* Returns
* See Function Return Codes
*
* Example
* CMS5000_Connect( &CMS5000_handle, _T("10.210.50.101") );
*
*****/
CMS5000API int CMS5000_Connect (CMS5000_HANDLE* CMS5000, const wchar_t*
```

```

CMS5000_ip_address);

/*****
* CMS5000_Disconnect
*
* Disconnects with CMS5000 and free's up associated resources.
* Each Successful Connect must be paired with a Disconnect.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Disconnect( CMS5000_handle );
*****/

CMS5000API int CMS5000_Disconnect (CMS5000_HANDLE CMS5000);

/*****
* CMS5000_Restart
*
* Restarts software running on CMS5000.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Restart( CMS5000_handle );
*****/

CMS5000API int CMS5000_Restart (CMS5000_HANDLE CMS5000);

/*****
* CMS5000_Reboot
*
* Reboots the unit.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Reboot( CMS5000_handle );
*****/
    
```

```
CMS5000API int CMS5000_Reboot (CMS5000_HANDLE CMS5000);
```

```

/*****
*
* CMS5000_Shut_Down
*
* Turns CMS5000 off.
* ** NOTE ** There is no way to remotely turn CMS5000 back on once it is Off.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Shut_Down( CMS5000_handle );
*
*****/

```

```
CMS5000API int CMS5000_Shut_Down (CMS5000_HANDLE CMS5000);
```

```

/*****
* CMS5000_Run_Method
*
* Runs a method
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*   method : [ IN] Full path to method (capitalization sensitive)
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Run_Method( CMS5000_handle, _T("/Method/CMS5000 Ck Std.mth") );
*
*****/

```

```
CMS5000API int CMS5000_Run_Method (CMS5000_HANDLE CMS5000, const wchar_t*
method);
```

```

/*****
* CMS5000_Set_Startup_Method
*
* Sets the Startup Method
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*   method : [ IN] Full path to method (capitalization sensitive)
*
* Returns
*   See Function Return Codes.
*
* Example

```

```

*   CMS5000_Set_Startup_Method( CMS5000_handle, _T("CMS5000 Ck Std.mth") );
*
*****/
CMS5000API int CMS5000_Set_Startup_Method (CMS5000_HANDLE CMS5000, const
wchar_t* method);

/*****
* CMS5000_Stop_Method
*
* Stops Currently Running Method.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Stop_Method( CMS5000_handle );
*
*****/
CMS5000API int CMS5000_Stop_Method (CMS5000_HANDLE CMS5000);

/*****
* CMS5000_Get_Hardware_Status
*
* Retrieves Hardware Status.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*   hw_status : [OUT] Pointer to a HardwareStatus stuct.
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Get_Hardware_Status( CMS5000_handle, &hw_status );
*
*****/
CMS5000API int CMS5000_Get_Hardware_Status (CMS5000_HANDLE CMS5000, Hardwar-
eStatus* hw_status);

/*****
* CMS5000_Get_System_Status
*
* Retrieves System Status.
*
* Parameters
*   CMS5000 : [ IN] Handle to a CMS5000
*   sys_status : [OUT] Pointer to a SystemStatus stuct.
*
* Returns
    
```

```

*   See Function Return Codes.
*
*   Example
*   CMS5000_Get_System_Status( CMS5000_handle, &sys_status );
*
*****/
CMS5000API int CMS5000_Get_System_Status (CMS5000_HANDLE CMS5000, SystemSta-
tus* sys_status);

/*****
* CMS5000_Get_Result_Info
*
*   Retrieves Results Info.
*
*   Parameters
*   CMS5000      : [ IN] Handle to a CMS5000
*   result_info : [OUT] Pointer to a ResultInfo stuct.
*
*   Returns
*   See Function Return Codes.
*
*   Example
*   CMS5000_Get_Result_Info( CMS5000_handle , &result_info );
*
*****/
CMS5000API int CMS5000_Get_Result_Info (CMS5000_HANDLE CMS5000, ResultInfo*
result_info);

/*****
* CMS5000_Get_Result
*
*   Retrieves Search Result for an unknown. This function can be used to iterate
*   through the array of found compounds.
*
*   Parameters
*   CMS5000      : [ IN] Handle to a CMS5000
*   search_result : [OUT] Pointer to a SearchResult stuct.
*   num          : [ IN] Index of specific SearchResult within the array of found
*                 compounds. The number of found compounds is provide by
*                 ResultInfo.SearchCount, obtained through CMS5000_Get_Result_Info().
*                 Valid range: 0 <= 'num'< SearchCount-1 [for SearchCount > 0]
*
*   Returns
*   See Function Return Codes.
*
*   Example
*   CMS5000_Get_Result( CMS5000_handle ,&search_result, num );
*
*****/
CMS5000API int CMS5000_Get_Result (CMS5000_HANDLE CMS5000, SearchResult*
search_result, int num);
    
```

```

/*****
* CMS5000_Get_All_Results
*
* Retrieves a pointer to a list of SearchResult struct.
*
* Parameters
*   CMS5000           : [ IN] Handle to a CMS5000
*   search_results[] : [OUT] Array of SearchResult structs.
*   max_results      : [ IN] Max number of results your buffer can hold.
*   num_results      : [ IN] Number of actual results recieved from CMS5000.
*
* Returns
*   See Function Return Codes.
*
* Example
*   CMS5000_Get_All_Results( CMS5000_handle, &search_result_buffer, 100, &num_results );
*
*****/
CMS5000API int CMS5000_Get_All_Results (CMS5000_HANDLE CMS5000, SearchResult
search_results[], int max_results, int* num_results);

```