Questor 5 for MAX300-CAT

Revision 2

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For further information or assistance, please contact:

Extrel CMS, LLC
575 Epsilon Drive
Pittsburgh, Pennsylvania 15238
USA

General Inquiries:	Telephone:	(412) 963 – 7530
	Fax:	(412) 963 – 6578
	Email:	info.pitt@process-insights.com
Technical Support:	Telephone:	(412) 967 – 5754
	Fax:	(412) 963 – 6578
	Email:	support.pitt@process-insights.com
Field Service:	Email:	schedule.pitt@process-insights.com
Sales:	Email:	info.pitt@process-insights.com
Website:	https://process-insights.com/	

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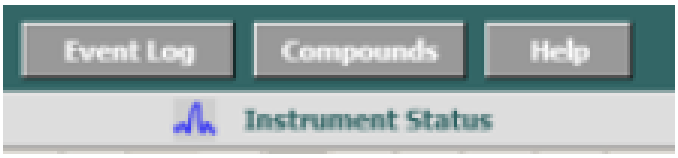
MAX-300 CAT Questor 5 Guide

1. Software Overview

1.1 Questor 5 Software: A Quick Tour

This section will give the user guided tour of Questor 5 and the generalized functions of its tabs.

Under the Questor5 main page, the *Instrument Status, Event Log, Compounds,* and *Help* buttons are located at the far-right of the screen and are always available when navigating Questor5.	
The *Instrument Status* icon changes based on the current state of the instrument.	Indicates the Instrument is Idle. Indicates the Instrument is in Tune mode. Indicates the Instrument is in Analysis mode. Indicates the Instrument is in Sequence mode. Indicates the Instrument is in Survey Scan mode. Indicates the Instrument is performing a Smart Start of downloading firmware.

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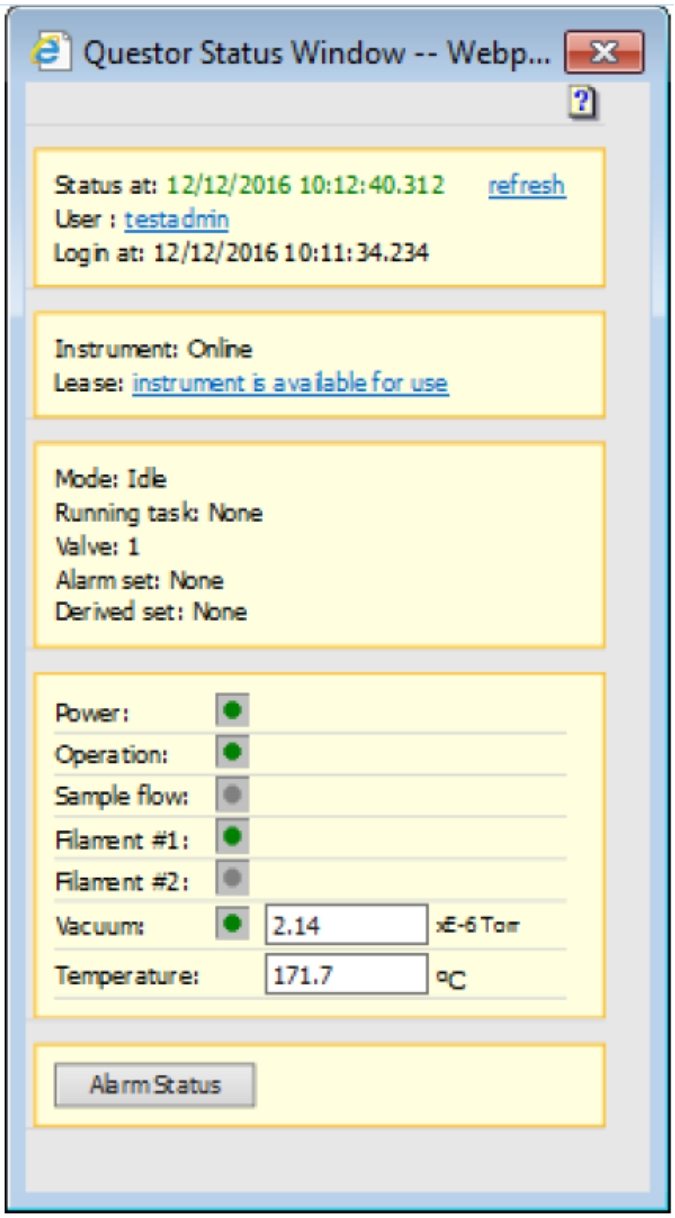
The status of the instrument can be displayed by letting the mouse pointer "hover" over the icon. Clicking on the icon will open the Instrument Status window. The Instrument Status window opens to display the Status of the instrument itself, as well as other parameters like the vacuum pressure and operation status.	
The *Home Tab* is the initial page that Questor 5 will open to. The home page allows for: • Editing of User profiles. • Booting and shutting down of the Questor 5 server. • Accessing of the Event Log.	

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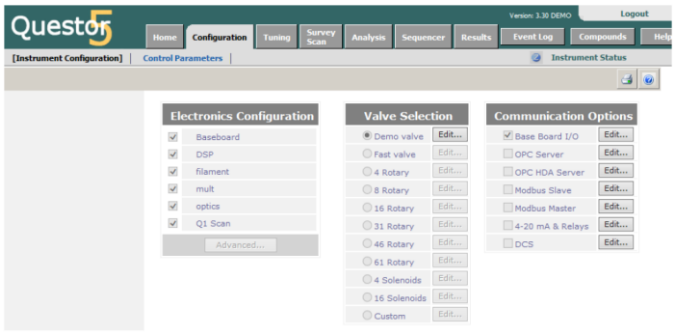
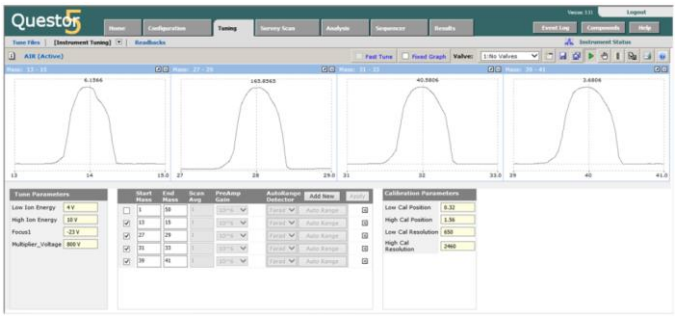
The *Configuration Tab* is used to define the hardware installed in the mass spectrometer, including the inlet valves and external communication methods that Questor 5 is using. This tab also allows the user control over certain physical parameters such as the main power to the instrument and filament selection and emission current.	
The *Tuning Tab* allows the user to select, create, and configure the files for defining the instruments basic operating parameters. The goal of the *Tuning Tab* is to define the parameters the instrument uses to create peaks suitable for analysis from the signals It receives from the samples.	

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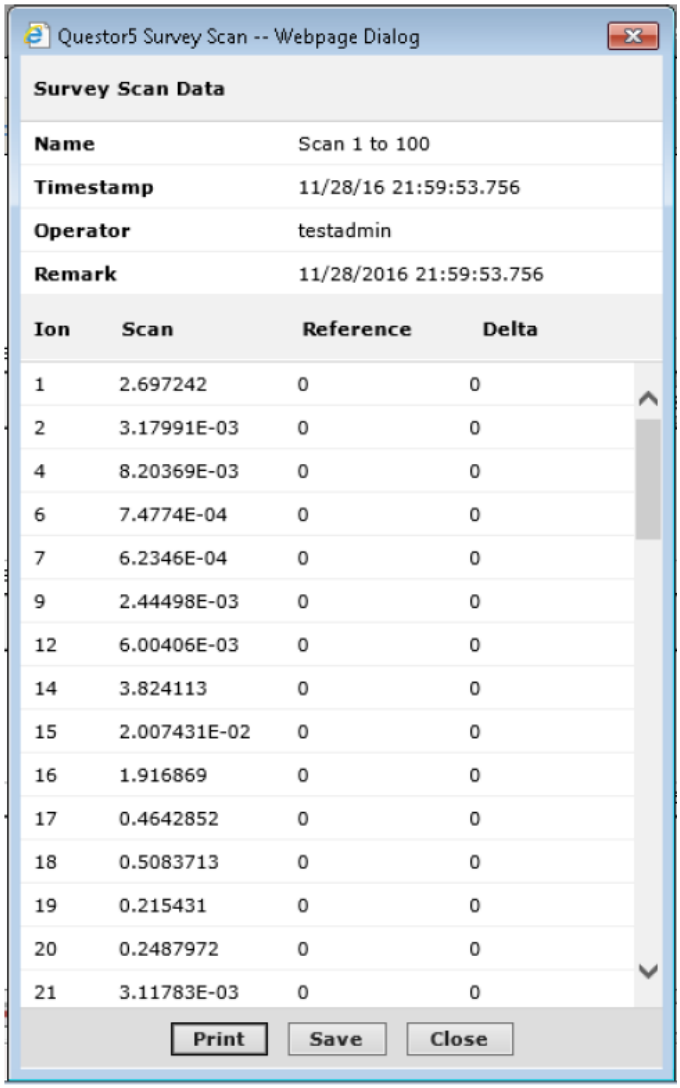
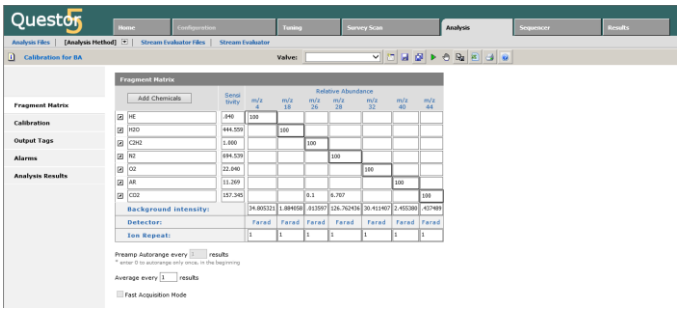
The *Survey Scan Tab* allows the user to use the mass spectrometer in its most fundamental mode: looking at everything that appears in user-defined mass range. The data is displayed in the form of a bar graph with M/z as the X-axis and the intensity as the Y-axis.	
The *Analysis Tab* is used to select, create, or edit files for the quantitative analysis methods used to generate and interpret the data from the mass spectrometer. **Note:** The results will be displayed under the *Analysis Results Tab.*	

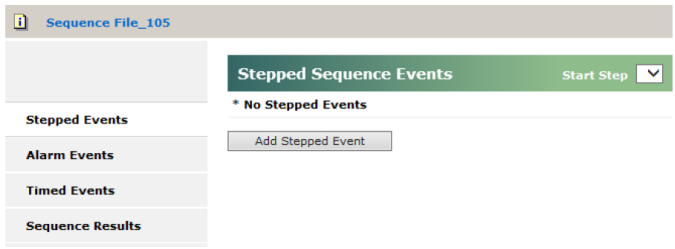
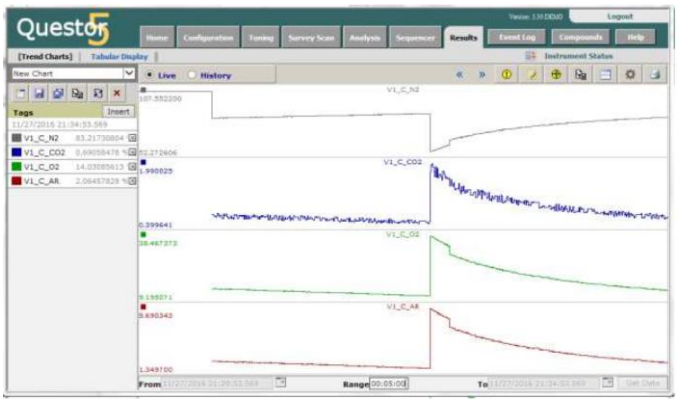
Questor5 Survey Scan -- Webpage Dialog

Survey Scan Data

Name	Scan 1 to 100
Timestamp	11/28/16 21:59:53.756
Operator	testadmin
Remark	11/28/2016 21:59:53.756

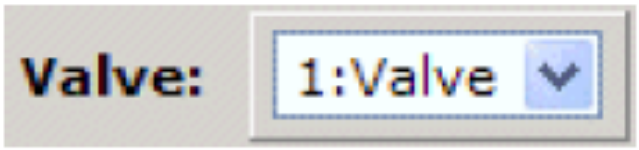
Ion	Scan	Reference	Delta
1	2.697242	0	0
2	3.17991E-03	0	0
4	8.20369E-03	0	0
6	7.4774E-04	0	0
7	6.2346E-04	0	0
9	2.44498E-03	0	0
12	6.00406E-03	0	0
14	3.824113	0	0
15	2.007431E-02	0	0
16	1.916869	0	0
17	0.4642852	0	0
18	0.5083713	0	0
19	0.215431	0	0
20	0.2487972	0	0
21	3.11783E-03	0	0

Print Save Close

The *Sequencer Tab* allows the user to create and edit files that define an automated sequence of operations Questor 5 will perform. There are three types of events; stepped events, alarm events, and timed events.	
The *Results Tab* allows the user to examine real-time and historical data. The data can also be exported from this tab into multiple forms, including an *Excel* [tm] spreadsheet.	

1.2 Button Descriptions

The Questor 5 Software *has buttons unique to it and its functions. This section will give the user a guided tour of these buttons and their functions.*

The *Valve Button* allows the user to select a specific valve and specific label of the port on that valve for the system to use. The valves can be called in other functions of Questor 5 and the format is <installed valve number>:<Valve port label>. The label for the valve port defaults to the number of the port. **Ex**: "1:Air" refers to valve port 1, assigned the description "Air". These labels can be changed into something more descriptive at *Configuration Tab > Instrument Configuration > Valve Selection> Edit*.	

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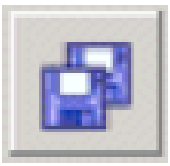
The *Create New File Button* allows the user to create a new file within the current window. **Ex:** If it is used within the *Tune Tab*, a new Tune file will be created.	
The *Save Button* allows the user to save files using the same name as the currently selected file, overwriting its current data. This button is accessed in the same windows as the *Create New File Button.* **Note:** This button is only available once a parameter has been changed so the user can save the modified parameter.	
The *Save As Button* allows the user to save the currently selected file under a different name, preserving the previously created file and creating a new one. This button is accessed in the same windows as the *Create New File Button.* **Note:** This button is only available once a parameter has been changed so the user can save the modified parameter.	
The *Start Button* allows the user to implement the currently selected file or set of parameters to control the instrument. This button is accessed in the same windows as the *Create New File Button.*	
The *Stop Button* allows the user to stop the current acquisition or applied process and put the instrument in idle mode. This button is accessed in the same windows as the *Create New File Button.*	

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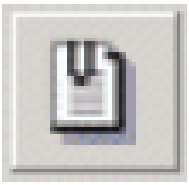
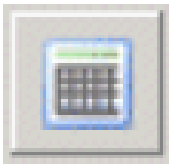
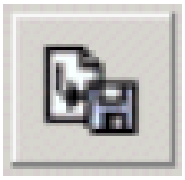
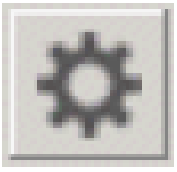
The *Set as Reference Scan Button* allows the user to use the currently displayed scan in a *Survey Scan* as the reference scan to be displayed in the *Reference Scan* plot area. This button is accessed only in the *Survey Scan Tab.*	
The *Show Data as Table Button* allows the user to display the latest set of acquired data in a table format.	
The *Show Derived Tags Button* allows the user to display the previously defined derived (Calculated) values derived from the lates set of acquired data.	
The *Export File Button* allows the user to export the template file to the Windows clipboard where it can be pasted into Notepad and saved as a .TXT file for future reference or importing to another installation.	
The *Export Data Button* allows the user to export the data acquired, into various formats useful in other applications like Excel™, .TXT, .CVS, and other file types.	
The *Trender Settings Button* allows the user to adjust the Trender (strip chart-like display) parameters.	
The *Print Button* allows the user to send a copy of the current screen to the Windows default printer screen.	

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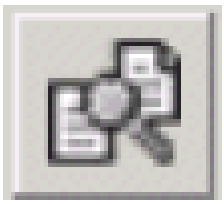
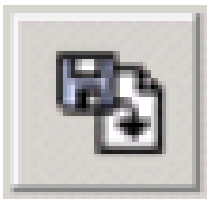
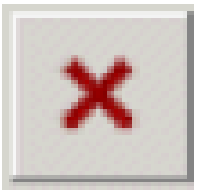
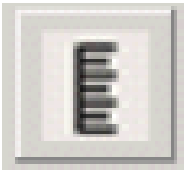
The *Help Button* allows the user to open the help system within Questor 5, which has a table of contents on the functions of Questor 5, and frequently asked questions.	
The *Import Reference Scan from Chemical Library Button* allows the user to use the mass spectrum specified in the Questor 5 chemicals and compounds library as the *Survey Scan* reference scan.	
The *Import Reference scan from .MSP Button* allows the user to use a mass spectrum in a NIST Library .MSP file as the *Survey Scan* reference scan.	
The *Delete Button* allows the user to delete the specified item currently in use (scan, tag, parameter, etc.)	
The *Auto Scan Button* in the *Tune Tab* allows the user to automatically adjust the scaling on mass windows to display the entire peak of all masses within the window, using the highest intensity signal as the reference point.	
The *Chart Forward Button* allows the user to move the window in which the data is displayed forward in time to display more recent data.	
The *Analysis Tab* has buttons to allow the user to navigate and configure the display of data collected over a period of time and will be discussed in the *Analysis Tab* section of the *MAX300-CAT Questor 5 User Guide*.	

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MAX-300 CAT Questor 5 Guide

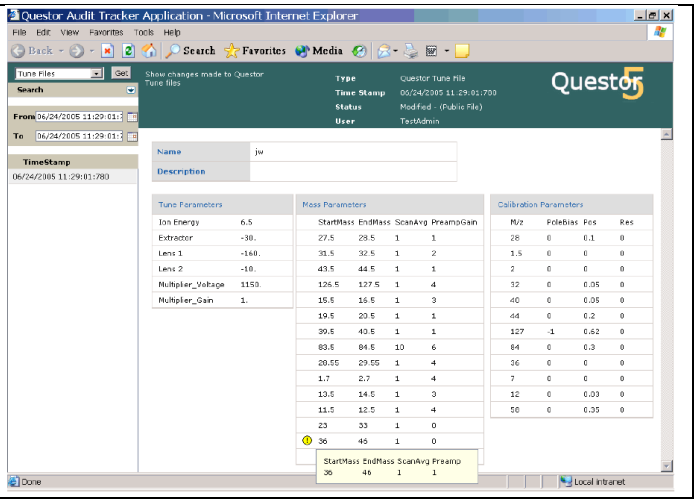
2. The Home Tab

2.1 Home Tab Introduction

This section will give the user an in-depth introduction to the Home Tab and outline the topics for further exploration in the Home Tab *section of the* MAX300-CAT Questor 5 Guide*. The main section of the* Home Tab *has links to the* Audit Tracker, Backup Manager, *and* Import Files *functions.*

2.2 Audit Tracker

The Audit Tracker *allows the user to search and display a list of files that have been changed since the last database backup.*

The user can access the *Audit Tracker* application in the *Home Tab.* The *Audit Tracker* allows the user to view and search for files that have been changed since the last database backup or archive. **Note:** The *Audit Tracker* only tracks changes to **files** that Questor 5 uses to define operation parameters and instrument procedures, not implementation or uses of those files.	

2.3 Backup Manager

The *Backup and Retore Manager* is only available to user with administrative privileges. The *Backup Manager* will allow creation of backup copies of the various databases used by Questor 5 to store data and operational settings. It will also allow the user to restore a backup copy and view its contents. The user can access the *Backup Manager* from the *Home Tab* in Questor 5 in the top left of the tab.

The user can perform Backups in two different ways: Automatic and Manual. A Manual Backup is performed through Questor 5 from a networked PC. Automatic backups are performed by the *Sequencer* by the user commanding it through a selected sequence within that tab.

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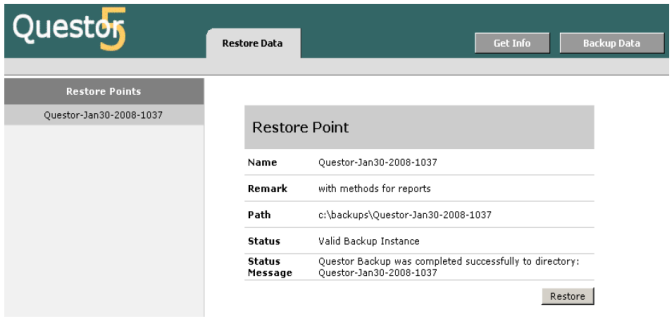
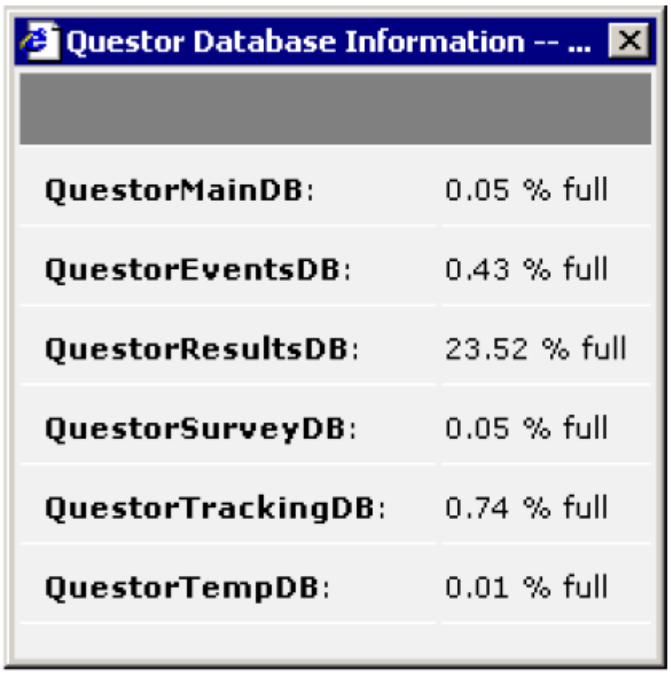
STOP AND REVIEW: Any existing data will be destroyed during a restore as it will be overwritten by the backup instance that has been selected. This means that any data, changes, or additions made after the date of the selected backup will be lost. ******The mass spectrometer must NOT be acquiring data during a restore******

2.3.1 Manual Backup

The user can perform a manual Backup by opening the *Backup Manager* window. The window will display all available restore points in the left pane. Selecting one of the restore points will show its status and give the user the opportunity to perform a restore. Clicking the Restore button will initiate the restoration of the Questor 5 software conditions that were saved on the date specified on the restore.	
The user can select the *Get Info button* in the window to display the information about the size of the current Questor 5 database. When the values approach full, a backup should be performed.	

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2.3.2 Automatic Backup and Purge

The user can schedule Backups at regular intervals through the *Sequence* feature in *Sequencer Tab*. The *Sequence* within the *Sequencer Tab* has aspects that command and control the instrument and the user can select time to be the triggering event for a *Sequence* to run.

The Macro command for a Backup is “Q5_BACKUP”. The user can command this to be run as a Time triggered step in sequencer. A Sequence takes 3 parameters:

1. How often to run the backup/purge procedure, in days. (0=run immediately regardless of last backup time)

2. Do backup - yes/no. (0=no, 1=yes)

3. Number of retention days for purge. (-1 = do not purge any data, 0 = purge all data after backup, 1 = purge all data older than one day, so on.)

Ex: Q5_BACKUP 30, 0, 90 - This will run the procedure every 30 days, will do a Backup, but it will also purge all data older than 90 days. To make this work add above line as a Command step in *Sequence Triggered Events* section.

The user could set this *Sequence* step to run every day. The step will remember the last time it ran the backup procedure. Every day when the step runs at the specified time, it will check if it is time to do the next backup. If yes, it will initiate the backup procedure., otherwise, the step will skip the procedure and will continue to next step.

NOTE: Make sure local user "Questor5" is added to the QuestorAdmin group in Windows, if not already added.

2.4 Import Files

The user can import files into Questor 5 through the *Import Files* selection in the *Home Tab*. All user types can make use of the *Import Files* function except for the *Viewer* type user. The *Import Files* function allows the user to more easily import Questor 5 operations files (*Tune, Survey, Method, Analysis, Calibration*, and *Sequence* files) from other instruments or backed up copies of these files. Any place in the Questor 5 software that allows the user the option to export .TXT or to copy information to clipboard, can be used to create the previously listed file types. The copied information can be pasted into a Notepad or other simple text editor and be saved as a text file. The *Import Files* function can recognize file content and associate them with the proper tab for later use.

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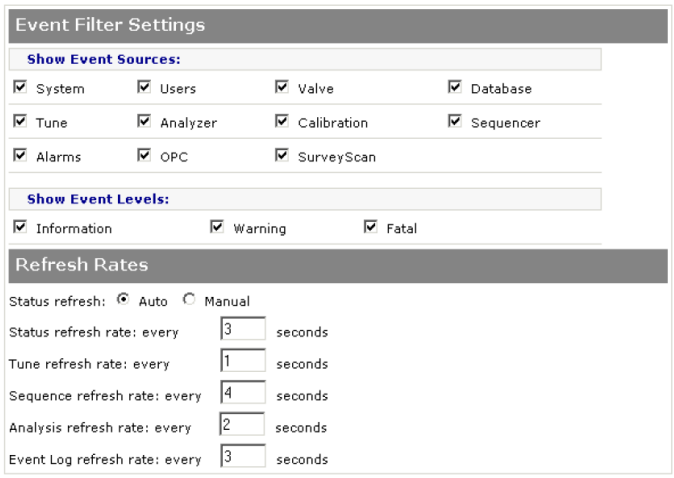
2.5 My Profile

The *My Profile* section of the *Home Tab* allows the user to view any information about the currently logged in user.	
The *Change Password* section allows the user to change the password for the current account, and it will be saved upon clicking the *Change* button.	

2.5.1 My Preferences

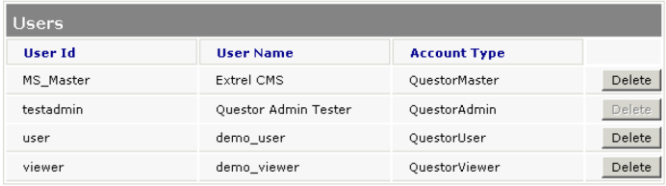
The *My Preferences* selection in the *Home Tab* allows various classes of events from the *Events Log* to be included or hidden when viewed by the user.

A check next to a class of event will display those events by default under the given user's instrument logs. The user may also adjust the refresh rate for some logged events.



2.6 Users List

The *Users List* section of the *Home Tab* allows the user to look at a display list of users currently authorized to use the system.
Administrator users can delete other users so long as they are accessing Questor 5 through either its host computer or computer linked to the network associated to the host computer.
A user account cannot be deleted while the user is logged in.



2.7 Events History

The *Events History* selection of the *Home Tab* will bring up a window where the user can view events that have been automatically logged. The user can click the calendar icon to the right of the *From* and *To* fields to select the time of the desired events. The user can use the *Filter* button to allow specific event classes to be included or excluded (See section 9 *Event Log* for more information on *Events.*) Items that affect Questor 5 performance will create a secure time stamped *Audit Trail* that can be used to comply with regulatory requirements (FDA 12 CFR Part 11.)

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2.8 Boot Server / Shutdown Server

The *Boot Server* and *Shutdown Server* selection of the *Home Tab* do not have screens associated with them. The user must select *Boot Server* to start the instrument and command it and use it for analysis. The user must select *Shutdown Server* to exit the software completely and shut down the instrument. If the user interface window (the Questor 5 web page) is close without the user selecting *Shutdown Server* then the software will keep running in the background.

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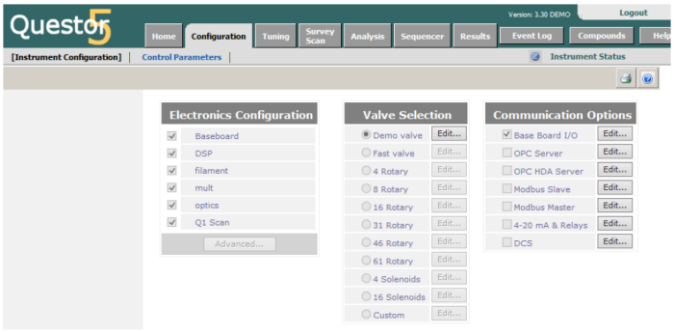
3.0 The Configuration Tab

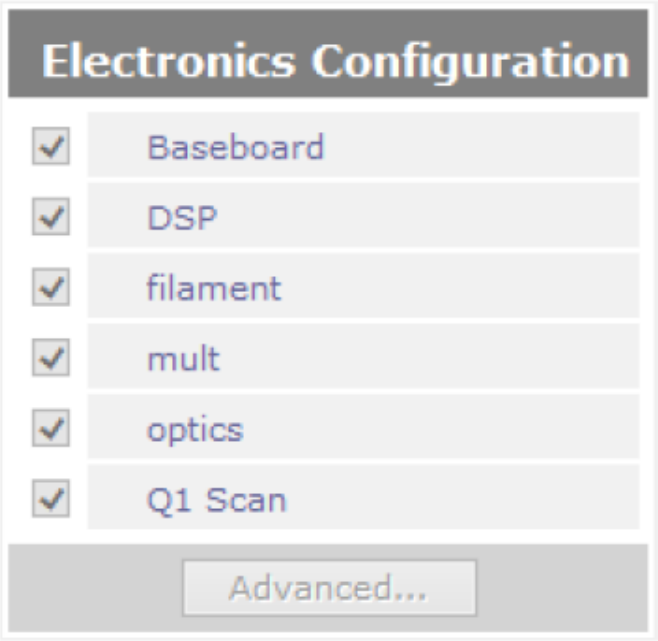
3.1 Instrument Configuration

The *Instrument Configuration* selection of the *Configuration Tab* allows the user to view the defined hardware installed in the mass spectrometer, as well as designate and change sample valves and external communication protocols that Questor 5 is using.



3.1.1 Electronics Configuration

The electronics modules installed in the mass spectrometer are listed in the *Electronics Configuration* table. The user can view the options selected through the *Electronics Configuration* table, but they cannot alter them.



NOTE: Only Extrel CMS service personal can change the components in the *Electronics Configuration*.

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3.1.2 Valve Selection

The user can look at the *Valve Selection* table view what types of valves are installed on the system. Installed valve options will have the radio button next to them checked and filled in.

The user cannot change the valve selection to change the hardware components but selecting *Edit* will allow the user to open the valve parameters dialogue box.

NOTE: Only Extrel CMS service personal can change the components in the *Valve Selection*.

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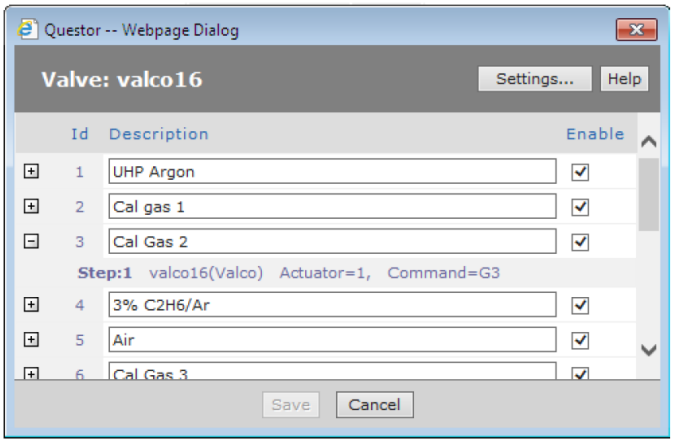
The valve parameters dialogue box. Each port (stream) shown on the valve will be identified by its *ID* number and *Description*. The *Description* filed can be edited to reflect what the valve is connected to.

By default, all ports on a valve are enabled, but users can disable them by unchecking the box on the right under the *Enable* column. Disabling a valve will prevent the rotor from stopping at the location that corresponds to it. The rotor may, however, rotate **through** that position.



3.1.3 Communication Options

The *Communications Options* table lists the external communications protocol options for Questor 5.

Only Extrel CMS service personnel can add or remove these communications options.

The user should contact Extrel CMS to make any adjustments to the *Communications Options*.

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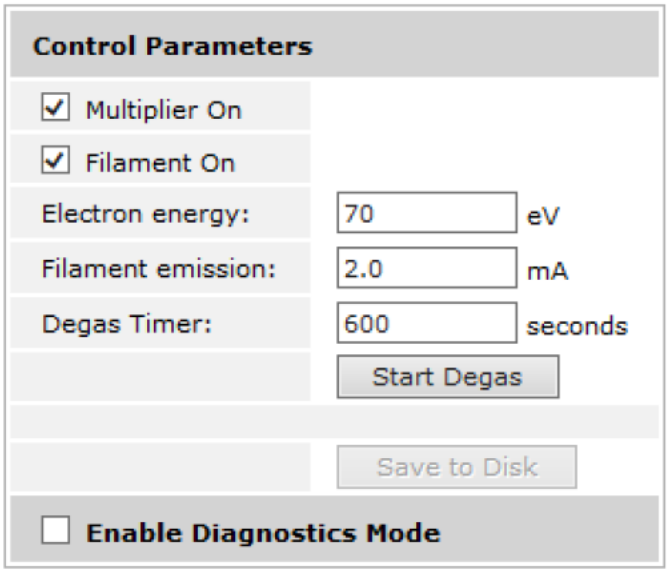
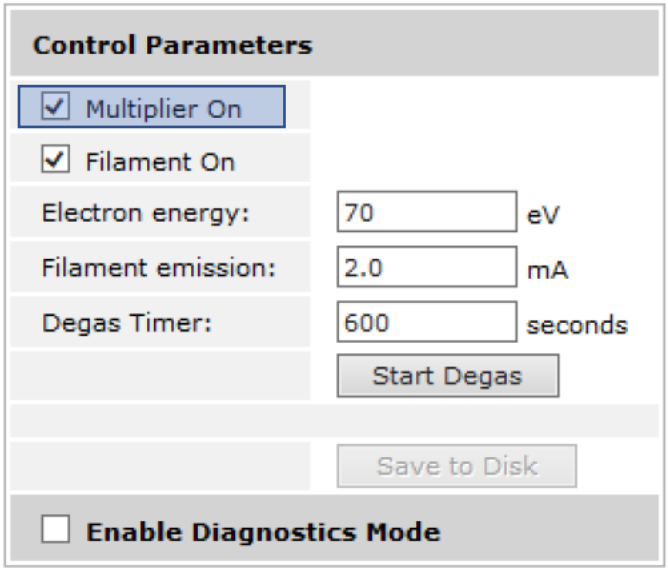
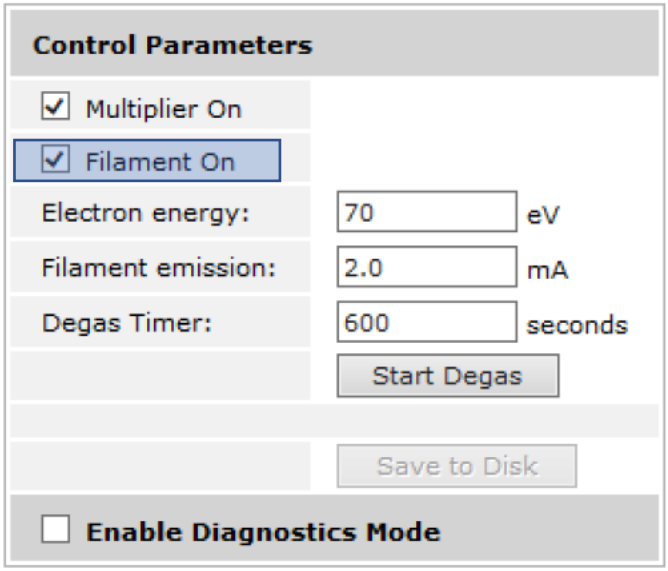
3.2 Control Parameters

3.2.1 Advanced Configuration

The *Control Parameters* selection of the *Configuration Tab* allows the user to view and adjust some aspects of the instrument that remail static during standard instrument function.	
The *Multiplier On* selection will only be available for systems that have a multiplier. It allows the user to turn on or off the multiplier based on experimental applications and the need for the multiplier. The multiplier serves to increase signal detection but can also be damaged through prolonged use in sample-dense environments. The user should attempt to use faraday detection before deciding upon multiplier-aided detection.	

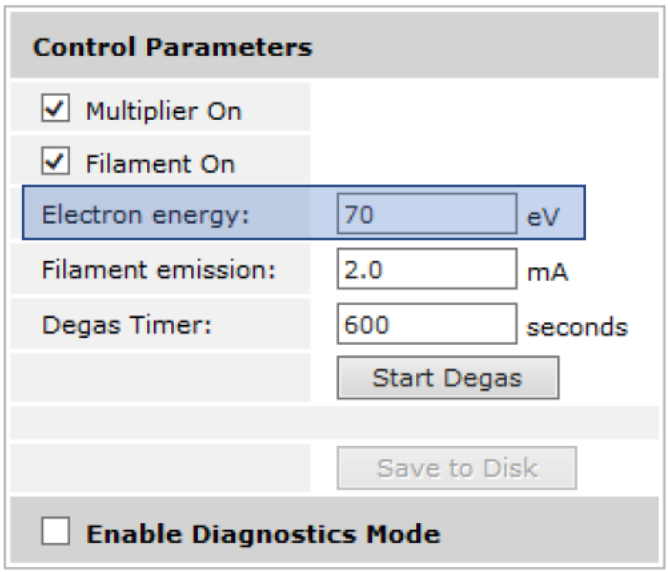
The *Filament On* selection allows the user to energize or deenergize the filaments. Placing a check in the *Filament On* checkbox will turn on the filaments in the ionizer. The user must check the box for the mass spectrometer to function, as these are the ionization source.



The *Electron Energy* is the potential placed between the filament electron source grid. The *Electron Energy* is the energy with which the electrons are emitted from the filament and impart on the molecules in the mass spectrometer. The factory value is 70 eV and the user should not change this value, as this will change how the molecules ionize. For advice and/or assistance, please contact Extrel Support:

Support@extrel.com

The *Electron Energy* is the potential difference placed between filament and source grid. The user must correct for the true electron kinetic energy by accounting for the contact potential difference between the thorium coated filament and the platinum coated source grid, and the voltage drop across the filament. The contact potential difference may place the electron kinetic energy as low as 3.7 eV below the *Electron Energy*.



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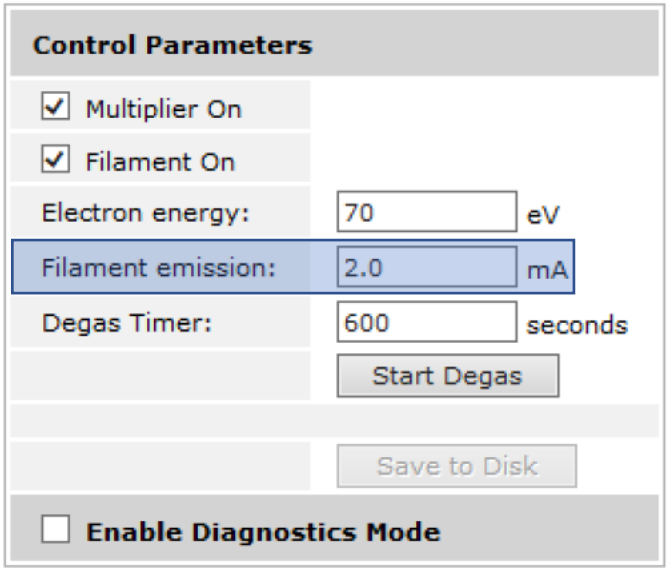
The *Emission Current* selection is the current leaving the filament and directed through the electron source grid. It is factory set for high sensitivity when operating at 70 eV electron energy.

The user may set the emission current between 0.1 mA and 4 mA, and the electron energy between 11 and 150 volts.

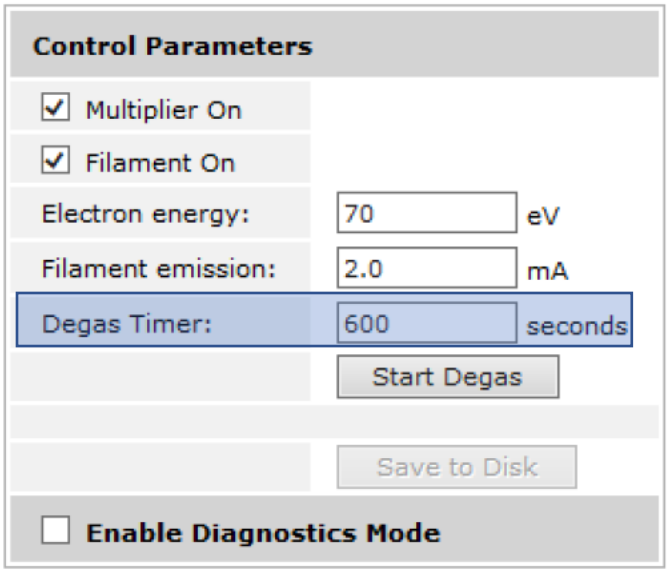
Not all combinations of emission current and electron energy may be set at once. At lower voltages, higher emission currents are not available.



The *Degas Timer* sets the *Filament Emission* to run with a high current to heat the element and purge minor contaminants/ impurities on the filaments and within the system. The *Degas Timer* sets how long the instrument will be in *Degas Mode*.

The user should use the *Degas Timer* if the sim of partial pressures is low compared to the total pressure the instrument is reading back. This indicates the instrument is not ionizing samples properly and could be due to a dirty ionization source. A contaminated ionizer may cause a different of one order of magnitude between measured pressure and real pressure.

The user should note that *Degas Mode* serves to clean the ionizer and if sensitivity does not increase, a new ionizer may be required.



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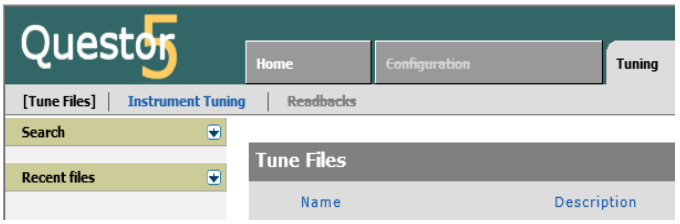
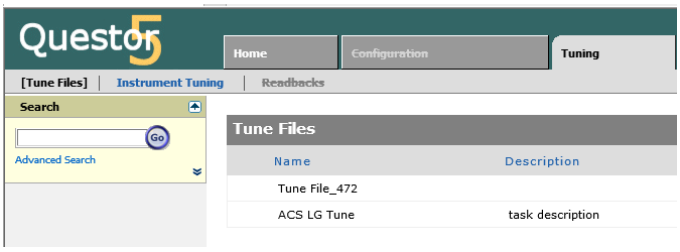
4.0 The Tuning Tab

The Tuning Tab *is the primary interface used to adjust the operating parameters of the mass spectrometer. The user can command the elements and parameters of ionizer, multiplier, preamp, and quadrupole from the* Tuning Tab*. The user can select the files that record the basic operating parameters of the mass spectrometer within this tab, as well as commanding the scan window and detector parameters. The purpose of the* Tuning Tab *is for the user to properly position and calibrate the signal peaks in a process called Tuning.*

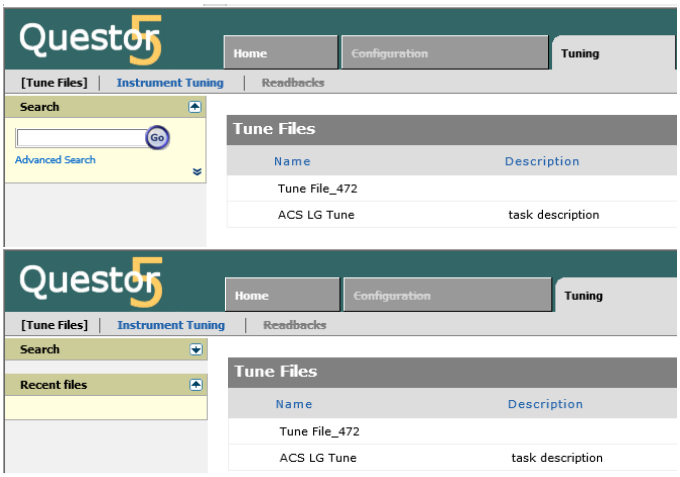
NOTE: The instrument cannot run in Tune Mode, Survey Scan Mode, or Analysis Mode at the same time.

4.1. Tune Files

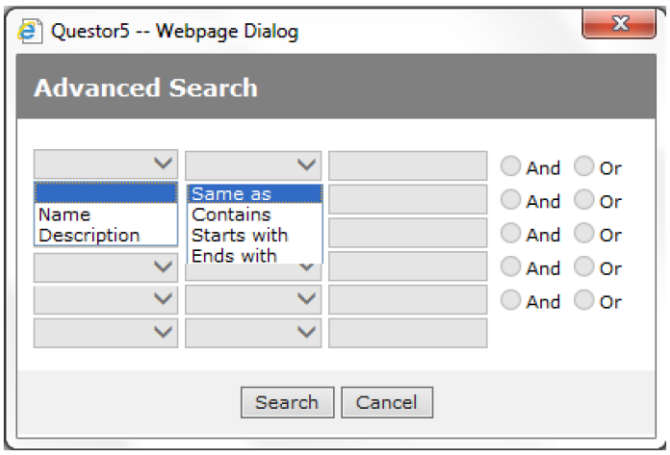
Tune Files are files the Questor 5 software calls upon to define the parameters by which the instrument will be run. The *Tune Files* section of the *Tuning Tab* contains a list of Tune files the instrument can call upon. They are listed by name, description, who last modified the file, and when.	
The system can have multiple tune files available for use. The user can search for a tune file using the *Search* function on the left of the *Tune File* window. The screen will have links where tune files can be searched for using keywords, as well as a list of the most recently used tune files.	

The *Search* box will allow the user to search using text names, words, or word fragments found in the description or name of the tune files.

The use of a wildcard "*" will search for anything that contains the given information.
Ex: *J* finds anything with a "J", *J finds anything that ends in a "J" or J* finds all things starting with a "J".



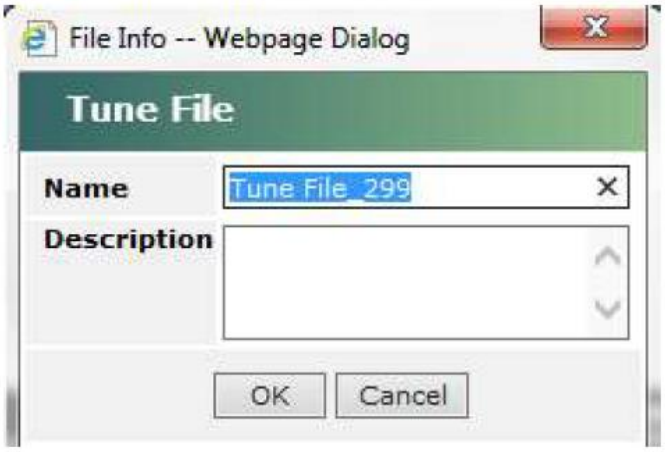
The user can perform more selective *Search* through the *Advanced Search* feature under the *Search* section of the *Tune File* window. The user can search the fields for directly matching content, or use logical operators, or chain logical operators together to find a specific tune file.
The selected tune file will become the active tune file only when the user enters the *Instrument Tuning* screen and starts tuning.



Along with selecting an existing tune file, the user can create a new tune file under the *Tune Files* section of the *Tuning Tab.*

The user will click in the *Create New…* button to start the process. From there, the user will be presented with a dialog box to name the tune and give it a description.

Once the user has named the new file and given it a description, a new dialog box will be presented to select an initial tuning mass. A value within the mass range of the instrument must be selected. The user can change the mass



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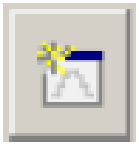
scan range and desired masses in tuning process. The software will automatically create a mass scan window of 1 amu centered on the selected mass.	

4.2 Instrument Tuning Buttons

The Instrument Tuning *window has buttons unique to it and its functions. This section will give the user a guided tour of these buttons and their functions.*

The *Start Tuning* button in the upper right of the window allows the user to implement the selected tune and commands the software to start displaying scan data.	
The *Create New Tune File* button allows the user to create a new tune file in a similar way to the process in the *Tune Files* window.	
The *Save Current Tune File* button allows the user to save the current tune parameters using the same name as the currently selected file, overwriting its current data. **Note:** This button is only available once a parameter has been changed so the user can save the modified parameter.	

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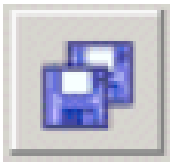
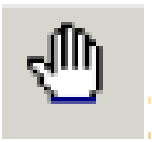
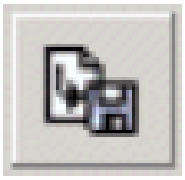
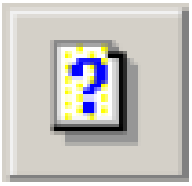
The *Save As Button* allows the user to save the currently selected tune file under a different name, preserving the previously created file and creating a new one. **Note:** This button is only available once a parameter has been changed so the user can save the modified parameter.	
The *Stop Tuning* button allows the user to stop currently running tune file, stopping the data from being collected and displayed.	
The *Scope Scale* button allows the user to command the software to set the vertical scale of the scan window(s) to be relative to the highest peak within the scan window.	
The *Export Tune File* button allows the user to export the tune file to the Windows clipboard where it can be pasted into Notepad and saved as a .TXT file for future reference or importing to another installation.	
The *Print Charts* button allows the user to send a copy of the current three tune tables and each of the mass windows to a local printer.	
The *Questor 5 Help* button allows the user to launch the Questor 5 help utility option for frequently asked questions and access to explanations of Questor 5 features within the software.	

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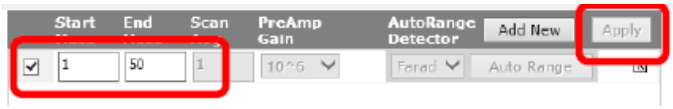
4.3 Calibration Parameters

The function of a mass spectrometer is to look for the appearance of signals (represented as peaks within the software) at various masses in the spectrum. The instrument will detect the peaks, but the user must calibrate the instrument to define the masses that are being ionized and observed in a process called Instrument Tuning.

The user can select or create a new tune file and start the tuning process. Once the user has selected a tune, the screen will open with multiple options functions. The user should start with the one on bottom of the screen where mass scan ranges are specified. The user can specify the scan range of the desired masses and the tune window will populate the desired masses. The *Add New* button will allow the user to specify a new mass range for the instrument to scan through. To make the scan range(s) active, the user must click the check box next to them, click the *Save* icon, and click *Apply*.
The *Start* and *End* sections allow the user to specify the range of masses being scanned with the scan window. If there are 4 or fewer windows, the scan windows will automatically scale to fit in the *Tuning Tab.*
Note: The instrument will slow with more scan ranges specified and selected.



NOTE: For a new instrument, the user should create a mass range from 27.5 to 28.5 and one from 1 to 50 and select for the instrument to scan through them. The user should let the instrument run for **at least 3 hours** with these selections before attempting to fine-tune the peaks. This allows the instrument to stabilize and return signals accurate to what will be seen in standard operation.

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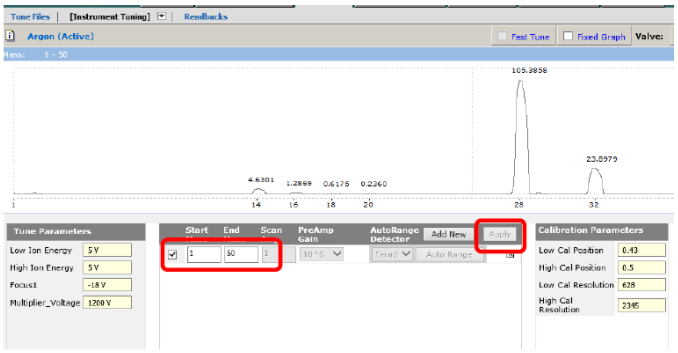
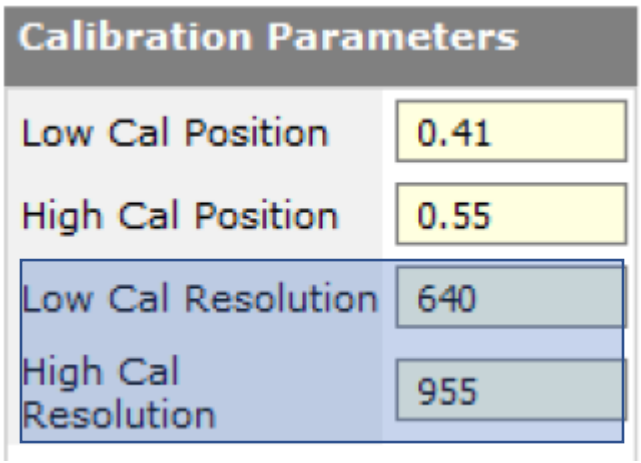
After the user has let the instrument run for **at least 3 hours with the previously mentioned parameters,** the fine-tuning procedure can begin. The user should identify at least three masses of interest (for scanning room air, 14, 28, 32, and 40 are recommended.) The user should use the *Add New* option to create new scans for each of the selected masses with a 2 amu window centered on the desired mass.
Ex: Nitrogen (N2) has a peak at 28 m/Z. The user should create a mass scan range of 27-29.



The user should begin the Tuning process by adjusting the *Resolution* parameters found at the bottom right of the *Instrument Tuning* window in the *Tuning Tab*. The user should adjust the *Resolution* parameters to manipulate the peaks to be approximately 1 amu wide at their base. Increasing the value will widen the peaks and decreasing it will thin the peak.
Note: To check the width of the peak, the user can place the mase to the left and right of each peak and the mass position will be shown in the upper right of the corresponding window.
Note: There are two *Resolution* parameters. The *High Cal Resolution* and *Low Cal Resolution*, which refer to the ends of the mass range (relative to the ultimate mass range for the instrument.) The user can adjust the peak width by the *Resolution* parameters, *Low Cal* for smaller masses and *High Cal* for larger masses.



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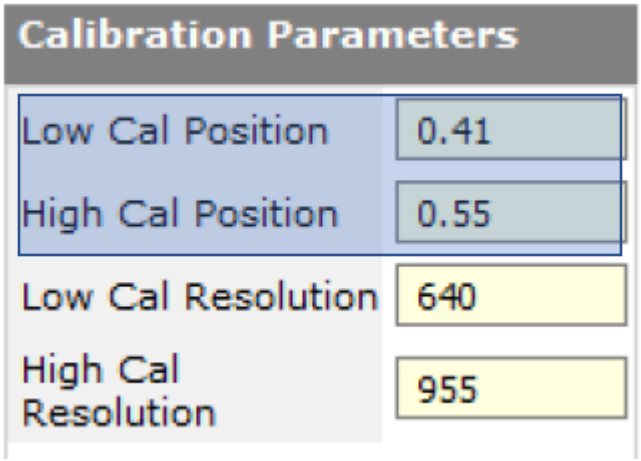
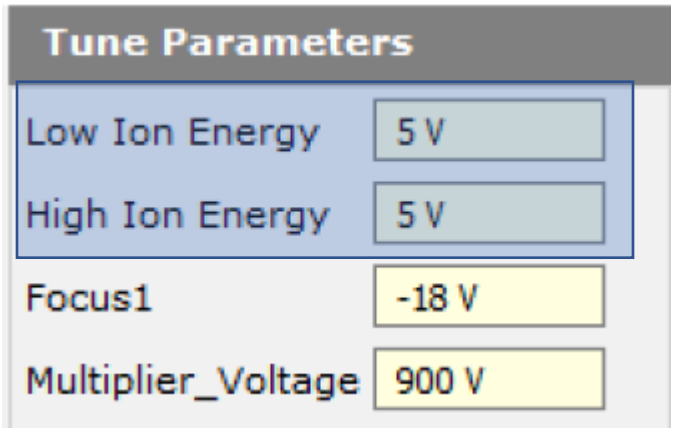
The user should continue the Tuning process by altering the *Calibration* parameters, found in the same window as the *Resolution* parameters. The *Calibration* parameters serve to correctly position the peaks. The *Calibration* parameters similarly have a *High Cal* and *Low Cal* parameter which affect the same masses as the *Resolution* parameters.	

4.4 Tune Parameters

The Tune Parameters *are found in the bottom left of the* Instrument Tuning *window in the* Tune Tab*. The* Tune Parameters *are used to refine he signal strength and consistency. Changing the voltages applied in this section will change the size and shape of the peaks.*

The *Ion Energy* allows the user to alter the energy that the filaments impart to the incoming samples. The user can increase the ion energy to increase sensitivity of the instrument, but the peak shape and quality will suffer when the ion energies are too high. *Low Ion Energy* & *High Ion Energy* settings are settings at Mass 1 and Last Mass, the ion energy is interpolated between and extrapolated beyond these two points for the rest of the mass scan window.	

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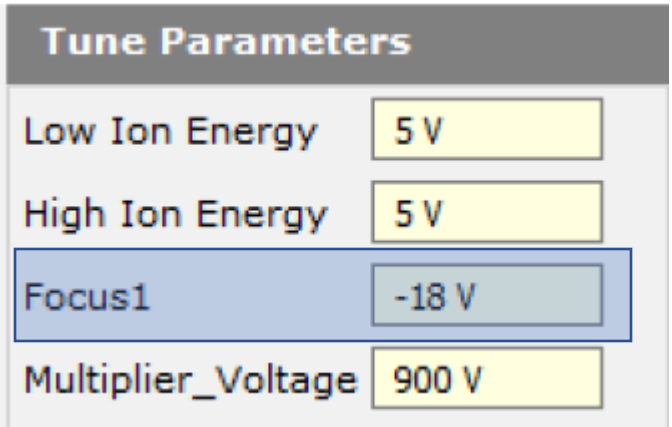
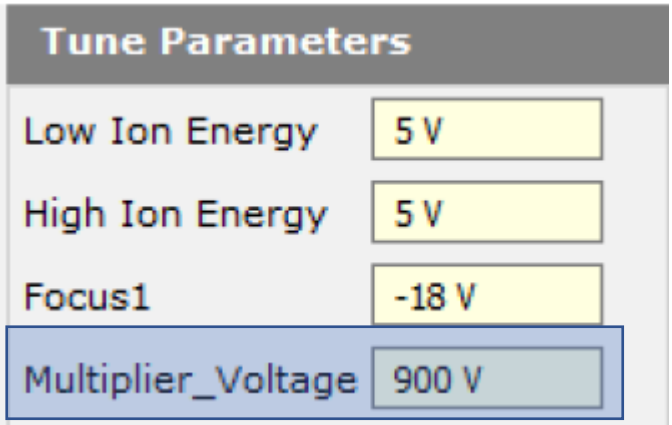
The *Focus1* parameter allows the user to control the potential which draws the ions out of the ion source grid. The factory setting is -18 V. The user can change the value of *Focus1* to change the signal peak intensity, as well as the peaks shapes.	
The *Multiplier_Voltage* parameter allows the user to adjust the voltage being applied to the multiplier. The user can increase the multiplier voltage to increase the sensitivity of the instrument, but signal quality will decrease if the applied voltage is too high.	

NOTE: The voltage applied to the multiplier will affect the lifespan of the component. Applying high voltages for extended period, operating in high sample concentration, or operating at high pressure will reduce the lifespan of the instrument.

Tips for Tuning

- The user should tune with the idea of maximizing peak intensity.
- The user should tune to have the peak shapes be nearly symmetrical, with sharp baseline resolution and a bell-shaped curve.

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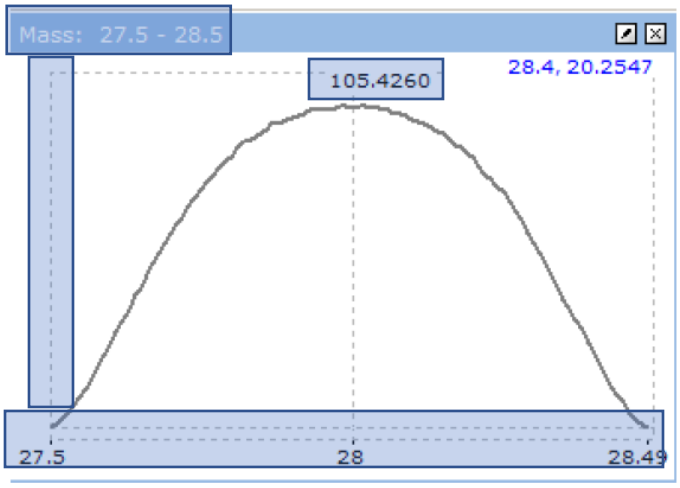
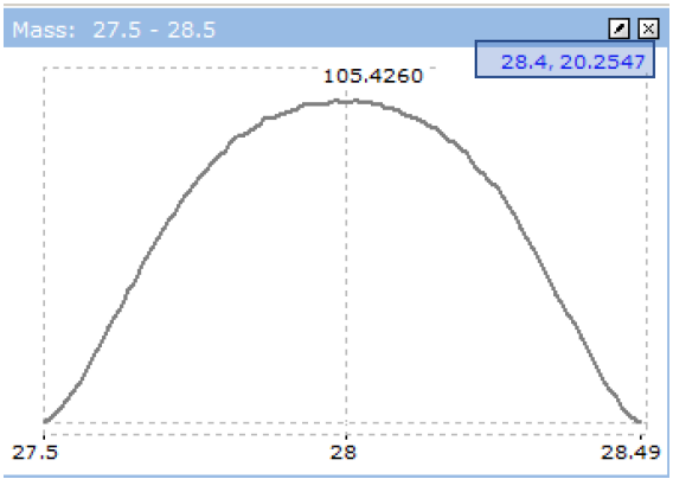
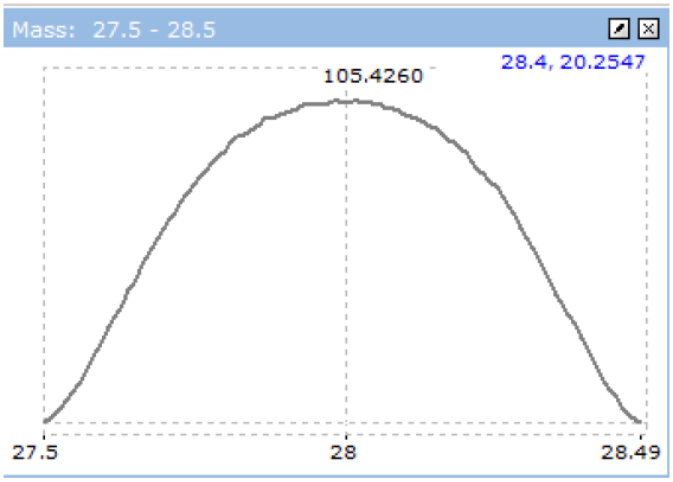
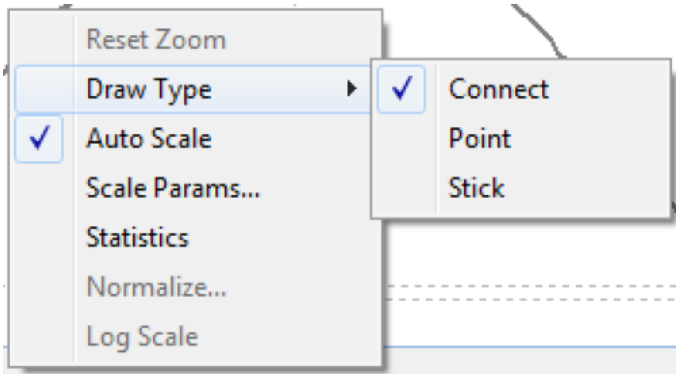
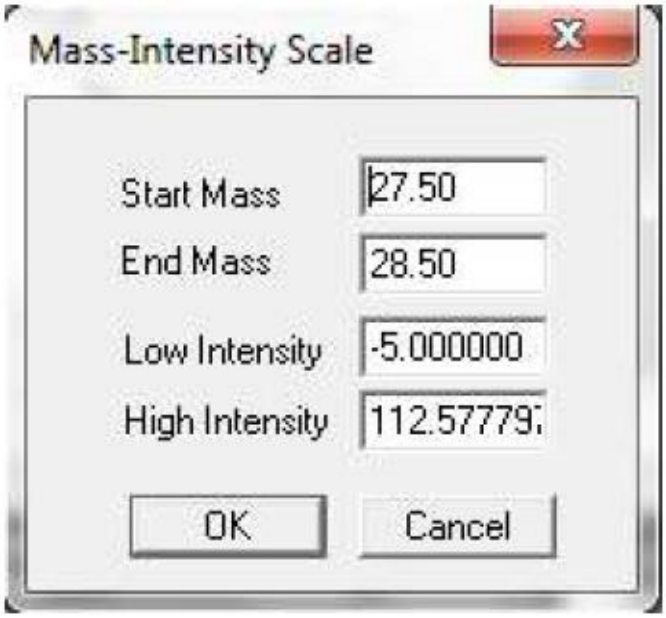
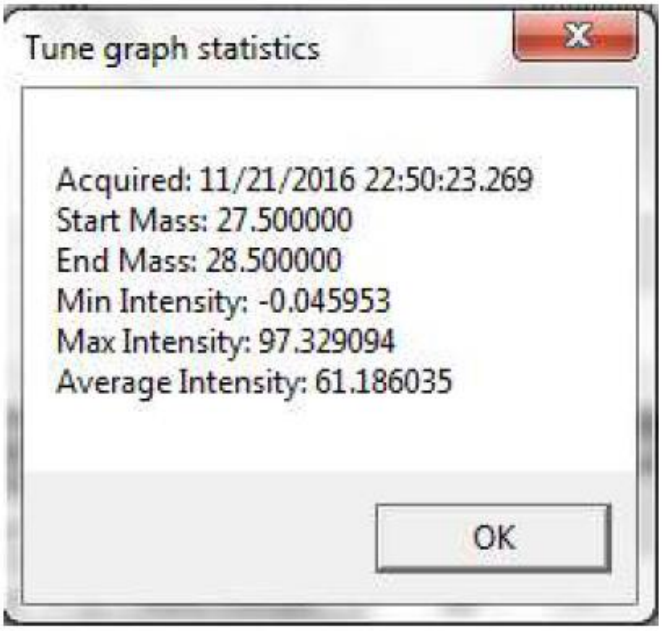
4.5 Mass Window Display Features

The user can manipulate the Mass Window Display Features*, allowing for a better display of the data acquired by the instrument.*

The user can view the current start and end point of the scan window as entered in the scan mass parameters in the title of the mass scan window. The scan window displays the active scan range, outlined with a gray dashed line. The user can view the center of the mass scan range at the top of the center gray dashed line. The bottom most allows the user to view the mass scale depicting the mass range being used.	
The user can use the mouse to hover over a point on the scan window. On the top right of the scan window, the user can view the mass where the mouse cursor is (left value) and the signal intensity that corresponds to the mass (right value.) **Note:** The user must keep moving the mouse cursor to continuously update the values in the top right. If the user stops using the cursor, the values disappear.	

The user can zoom into the display by left clicking and dragging the mouse pointer diagonally to define a new area. The display can be redrawn to show he newly defined area. The user can reset the zoom by right clicking the mass window and selecting the *Reset Zoom* option from the window that appears.	
The user can right click the mass window to bring up further display parameters. The user can select different draw types under the *Draw Type* selection. • *Connect* gives the standard display that plots the points collected and connects them to create the peaks. • *Point* shows the individual data points as "+", without continuity between points. • *Stick* creates a bar graph with each point acquired being represented by its own line.	
The user can select the *Auto Scale* option to have the mass window always set its vertical scale based on the top of the most intense peak within the mass scan range.	

The user can select *Scale Parameters* to manually edit the mass scan range and vertical scale parameters for the selected mass scan window.	
The user can select the *Statistics* selection to display some statistics about the current data in the mass scan window.	

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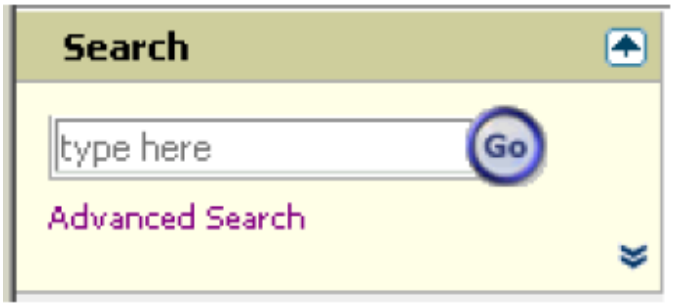
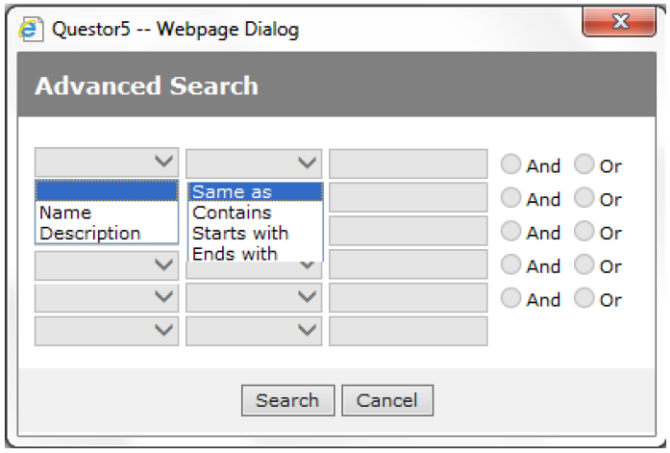
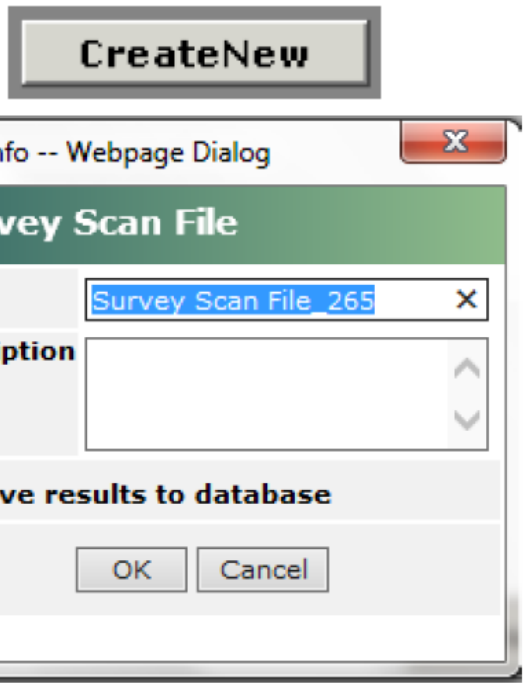
5.0 The Survey Scan Tab

The Survey Scan Tab *is where the user can use the mass spectrometer in it most fundamental mode: to look at everything that appears within the defined mass range. The default scan takes the form of a bar graph, with mass as the x-axis and intensity as the y-axis.*

5.1 Survey Files

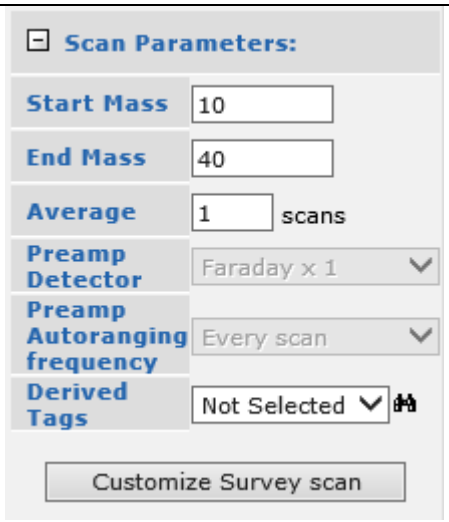
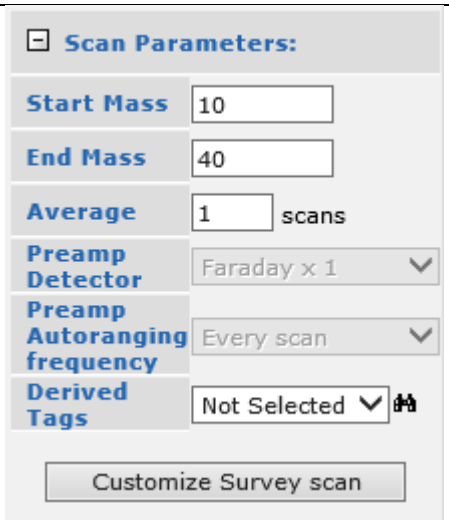
The Survey Files *selection under the* Survey Scan Tab *present a list of files much like those encountered in the* Tune Files *window under the* Tuning Tab*.*

The *Survey Files* selection on the *Survey Scan Tab* allows the user to access a list of survey files currently available on the system. The files are listed by name, description, who last modified the file, and when it was last modified.	
The user can use the *Search* function to find files by their text names, or file descriptions using whole words or word fragments (similarly to the *Search* function in the *Tune Files* window under the *Tune Tab.*)	
The user can use a wildcard "*" to search for anything that contains the given information. **Ex**: *J* finds anything with a "J", *J finds anything that ends in a "J" or J* finds all things starting with a "J".	

The user can perform more selective *Search* through the *Advanced Search* feature under the *Search* section of the *Survey File* window. The user can search the fields for directly matching content, or use logical operators, or chain logical operators together to find a specific survey file. The selected survey file will become the active survey file only when the user enters the *Survey Scan* screen and starts acquiring data.	
The user can select the *Survey File* by clicking on it, and this will transport the user to the *Survey Scan* screen, loading the selected *Survey File* in the process. The file selected by the user will not become the active file until the *Start Survey Scan* button is clicked in the top right of the window.	
Once the user selects a new *Survey File*, a window will be created to allow the user to name the file and write a description. The user can also instruct the software to save the results to the Questor database by checking the designated box. The box is checked by default to specify that data generated during a survey will be saved and available as historical data. If the user clicks *Okay*, the software will shift to the *Survey Scan* tab with the survey files default values displayed but will not be commanding the instrument yet. The last set of tune parameters will also be loaded.	

5.2 Survey Scan

The Survey Scan *selection under the* Survey Scan Tab *presents a data acquisition mode that uses the mass spectrometer in its most fundamental way, and allows the user to view real time data, as well as historical data, and gives the user the ability to compare the two.*

The user can use the *Survey Scan* window in the *Survey Scan* tab to adjust a limited number of parameters.	
The user can change the parameters for the *Start Mass, End mass, Average,* and the set of *Derived Tags.* The user can edit the settings by either selecting the window and tying new values or selecting an option from the drop-down list. **Note:** All changes made to the *Scan Parameters* will take effect only after the user restarts the scan. **Note**: The *Customize Survey Scan* button is not present in the MAX300-CAT Questor 5 software.	
The *Start Mass* and *End Mass* settings specify the scan range used in the survey scan. The *Average* function will specify how many scans are taken per point and averaged together. The user can increase the scan average to acquire more stable and sensitive data, but this will reduce the speed of the isntrument. The *Derived Tags* option will allow the user to select speific data to be recorded and analyzed beyond the general spectrum presented by the *Survey Scan.*	

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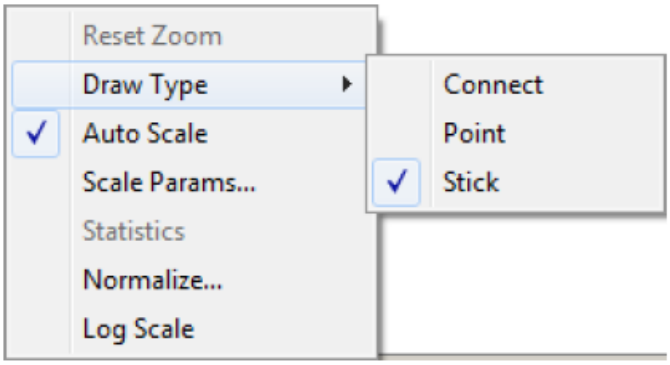
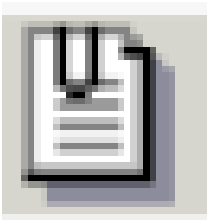
The user can edit the *Survey Scan Window* in much the same ways as those found in the *Mass Window* in the *Tune Tab.* (See the *Mass Window* section.) The user can right click the *Survey Scan* window to access the edit options. The *Survey Scan* allows the user to select a *Log Scale* option in the edit window to set the peak scaling to logarithmic to view small peaks relative to large peaks more easily.	

5.3 Survey Scan Data Display

The Survey Scan *window has unique functions and capabilities. This section will give the user a guided tour of these functions and how to access and use them.*

The user can use the *Set Current Scan as Reference Scan* button on the top right of the *Survey Scan* window to set a reference scan. The data from the current scan is copied to the *Reference Graph,* where it will be used as the reference scan to populate the *Delta Graph.* **Note:** The user can use all formatting and editing techniques for the other graphs in the *Survey Scan* window.	
The user can access the *Reference Graph* window by left clicking the *Reference Graph* icon in the middle-left of the screen. The *Reference Graph* is used as the set point for the *Delta Graph* to measure dynamic changes of data over time.	
The user can access the *Delta Graph* window by left clicking the *Delta Graph* icon in the middle-bottom of the screen. The *Delta Graph* measures changes in the data acquired by the *Survey Scan* against the *Reference Graph* over time.	

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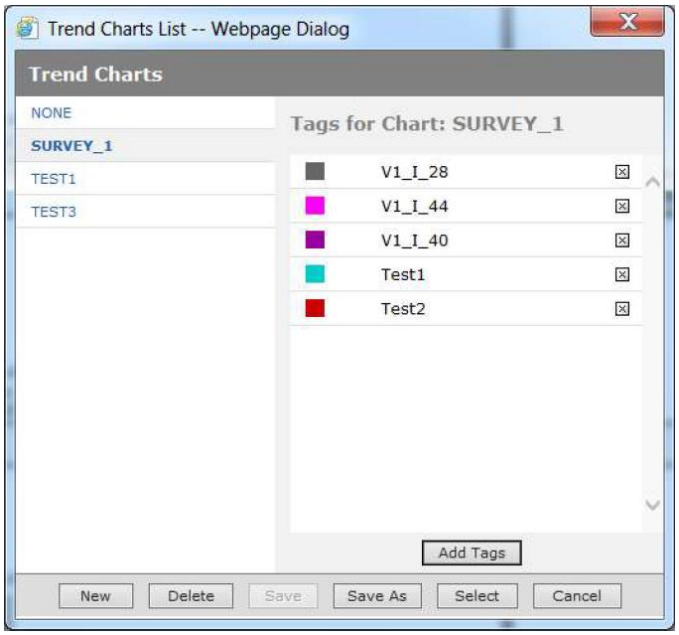
The user can graph any mass or derived tags versus time along with viewing the entire spectrum over time. The user can access this function by clicking the check box labeled *Show Charts* in the toolbox at the top of the window.	
The user can select a user defined chart from a list through interacting with the tool bar at the bottom of the *Charts* window on the bottom of the *Survey Scan* window with *Show Charts* enabled. The user can view a list of available chart files by selecting the first button on the tool bar, the second button allows the user to modify the settings of the displayed chart, and the last button allows the user to clear the chart display.	
By selecting the option to view the available charts, the user will be presented with a window with the capability to edit, create, and delete charts. The user can create a new chart by clicking the *New* button on the bottom of the presented window. This button allows the user to create a named chart with a description. Within the new chart, the user can select the *Add Tags* button to add a mass to monitor, a valve position for said mass to be introduced into the mass spectrometer, and a derived tag for the selections made. The *Select* button allows the user to select the chart type that will be made active within the *Survey Scan* tab.	

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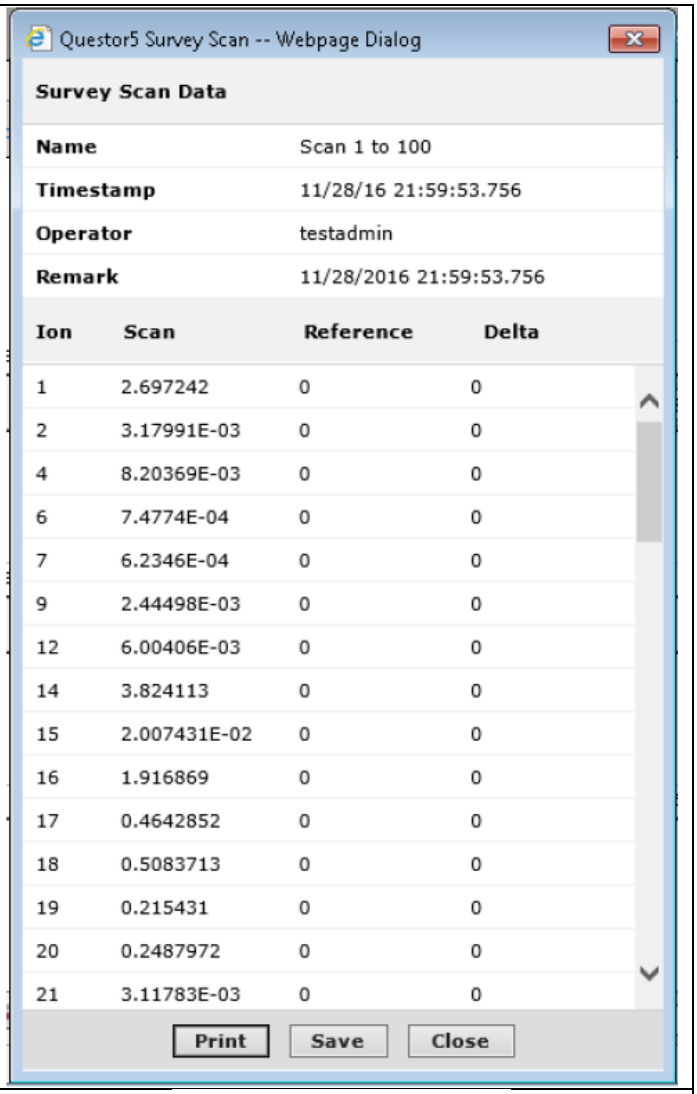
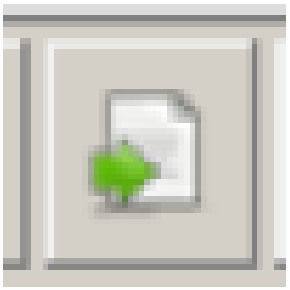
The user can display the results of the *Survey Scan* data in a tabular format as well as graphical. The user can select a button at the top right of the *Survey Scan* window to display the *Survey Scan* data, the delta, and reference data.



The user can also use the tool bar at the top right of the screen to export the data acquired in the *Survey Scan* into various formats in much the same way at the *Instrument Tuning* window in the *Tune Tab.*



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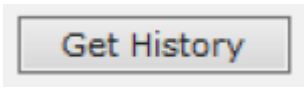
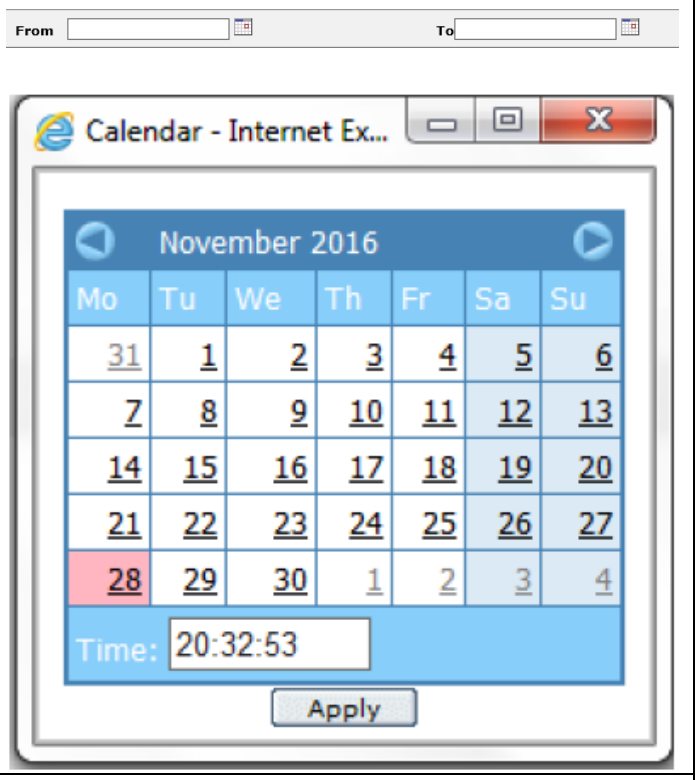
5.4 Survey History

The Survey History *window allows the user to view the saved* Survey Scan *data generated from a manual scan or* Survey Scan *generated from a step in an automatic sequence.*

The user can access the information in the *Survey History* scan through the *Get History* button in the tool bar. The display windows will be initially blank, as the user needs to specify the data for the window to call up. The *Get History* button allows the user to view a list of the most recent *Survey Scans* in the database.	
The user can specify the dates and times for the *Get History* button to find the data in two ways. The user can first specify the ranges in the *To* and *From* boxes in (mm/dd/yyy hh:mm:ss) format. Or the user can use the calendar icons next to the *To* and *From* text boxes to specify the ranges. Once the user has selected the date and time and applied them, the user can click the *Get History* button to populate the *Survey History* graphs and data tables.	
One the user has selected the historical data the *Survey History* window will be populated. The user can manipulate the data windows in the same way as the other data windows under the *Survey Scan* tab.	

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6.0 The Analysis Tab

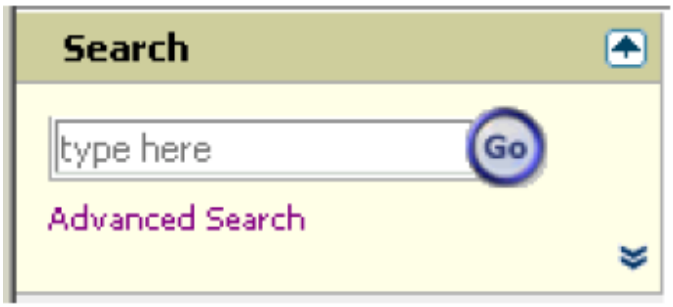
The user can use the Analysis Tab *to select, create, or edit files that define a method used to generate and interpret the data from the mass spectrometer.*

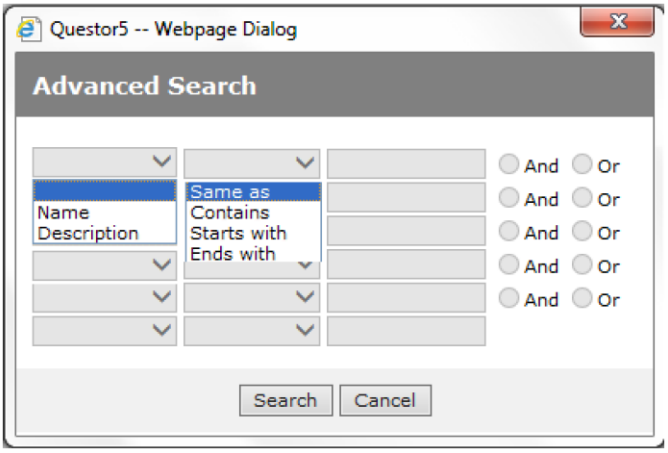
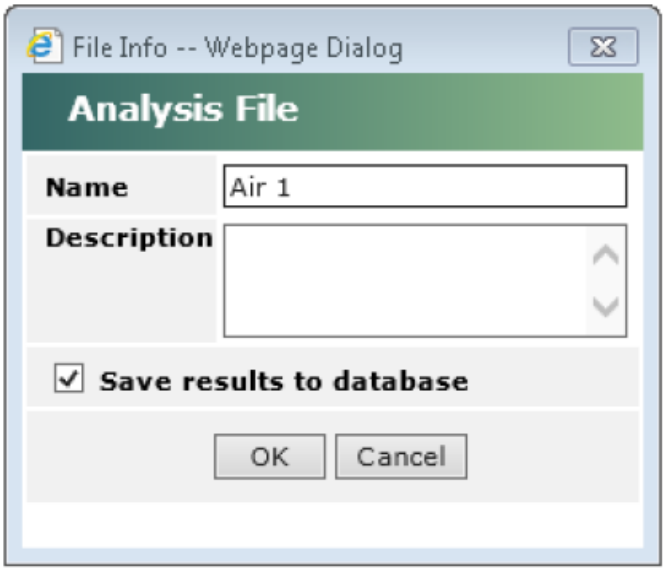
NOTE: The functionality of the *Analysis Tab* is dependent on a proper instrument Tune. If the instrument is not properly tuned, the *Analysis Methods* will not be able to accurately detect the analytes.

NOTE: The instrument cannot run in Tune Mode, Survey Scan Mode, or Analysis Mode at the same time.

6.1 Analysis Files

The Analysis Files *selection on the* Analysis Tab *allows the user to view and edit a list of analysis files listed by name, descriptions, who last modified the files, and when they were last modified.*

The user can use the *Search* function to find files by their text names, or file descriptions using whole words or word fragments (similarly to the *Search* function in the *Tune Files* window under the *Tune Tab.*)	
The user can use a wildcard "*" to search for anything that contains the given information. **Ex**: *J* finds anything with a "J", *J finds anything that ends in a "J" or J* finds all things starting with a "J".	

The user can perform more selective *Search* through the *Advanced Search* feature under the *Search* section of the *Analysis File* window. The user can search the fields for directly matching content, or use logical operators, or chain logical operators together to find a specific analysis file. The selected analysis file will become the active survey file only when the user enters the *Analysis* screen and starts acquiring data.	
Once the user has selected a file and clicked it, the software will direct the user to the *Fragmentation Matrix* screen. The selected file will not become the active file until the user selects the *Start Analysis* button in the upper right of the browser window.	
The user can create a new *Analysis File* by selecting the *Create New* button in the *Analysis Files* selection of the *Analysis Tab.*	
Once the user selects a new *Analysis File*, a window will be created to allow the user to name the file and write a description. The user can also instruct the software to save the results to the Questor database by checking the designated box. The box is checked by default to specify that data generated during a sequence will be saved and available as historical data.	

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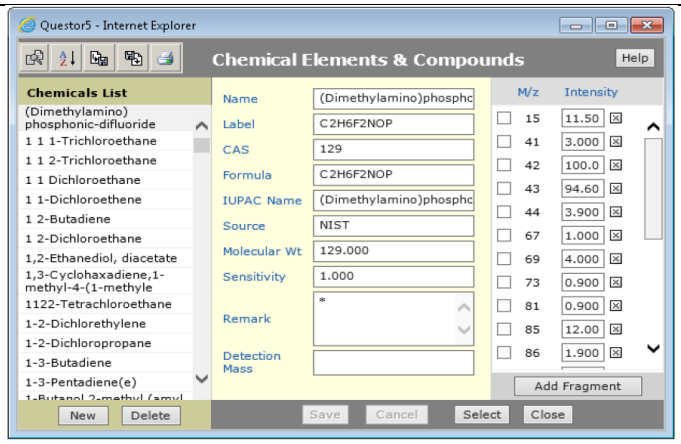
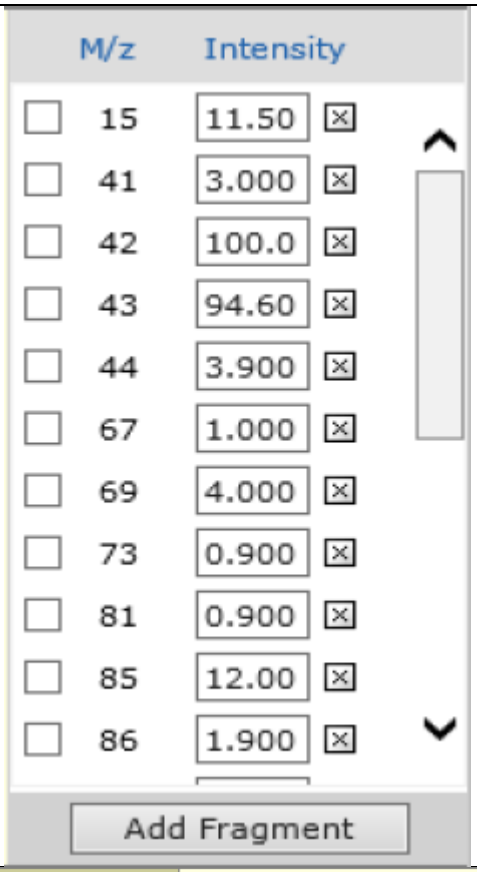
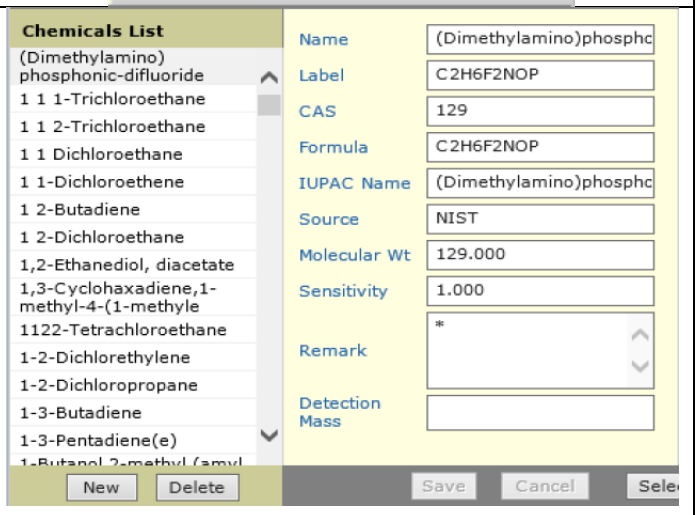
6.1.1 Chemical Elements and Compounds

The user has access to a searchable and editable library of mass spectra designed to be used to create a table of detection masses that Questor 5 can use to evaluate samples in a selected sample stream.

When creating a new *Analysis Method*, the user will be presented with the *Chemical Elements and Compounds* table to specify the analytes of interest and the masses of interest from those analytes. The user can select the chemicals from the list on the left, and from there the user can select one or multiple peaks at which the analyte will be identified, as well as relative intensity values of those mass fragments. The user can search the list of chemicals available through the toolbar in the top left of the screen. The same search functions and rules from the other windows persist for this *Search* function as well (See *Tuning Tab – Tune Files* for details.)	

The user can also add masses and mass fragments to the *Chemical Elements and Compounds* table. To add a fragment to an existing mass, the user selects the *Add Fragment* option and specifies the mass of the desired fragment and the expected relative intensity of the fragment.	
The user can add chemicals to the *Chemical Elements and Compounds* table by selecting the *New* button on the bottom left of the screen. The user will be prompted to fill out a name, label, formula, molecular weight, and sensitivity of the desired molecule or element. From there, the user will have to specify fragments the molecule will break into when ionized, as well as their expected relative intensities. **Note:** The *Sensitivity* parameter of the molecule is a measure of how easy the molecule is to ionize relative to *Nitrogen*, which is assigned a *Sensitivity* value of 1 in the software.	
The *Detection Mass* field is left blank intentionally. The *Detection Mass* is the designated point on the mass spectrum where the molecule will be monitored.	

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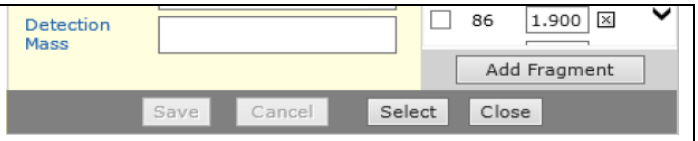
The user must have *Detection Mass* field unique to each component analyzed.	
The user can specify the *Detection Mass* manually or allow the system to automatically populate it. To select the *Detection Mass* the user can either: place a check mark next to the desired fragment and click *Select,* type a number from the listed fragments into the *Detection Mass* field and click *Select*, or double click a value in the fragments column and click *Select.* The user can allow the system to determine the *Detection Mass* by clicking the *Select* button while having the desired chemical compound open, and the system will automatically select the highest intensity fragment to be the *Detection Mass*. **Note:** If the user has multiple fragments designated to be used in the analysis method for detection, and does not specify a *Detection Mass* the system will automatically select the fragment with the highest intensity to be the *Detection Mass.*	

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6.2 Analysis Method

The Analysis Method *selection on the* Analysis Tab *allows the user to specify parameters for the instrument to follow when acquiring, interpreting, and displaying data.*

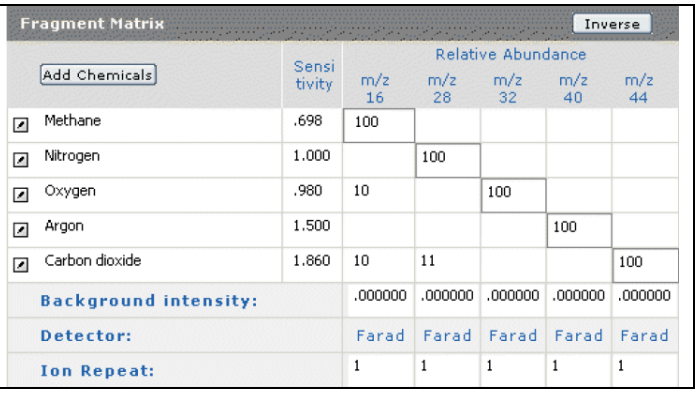
NOTE: The instrument cannot run in Tune Mode, Survey Scan Mode, or Analysis Mode at the same time.

The mass spectrometer will not implement an *Analysis Method* without the user selecting the *Start Analysis* button in the upper right of the screen and selecting a valve for the *Analysis Method* to analyze. **Note:** The user must save all methods and steps after changes have been made to run them.	

6.2.1 Fragmentation Matrix

The Analysis Method *selection on the* Analysis Tab *has multiple subsections, the first of which is the* Fragmentation Matrix. *This subsection allows the user to view and edit the compounds in the analysis stream that the software will look for, as well as some detector parameters.*

NOTE: The user should recalibrate the instrument each time a new sample gas or experimental change is made. The user can reuse previously created calibrations from similar experiments. It is recommended the user make multiple calibrations rather than recalibrate the same file.

The *Fragmentation Matrix* subsection allows the user to view the masses and molecules selected to be analyzed. The display also allows the user to edit the values associated with the compounds (*Relative Abundance, Sensitivity, Ion Repeat, and Background Intensity* values.)	

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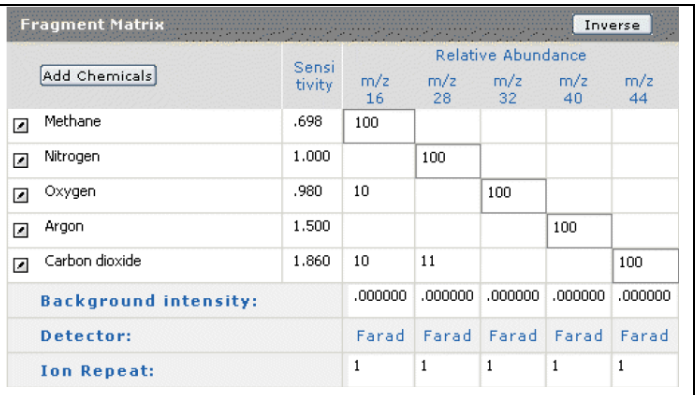
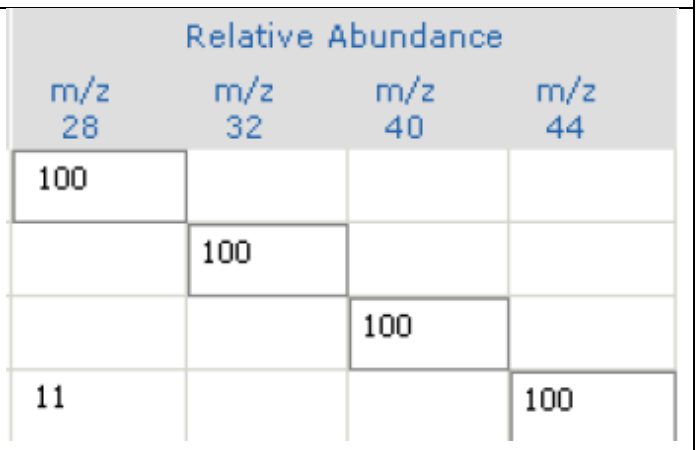
The *Sensitivity* parameter is a measure of how easy the molecule is to ionize relative to *Nitrogen*, which is assigned a *Sensitivity* value of 1 in the software. The software has a calibration sequence to determine values accurate for the instrument and the samples being used. The software has library values that are estimates, but they are not specific to the application or instrument.	
The *Relative Abundance* values allow the instrument to properly account for the relative values of molecules present in a gas stream based off their signal intensities and what is the expected contribution of one signal peak relative to the true concentration of the molecule within the gas stream. The *Relative Abundance* values also allow the instrument to determine what proportion of the mass signal is generated by each of the molecules that contribute to the signal at the m/z.	
The *Background Intensity* allows the user to view and edit the values for the intensity at each mas that is contributes from the background gases and materials in the mass spectrometer vacuum system. The *Background Intensity* is subtracted form the total ion signal, and the user needs to calibrate for accurate values to achieve quantitative analysis.	
The *Ion Repeat* field allows the user to view and edit how many times a given mass window will be scanned before the data is averaged and recorded in the *Analysis Results* tab.	

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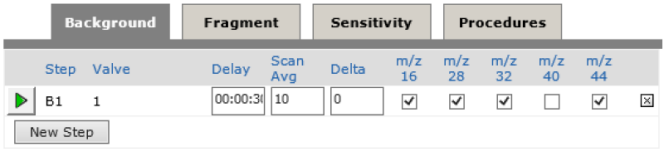
6.2.2 Calibration

The Analysis Method *selection on the* Analysis Tab *has multiple subsections, the second of which is* Calibration*, where the user can adjust the parameters for three types of calibration and define steps to be included in a complete calibration procedure.*

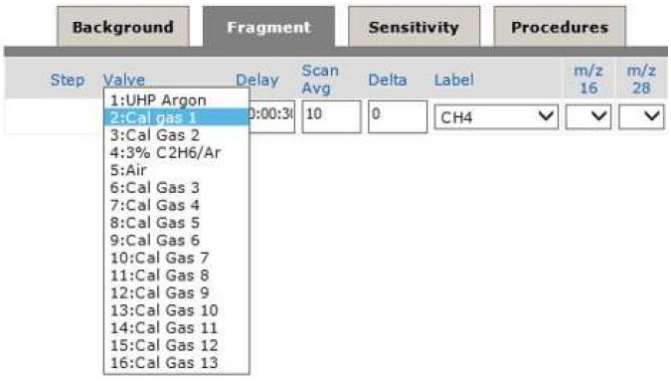
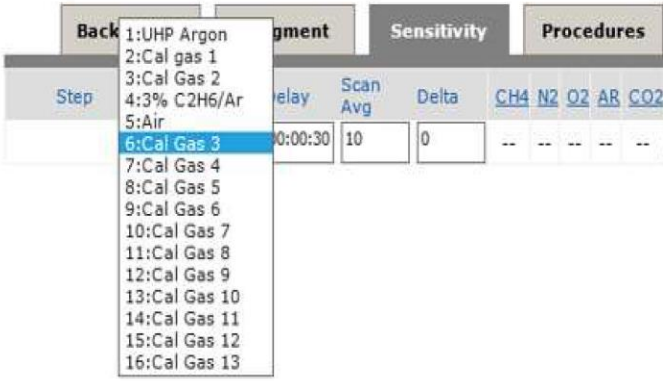
NOTE: The user should remember the isotopic forms of their gasses when performing *Calibrations.* If an isotope of a gas would overlap in its m/z signal with another gas, it must be accounted for in the *Calibration* steps.

The software determines a components concentration accurately through four calculations applied to the raw intensity signal:

- Correct total intensity for background intensity.
- Correct the intensity signal for the fragment ion interference.
- Convert the corrected intensity to concentration by factoring in the sensitivity.
- Normalization of all component concentrations to 100%.

The user can create multiple *Background Calibration* can have multiple steps to correct multiple sample gas streams. The user can create new steps by selecting *Create New.* The user must create two septs per gas mixture: one for the components with the bulk gas not selected, and then another with just the carrier gas selected. Each step allows the user to specify the gases in the stream, the valve position to be used, a time delay once the step has been started, and the number of scans taken and averaged together before a data point is plotted. The user can also specify a *Delta* value, which will let the software know that if the calibration values are different by more than +/- *Delta*, the software will reject them. **Note:** Leaving the *Delta* as "0" will allow the software to automatically accept the values.	

STOP AND REVIEW: ***For a proper *Fragmentation Calibration*, the sample gas must **NOT** have any components with overlapping fragments (e.g.: only one gas could have a fragment at mass 16.) A binary mixture of non-interfering gases is recommended***

The user can create multiple *Fragment Calibration* can have multiple steps to correct multiple sample gas streams. The user can create new steps by selecting *Create New.* Each step allows the user to specify similar parameters to the *Background Calibration* steps, but the *Fragment Calibration* step has **additional functions**. In the *Fragment Calibration* step the user specifies an **individual gas to be measured rather than multiple gases** in the stream. The gas selected is designated in the *Label* section, and the options are generated from the *Fragmentation Table* created in previous steps. The user will have to select a *Base Peak* (labeled "B") to be used as the primary mass (most abundant typically), and the other masses present will be designated as *Fragments* (labeled "X".)	
The user can create multiple *Sensitivity Calibration* can have multiple steps to correct multiple sample gas streams. The user can create new steps by selecting *Create New.* Each step allows the user to specify similar parameters to the *Background Calibration* steps, but the *Sensitivity Calibration* step has **additional functions**. The user can select the gases being used, similarly to *Background Calibration*, but the user must also designate the concentrations of the gases being used, with the bulk gas being designated "B" for base.	

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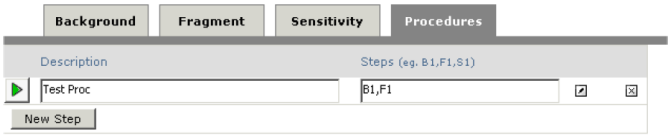
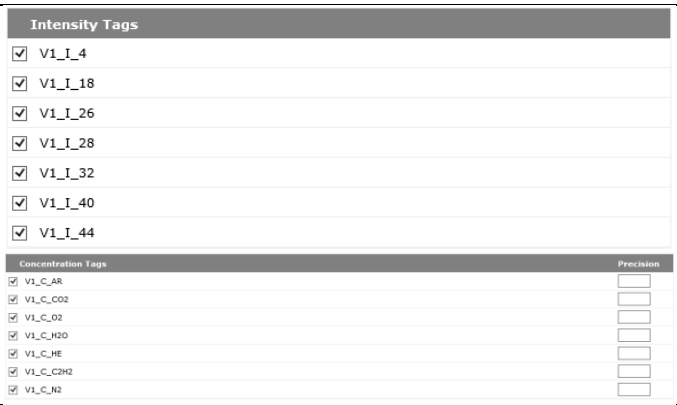
The user can create multiple steps to be ran for each of the *Calibration* procedures, and each step can be ran individually. The user can also specify that all steps in the current method be ran as well, by selecting the *Start* button at the top of the *Analysis Method* tab in the software. However, the user can also designate specific sequences of steps to be ran in a certain order. The *Procedures* window allows the user to create a new step and specify steps to be ran based off the designations of the steps from the previous windows. **Ex:** B1, F1 ,S1 instructs the instrument to run the first *Background Calibration,* then the first *Fragmentation Calibration,* and then run the first *Sensitivity Calibration.*	

6.2.3 Output Tags

The Analysis Method *selection on the* Analysis Tab *has multiple subsections, the third of which is* Output Tags*, where the user can view and edit software derived data tags.*

When the user first views the *Output Tags* window, the software will have two types of automatically generated tags: *Mass Intensity* tags and *Compound Concentration* tags. **Note:** Only the data tags with a check mark next to them will be saved to the Questor 5 database.	
The *Output Tags* are structured with the Valve Position of the analyte, the identifier for the type of data tag, and then the component or mass of interest depending on the identifier, with each of these fields being separated by an underscore.	V1_I_4

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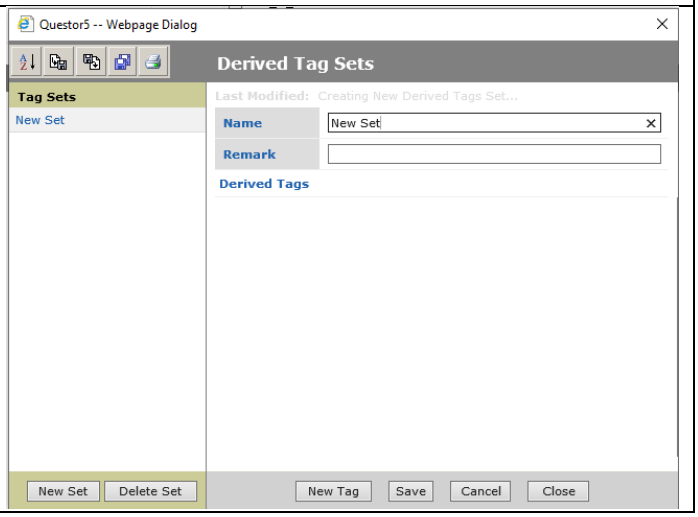
The *Mass Intensity* tag is a background subtracted ion intensity at the specified m/z. These tags have an identifier “I”. The *Compound Concentration* tag is a percentage concentration of the specified compound that has been normalized so the total of all compounds is 100%. These tags have the identifier “C”.	V1_I_4 V1_C_HE
The *Derived Value* tags are a tool within questor that allows the users to define customized expressions to calculate and maximize the information received from the mass spectrometer. The *Derived Value* tags are automatically calculated and dependent on the *Analysis Method* selected by the user.	
Along with the software creating tag set, the user can also create derived tag sets. The user can create a new set of tags by clicking the *New Set* button in any *Tag Sets* dialog box. One of the ways to do this is for the user to go through the *Output Tags* section of the *Analysis Methods Tab*.	
To create a new *Derived Tag* set, the user can *Output Tags* selection in the *Analysis Method* and click the *Derived Tag Sets* button. Questor 5 will bring up a window where the user can create a new tag set. The user can click the *New Set* button where the user will be prompted to create a name for the new tag set and give it a description.	

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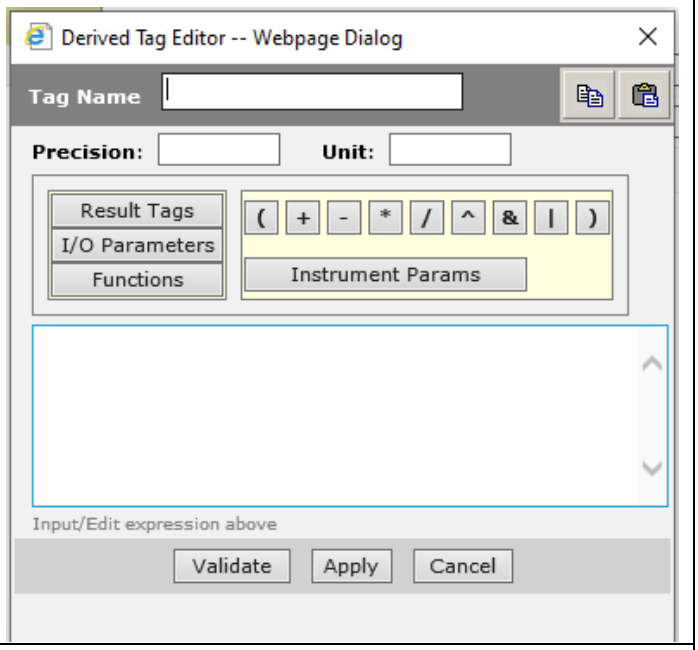
Once the user has created the new tag set, new tags can be added by selecting the *New Tag* button on the bottom of the window. Questor 5 will open a new window where the user can name the new tag and control all aspects of the created tag. The *Results Tags* button will allow the user to view a list of automatically generated tags from the currently active *Analysis Method.* **Note:** There are specific syntax rules the user must follow to create tags (see types of output tags for examples.)	
The user can edit previously created tag sets as well as creating new ones. The currently selected tag set will be highlighted in the list of *Tag Sets* on the left of the window. The user can add tags in the same way as when creating a new set, and tags can be removed by clicking the ”X” button next to the desired tag. By default, all tags within a set are selected and enabled but the user can choose to remove a tag from the set by unchecking the box next to the tag. **Note:** The user can export and import tag sets in .XML formats across other save files from Questor 5.	

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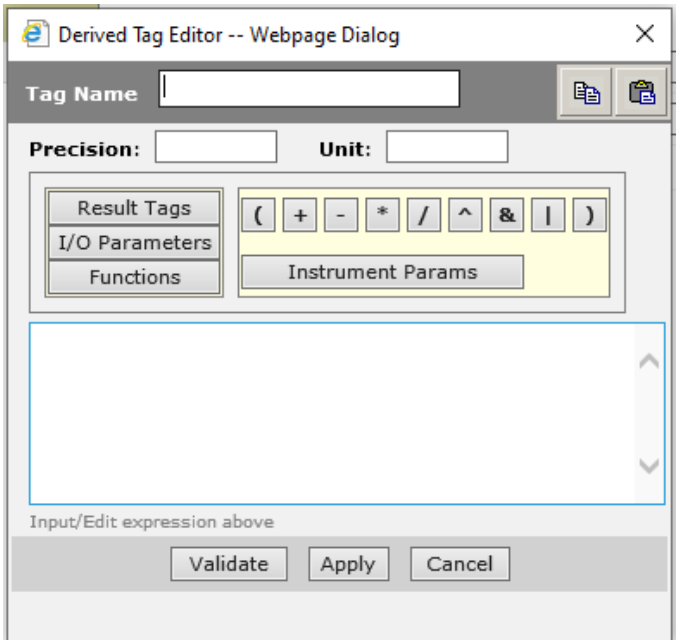
The user can create tags with multiple different types of information and parameters. The user can create tags that make use of different valve numbers as well to allow for calculations across sample streams. The " * " wildcard will apply the tag to all valves available on the instrument. **Ex**: "V*_C_CO2" would report the concentration of CO2 on all the valves on the system. The " - " wildcard will include all valves within a range of values (lowest to highest). **Ex:** "V5-8_C_CO2" would report the concentration of CO2 on valve positions 5, 6, 7 and 8. The comma " , " is used to separate a list of valves in ascending numerical order. **Ex:** "V1,5,8,12_C_CO2" would report the concentration of CO2 on valve positions valves 1,5,8 and 12. **Note:** The " , " and " - " can also be combined in an expression to define a series of valves. The user should validate the commands, by selecting the *Validate* button, after creating them to ensure the software can interpret it.	

The user can incorporate five derived data types in addition to the arithmetic operators.

Concentrations: from the concentration type tags.

Intensities: from the Intensity type of tag.

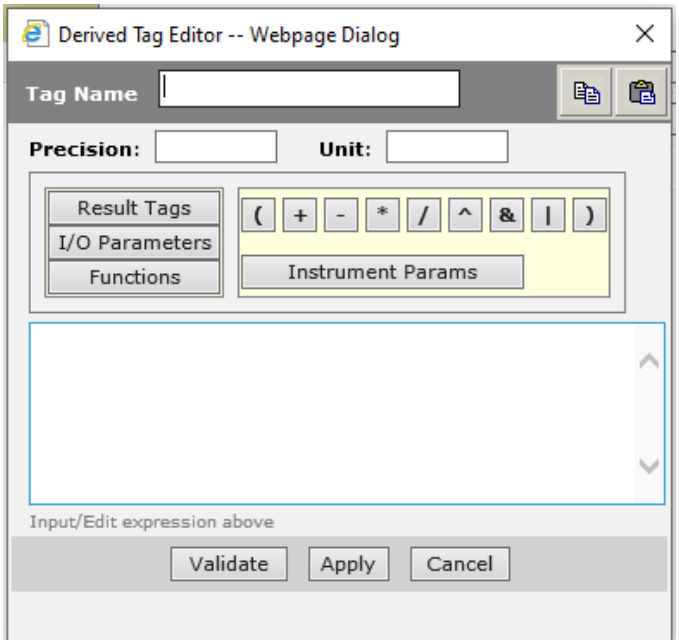
Derived Values: from other Derived Value tags. (This is useful when calculating derived values using data from several streams and/or several analysis methods).

Instrument Parameters: The user can incorporate tags relating to Instrument Parameters and instrument status. Clicking on the *Instrument Params* button will bring up a list of available instrument parameters that can be included in the derived value tag.

I/O Parameters: The user can incorporate external communications protocols installed on Questor5 to import readings from external instruments into derived value tags.

Contact Extrel Support to utilize I/O Parameters.

Support@Extrel.com



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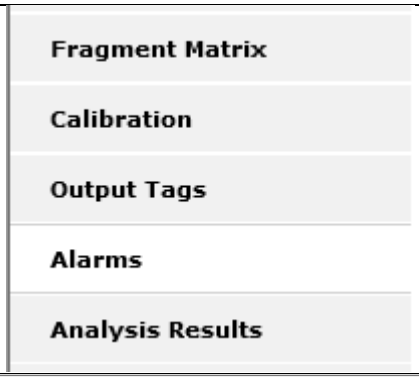
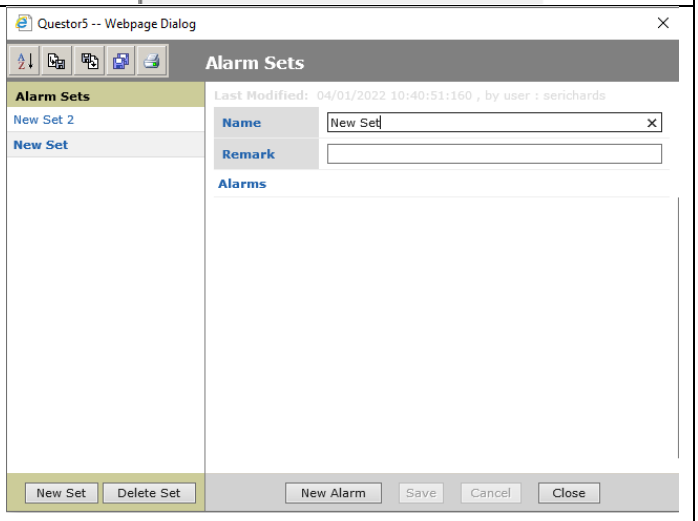
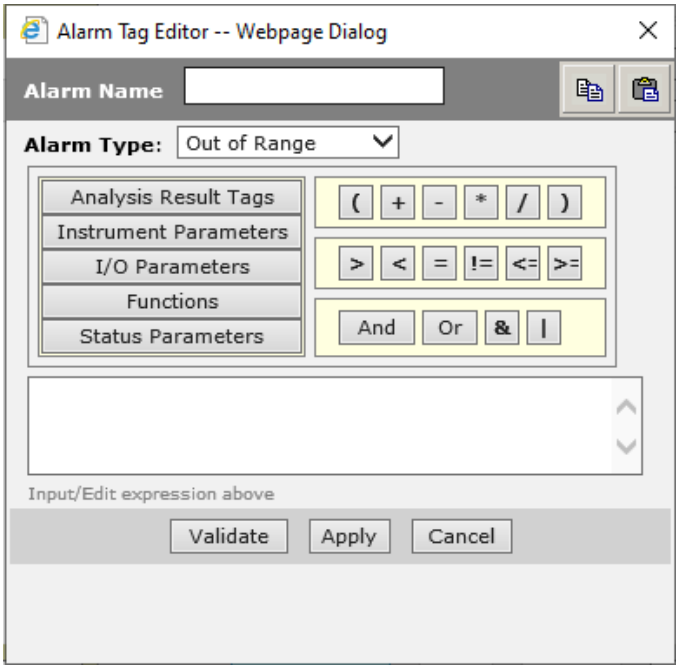
6.2.4 Alarm Tags

The Analysis Method *selection on the* Analysis Tab *has multiple subsections, the fourth of which is* Alarm Tags*, where the user can view and edit user defined alarms.*

NOTE: All *Alarm Tags* must be included in an *Alarm Tag Set* and will only be ran as part of a *Sequence*.

The user can create *Alarm Tags* to trigger upon certain user defined criteria. The user can create an *Alarm Tag Set* in a similar way to *Derived Tag Sets*. The user can go through the *Alarms* option in the *Analysis Methods* selection of the *Analysis Tab.*	
The user will have the option to create a new tag in an existing set or create a new set and populate tags within the set. The currently selected tag set will be highlighted in the left of the window and the user can select the *New Alarm* button on the bottom of the middle of the window to create a new alarm even within the existing set. The user can also click the *New Set* button on the bottom left of the new window to create a new tag set where the user will name and create a description for the tag set.	

When the user creates a new alarm, the software will create a new window where they can define parameters to trigger the alarm; *Analysis Results Tags, Instrument Parameters, I/O Parameters, Functions,* and *Status Parameters.* The user can create tags with the same syntax rules as those found when creating the *Derived Tag Set*, with some additional functions as well. The functionality of the tags is also similar, however there are some additional features. The user can create alarms to trigger based on the instrument *Status Parameters*. Depending on definitions of the user, the instrument will create an alarm status when a desired *Instrument Parameter* falls outside of the user-defined limits. The user can create alarms to trigger based on the *Analysis Result Tags*. Depending on definitions of the user, the instrument will create an alarm status when a desired *Analysis Result Tag* falls outside of the user-defined limits.	

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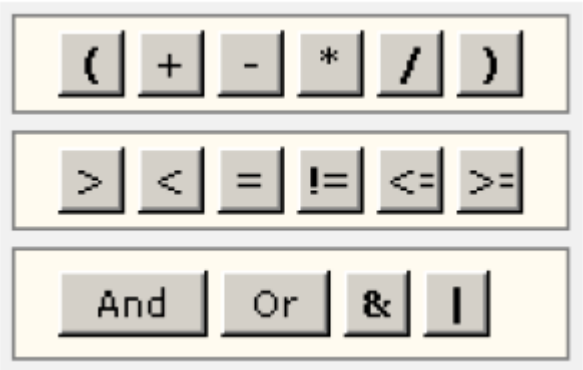
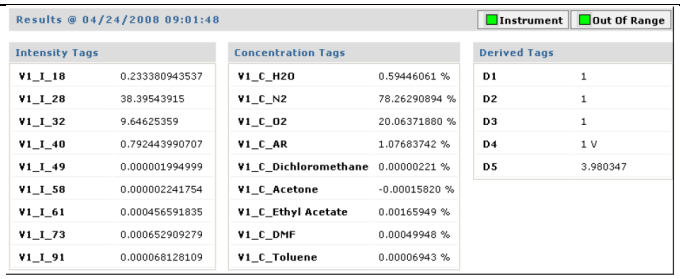
The syntax of the *Alarm Tags* is similar to the *Derived Tags*; however, alarms have additional functionalities. The user has access to equalities to define ranges or exact values for the *Alarm Tags* to follow, as well as a "!=" button to define a "not equal to" function. The user should validate the commands, by selecting the *Validate* button, after creating them to ensure the software can interpret it.	

6.2.5 Analysis Results

The Analysis Method *selection on the* Analysis Tab *has multiple subsections, the fifth of which is* Analysis Results*, where the user can view and edit user defined alarms.*

To populate the *Analysis Results* option, the user must click the *Start Analysis* button in the upper right of the window. The software will change the display to the *Results* subsection of the *Analysis Tab* and display the real-time results of the running analysis in a tabular format. The data displayed is dependent on the *Derived Tag* set defined by the user.	

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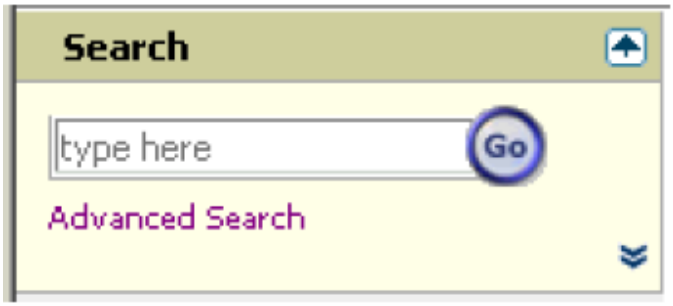
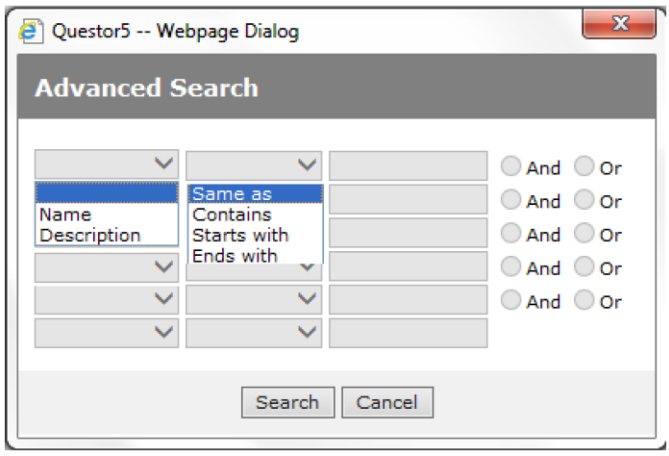
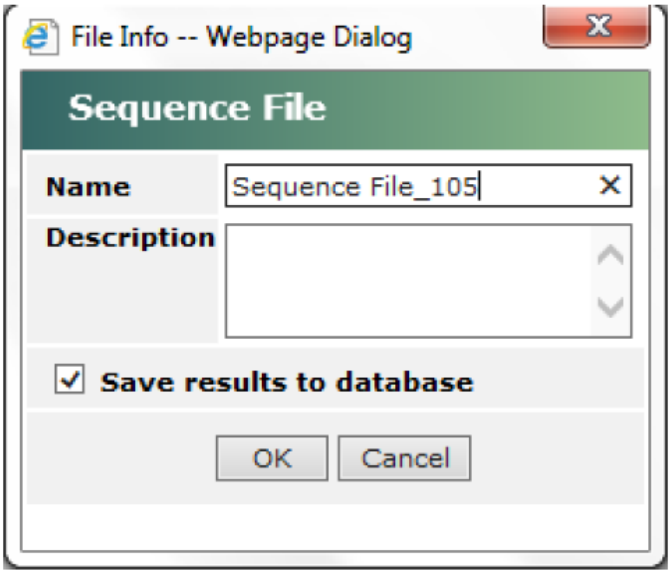
7.0 The Sequencer Tab

The Sequencer Tab *allows the user to create an automated process that will use both existing and newly created files to run an order of operations when user-defined criteria are reached.*

7.1 Sequencer Files

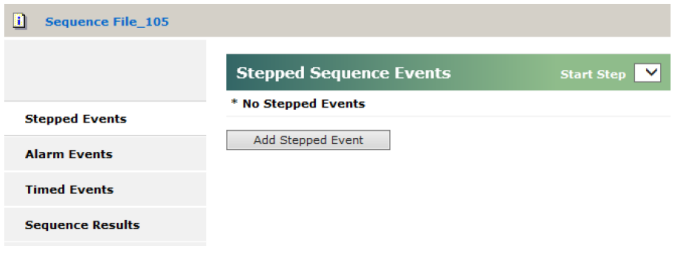
The Sequencer Files *selection on the* Sequencer Tab *allows the user to view and edit a list of files listed by name, descriptions, who last modified the files, and when they were last modified.*

The user can use the *Search* function to find files by their text names, or file descriptions using whole words or word fragments (similarly to the *Search* function in the *Tune Files* window under the *Tune Tab.*)	
The user can use a wildcard "*" to search for anything that contains the given information. **Ex**: *J* finds anything with a "J", *J finds anything that ends in a "J" or J* finds all things starting with a "J".	
The user can perform more selective *Search* through the *Advanced Search* feature under the *Search* section of the *Sequencer File* window. The user can search the fields for directly matching content, or use logical operators, or chain logical operators together to find a specific analysis file. The selected sequence file will become the active survey file only when the user enters the *Sequence* screen and starts acquiring data.	

Once the user has selected a file and clicked it, the software will direct the user to the *Sequence Selection* screen. The selected file will not become the active file until the user selects the *Start Sequence* button in the upper right of the browser window.	
The user can create a new *Sequence File* by selecting the *Create New* button in the *Sequence Files* selection of the *Sequencer Tab.*	
Once the user selects a new *Sequence File*, a window will be created to allow the user to name the file and write a description. The user can also instruct the software to save the results to the Questor database by checking the designated box. The box is checked by default to specify that data generated during a sequence will be saved and available as historical data.	

7.2 Sequencer

The Sequencer *selection on the* Sequencer Tab *allows the user to define a sequence of procedures/events that Questor 5 will go through under user defined circumstances.*

The user can create a series of *Events* that are executed according to a user-defined sequence while in *Sequence Operation* mode. The *Sequence Operation* mode allows the user to create and continuously run an automated sequence without use intervention.	

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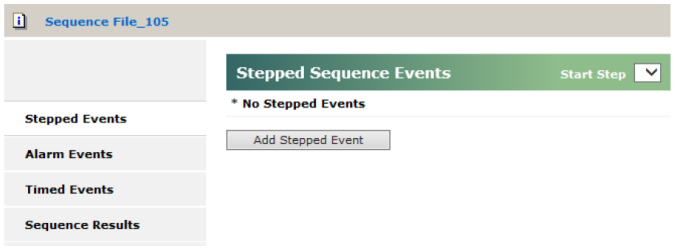
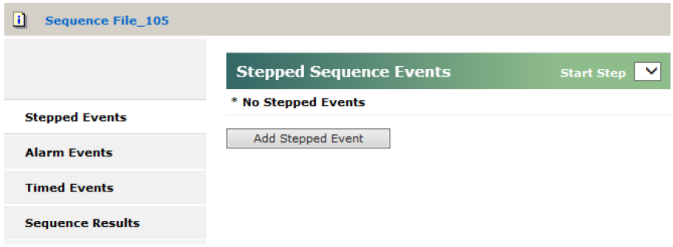
The user can create, edit, save, open, and deleted sequences through lines in the *Sequencer Tab.* A sequence includes events triggered by one of three types of triggers classified by the nature of the triggering event. The user can set any type of event to be executed from any type of trigger.	

7.2.1 Stepped Events

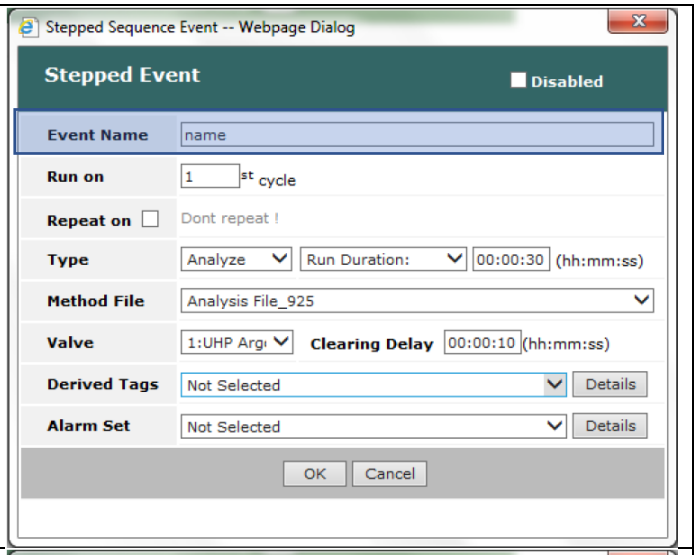
The Sequencer *has different types of events, one of which is the* Stepped *event.*

A *Stepped Event* is a sequence event that follows a user-defined step pattern. The steps are executed according to a user-defined loop series. The user will define the steps and their order, and the *Sequencer* will run through the steps in the list as written. The software will run through the steps until the end is reached, at which point it will begin the loop again. A sequence of *Stepped Events* is recommended for continuous process stream analysis, with each stream analysis being a step in the loop.	

NOTE: All sequences must include at least one *Stepped Event.*

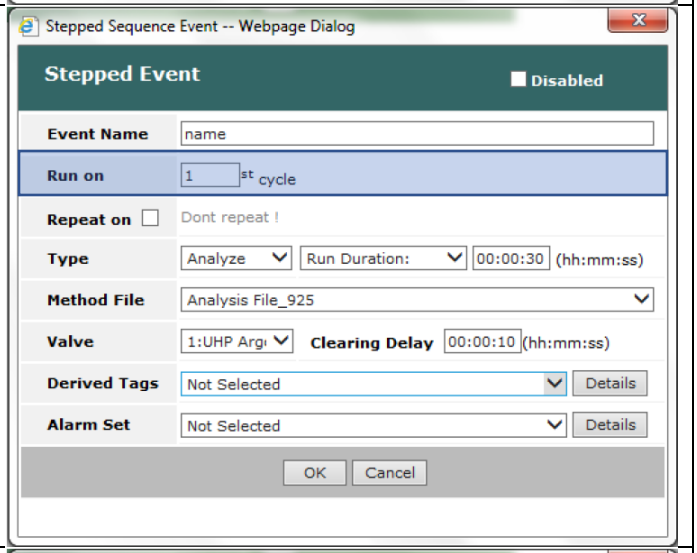
The user can create a *Stepped Event* from the named sub section in the *Sequencer* window. The user can click the *Add Stepped Event* button to bring up a dialogue box where all aspects of a new *Stepped Event* may be specified.

The user must create a unique name for the new *Event*, and it is recommended the user specify a name that relates to the function of the *Event*.



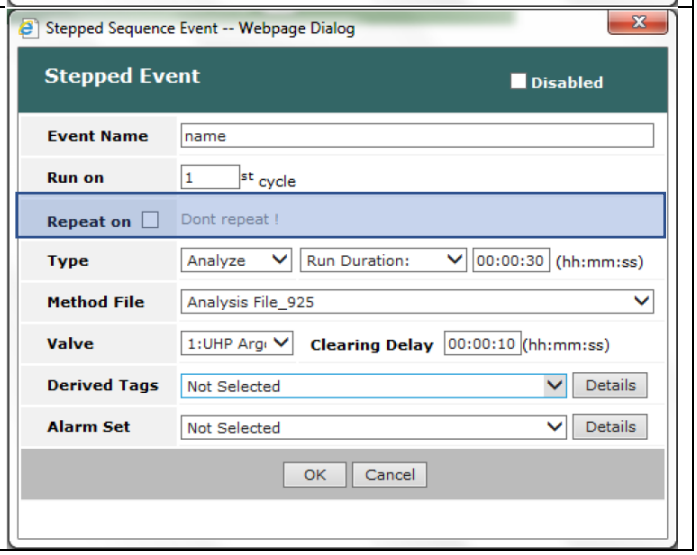
The *Run On* field allows the user to define which cycle the event will start running on.

Ex: If the user sets the field to 2, the *Event* will start to run on the second run through of the loop.



The user can select the *Repeat On* check box and assign a *Stepped Event* to be executed multiple times in a loop.

Ex: If the user selects the *Repeat On* option and sets the value to 2, the *Event* will repeat twice in that loop.



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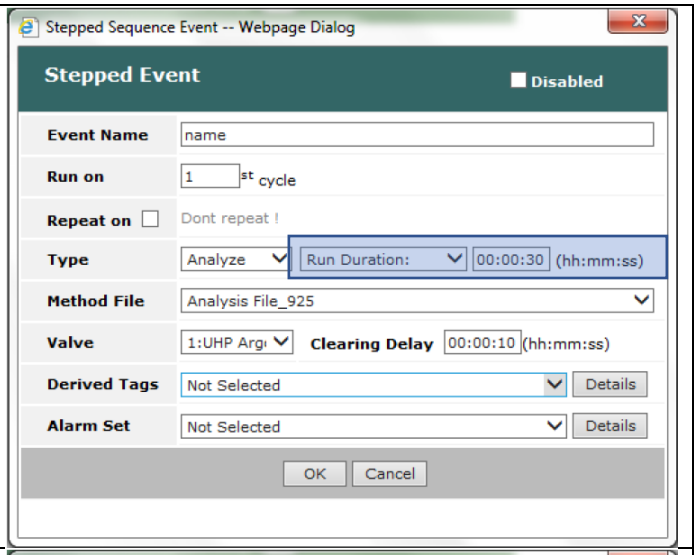
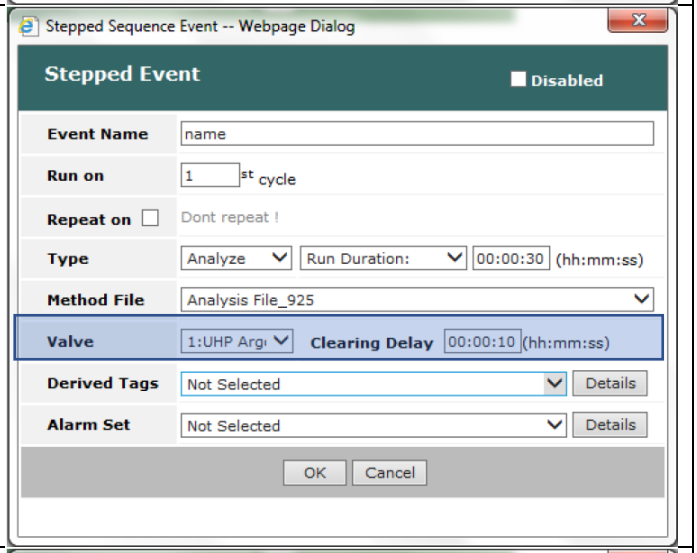
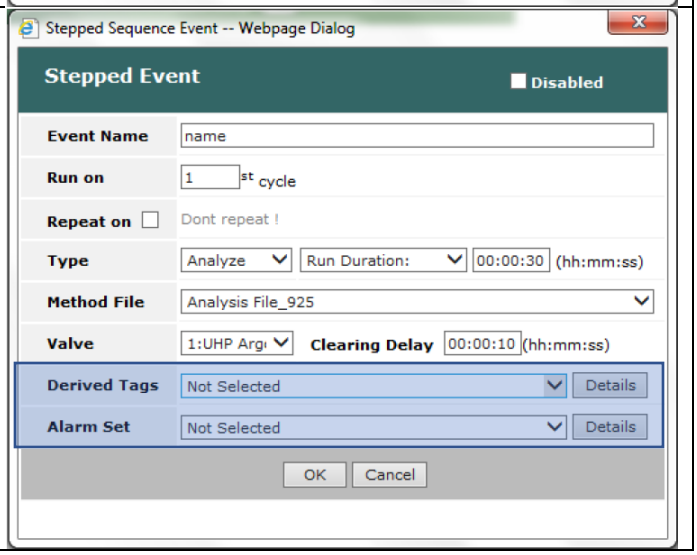
The user can use the *Run Duration* field to determine the length of time the *Event* will run for within the sequence. The default time is 30 seconds, but the user can define any amount of time in hh:mm:ss format. **Note:** The *Run Duration* field will only be displayed for *Analyze* and *Survey* event steps.	
The user can select the *Valve* to be used for the created step, as well as specify a *Clearing Delay* that will pause data collection for the duration specified so the transfer lines and system have time to purge away previous samples. The user can define the clearing delay using the same format as other time definitions.	
The user can define *Derived Tags* and *Alarm Sets* to be used in the *Stepped Event.* The *Derived Tags* field allows the user to define where to save the data created by the *Event* outside of the standard save type for the *Sequencer*. The *Alarm Set* field allows the user to define an alarm to be used for the duration of the step, and if the user-defined alarm is triggered within the step, the defined response will also be executed.	

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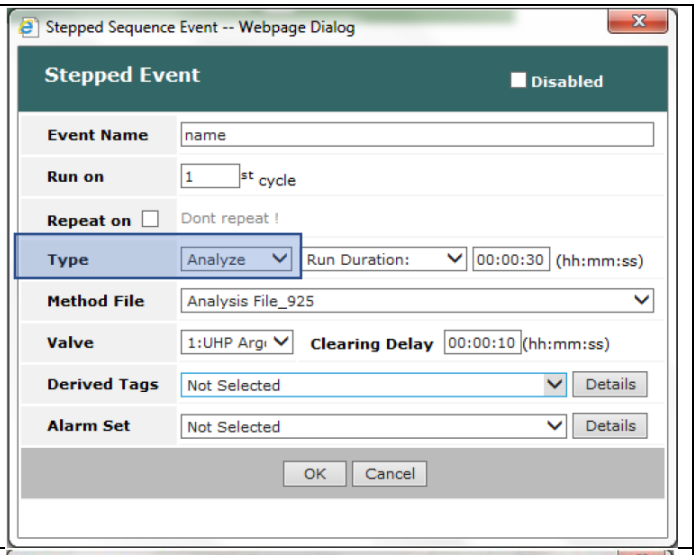
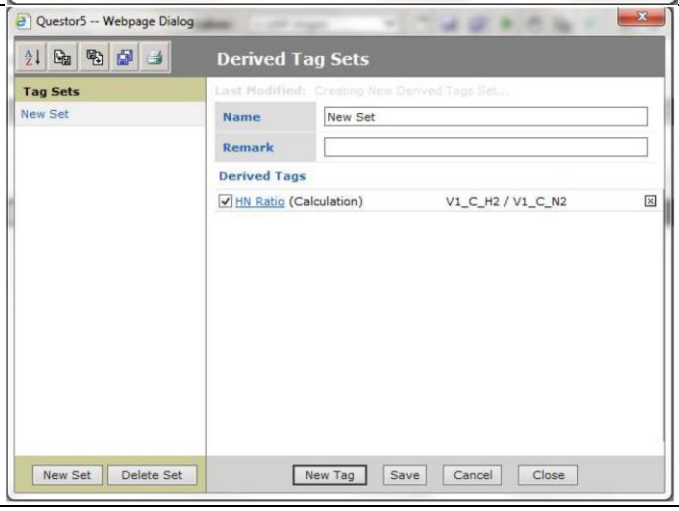
The user can define the type of *Event* from a drop-down menu. The user can select from *Analyze, Calibrate, Sequence,* or *Survey.* Each type of *Event* provides different functionality to the *Stepped Event* and will affect the options allowed within the *Stepped Event.* The user may be required to choose a method file, valve number, delay time, calibration type, sequence step or other parameters depending on the event type chosen.	
The *Analyze Type* of *Event* will allow the user to specify *Derived Value* tags and *Alarm* tags. The user can view the tags within the selected set by clicking on the *Details* button. The user can edit or create new tags in the same way as the previous methods specified in the *Analysis Tab* section.	
The *Calibrate Type* of *Event* allows the user to specify a previously made *Calibration* procedure to be ran. The possible steps are those premade in the *Analysis Tab.*	
The *Sequence Type* of *Event* allows the user to specify a *Sequence* procedure to be ran. The possible options are those that were previously made *Sequences*, to allow for nested loops of procedures to be ran.	
The *Survey Type* of *Event* allows the user to specify a previously made *Survey* procedure to be ran. The possible steps are those premade in the *Survey Tab.*	

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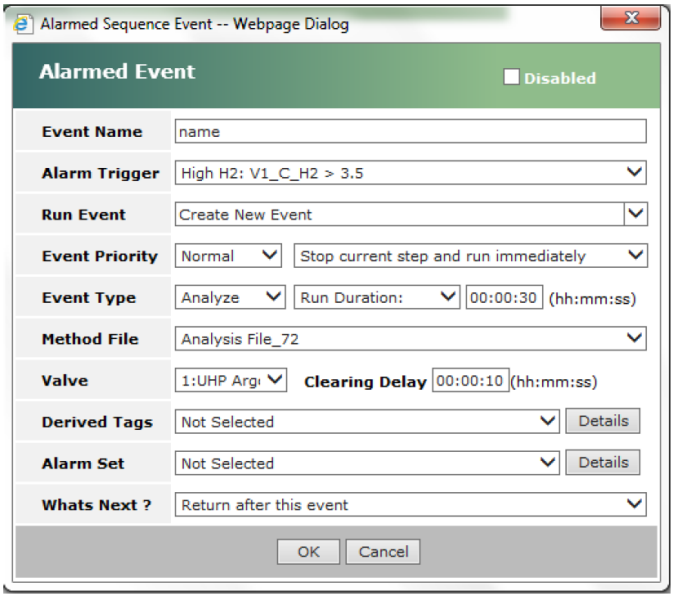
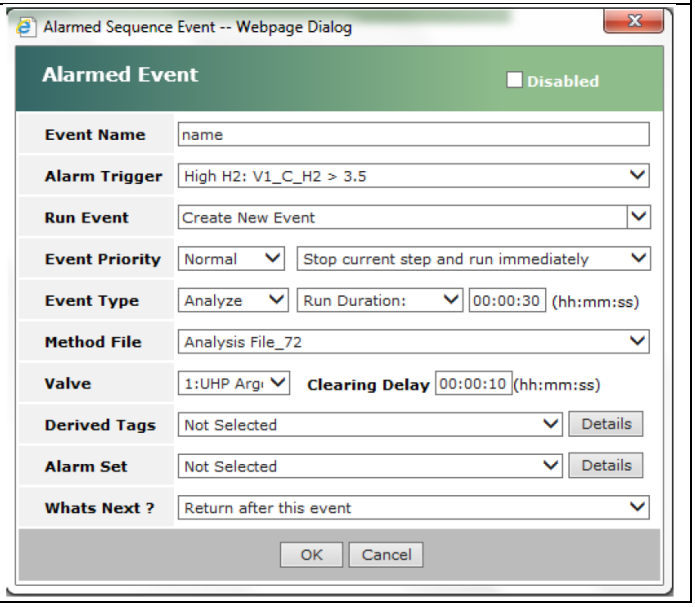
7.2.2 Alarm Events

The Sequencer *has different types of events, one of which is the* Alarm *event.*

The *Alarm Event* is one that will instruct Questor to perform a user-defined action if some parameter in the data meets the defined conditions. The user-defined event can be any previously defined event, or a newly created event to be only used in the specific *Alarm Event*. **Ex:** The user can set an *Alarm* sequence to calibrate upon failure of a checked bottle. The user can designate a range of acceptable values for the concentrations of gasses within the bottle, and the instrument can run an automatic calibration as soon as the detected values fall outside of the acceptable specified range.	
The user can create an *Alarmed Event* from the named subsection within the *Sequencer* tab. After the user has selected the *Add Alarmed Event* a window will appear where the user can specify all aspects of the *Alarmed Event*.	

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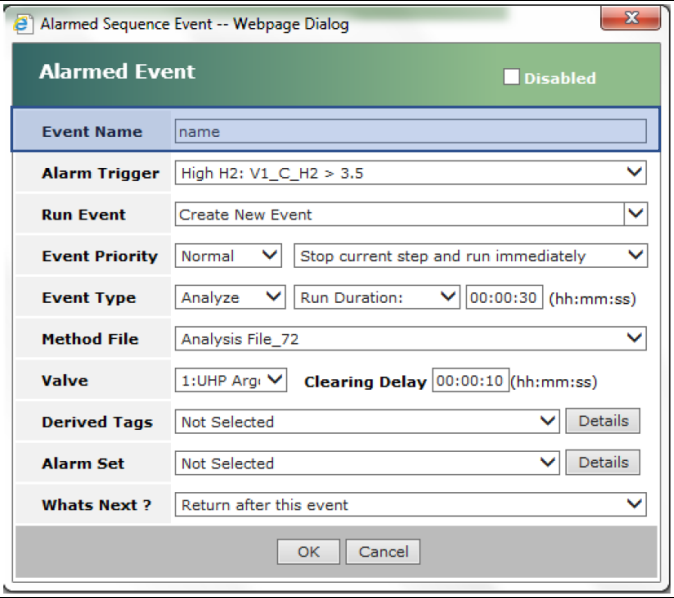
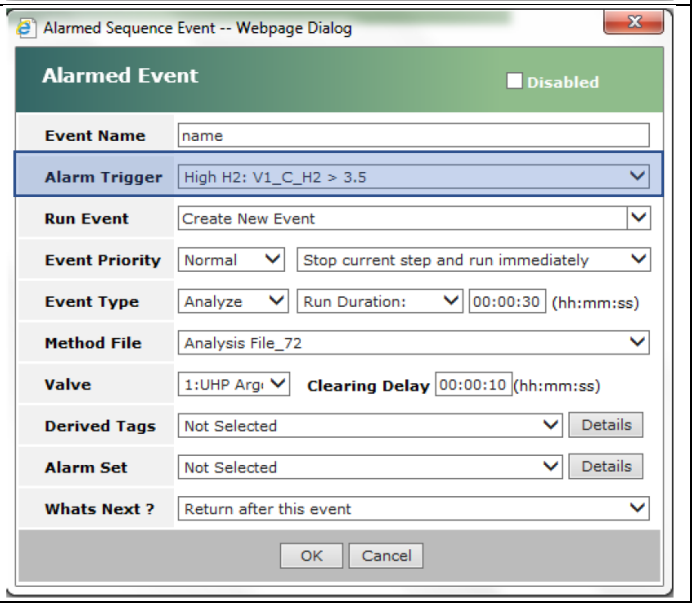
The user must create a unique name for the new *Event*, and it is recommended the user specify a name that relates to the function of the *Event*.	
The user must specify an *Alarm Trigger* from a drop-down menu that contains a list of alarm tags generated from a previously created *Alarm Set*. The user any select and previously made tag to act as eth trigger for the *Event.* If the user fails to select an *Alarm Trigger*, the *Event* will not be created.	

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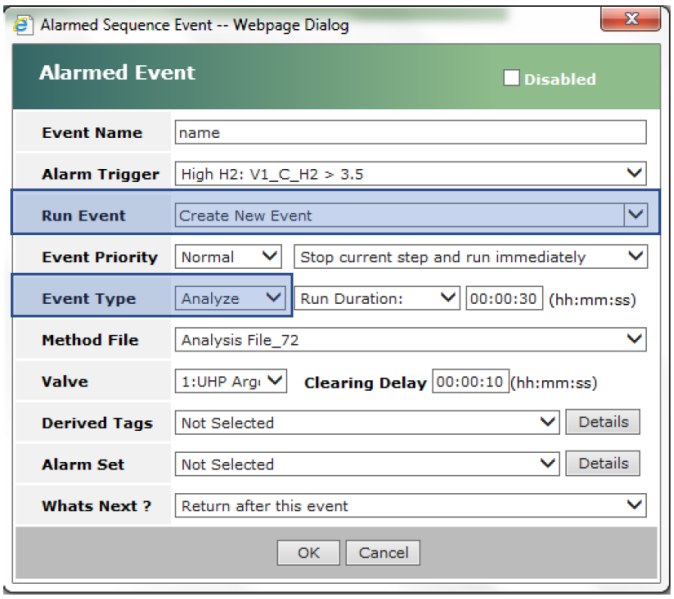
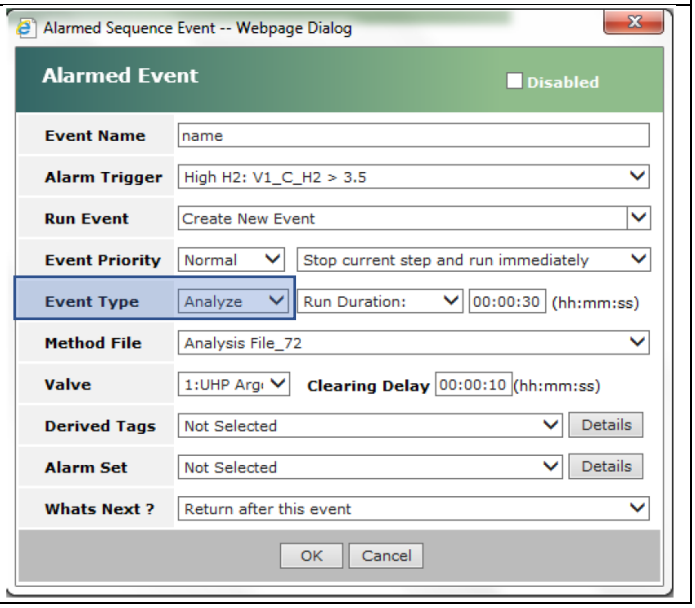
Once the user has specified the conditions that will trigger the *Alarm Event*, the user must specify the actions the software will take in response to the conditions. The user must specify the actions in the *Run Event* field from a dropdown menu. The user can select from premade processes from previous *Events,* or new events can be made. The software will either populate the other fields, if the user selected an existing option, or the user must populate the remaining fields if they selected *Create New Event.* **Note:** The available fields may change based on the selections made in in the *Event Type* field.	
If the user selects *Analyze* as the *Event Type*, then the user will be able to select a derived value tag and alarm tag. The user can use previously made tags or create new ones through the same process defined in previous sections (see *6.2 Analysis Method.*) The software defaults to having all tags enabled within each set.	

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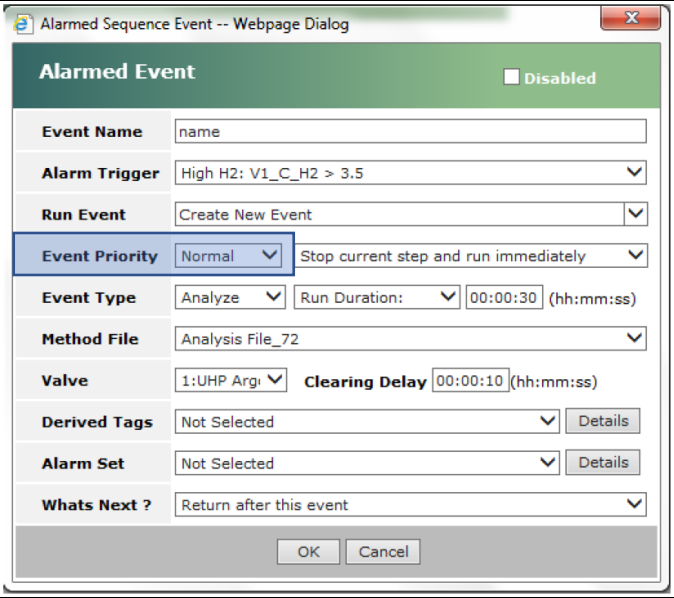
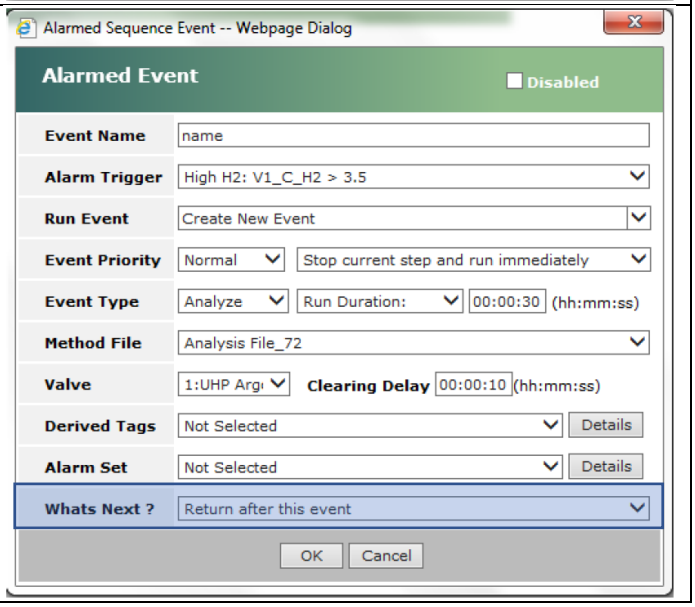
The user will have a new field to populate regardless of the *Run Event* selected. The *Event Priority* section allows the user to designate how Questor responds if multiple *Alarm Events* are triggered. The user can select from five levels of *Event Priority: Very Low* to *Very High*. The software will execute the *Alarms* in the order of the priority assigned to them. **Note:** If the user has specified two alarms to have the same priority, the software will execute the *Alarms* the order in which they were created.	
The user must also make a designation in the *What's Next?* field. The user will be presented with different options based on whether the *Run Event* is a *New Event* or premade event. If the user has created a *New Event,* then they will have the options to *Stop sequencer after this event* or *Return after this event.* If the user designated a preexisting *Event*, then the user will have access to the previous options as well as *Continue from here*.	

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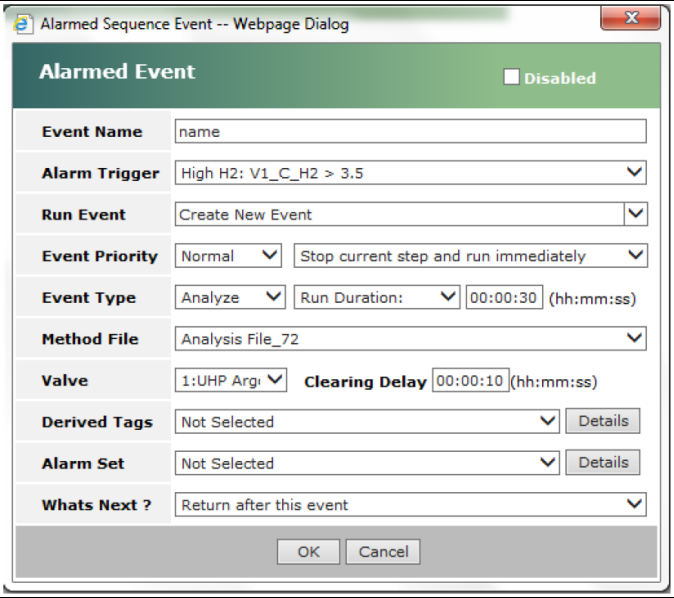
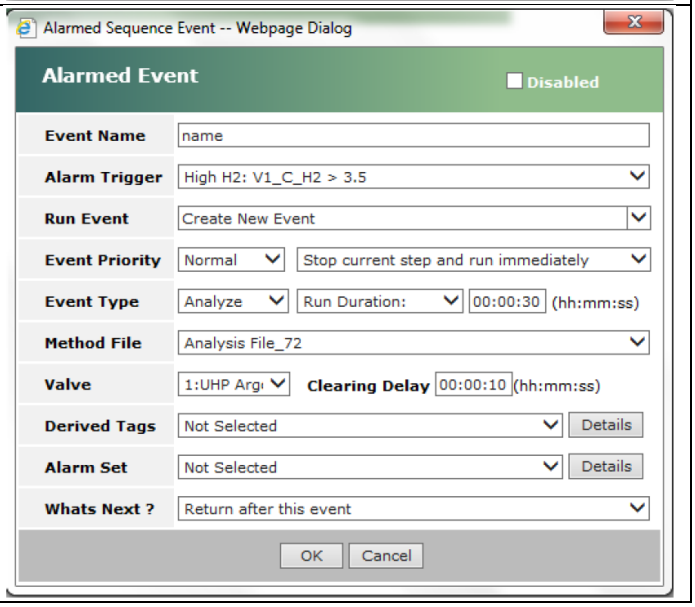
If the user selects *Stop sequence after this event* the mass spectrometer will stop operation and stop collecting data as well.	
If the user selects *Return after this event* the software will resume operation at the next point in the sequence after where the *Alarm* was triggered.	

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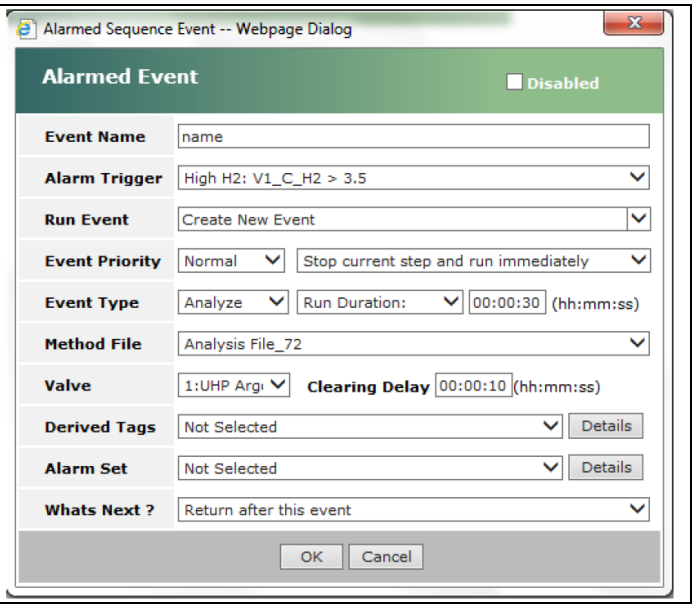
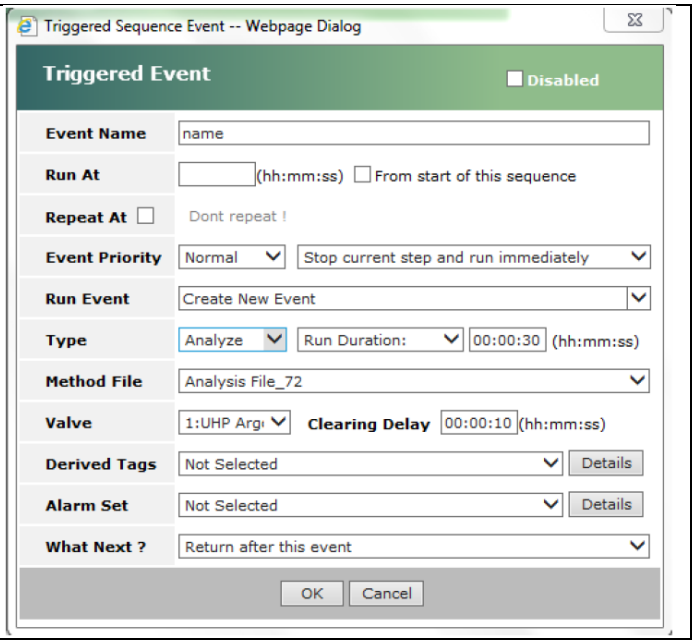
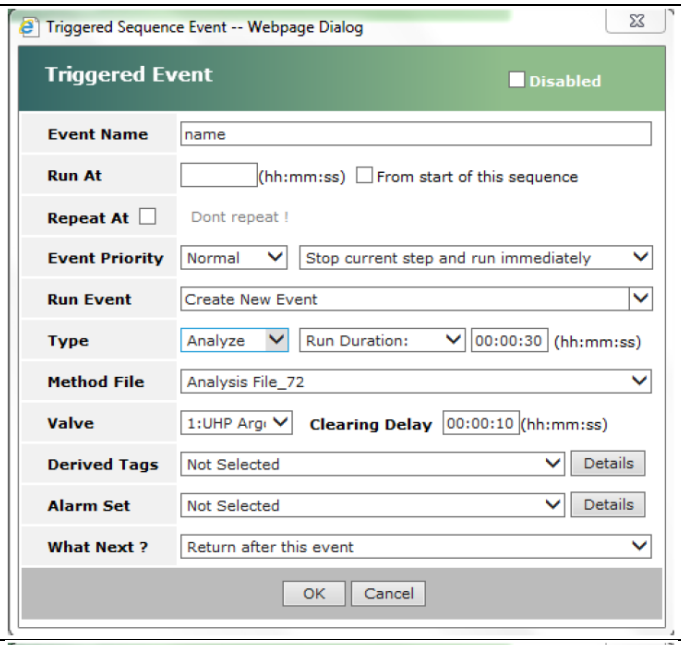
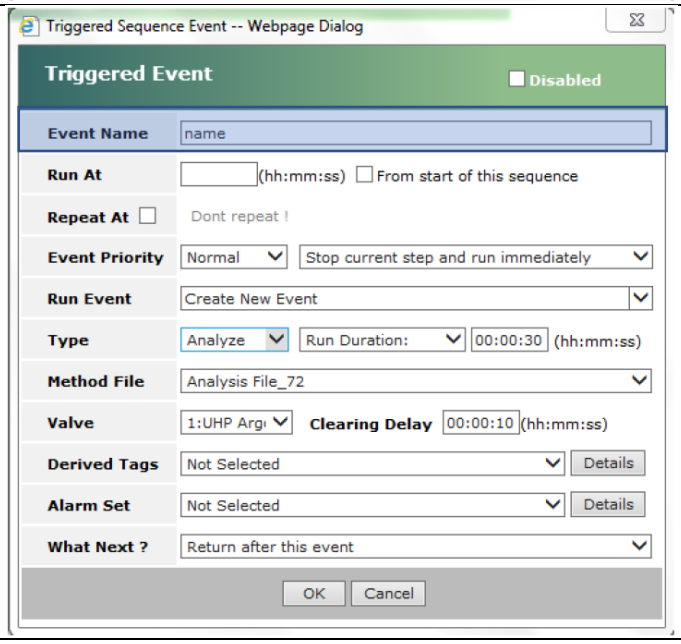
If the user selects *Continue from here* the software will continue the sequence with whatever occurs after the step called by the *Alarm Event.* **Note:** The user can only select the *Continue from here* option if they selected a preexisting sequence step for the *What's Next?* field.	

7.2.3 Timed Events

The Sequencer *has different types of events, one of which is the* Timed *event.*

The *Time Event* one the user can use to instruct the software to perform an action after a specified time condition. The user can set the time condition to be based on an interval or a specified time in the system clock. The user can have the event be based off something previously defined, or a newly created event. **Note:** The *Timed Events* are based on local time and follow a 24 -hour format.	

The user can create a new *Timed Event* in the *Timed Events* subsection of the *Sequencer Tab*. The user must select the *Add Triggered Event* button and a dialogue box will be created where the user can define all aspects of the newly created *Timed Event.*	
The user must create a unique name for the new *Event*, and it is recommended the user specify a name that relates to the function of the *Event*.	

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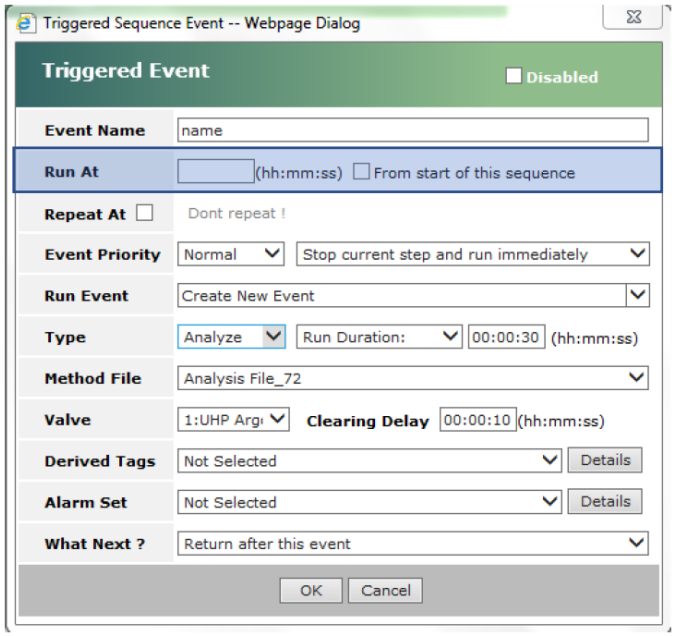
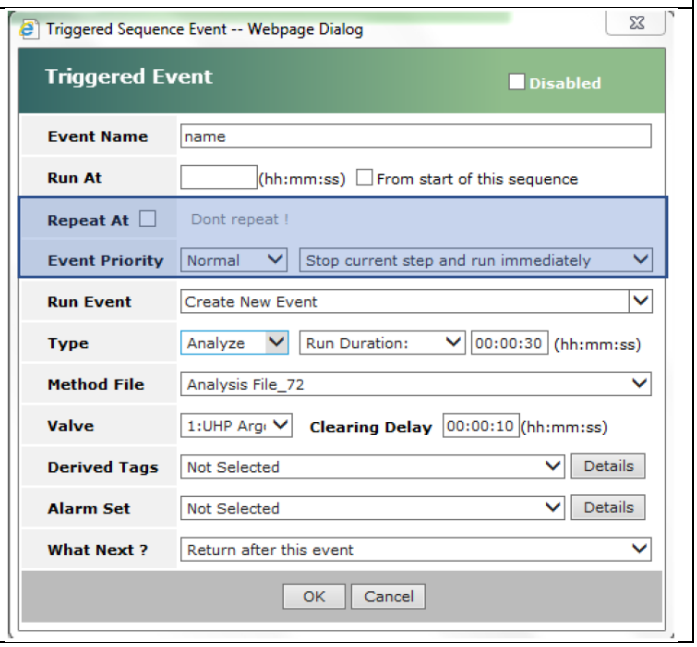
The user must designate a time element to trigger the *Timed Event*. The user must fill out the *Run At* section of the window with a time specification, following the same format as other time elements within the software. The user can specify the trigger to be after an increment of time by checking the box *From the start of this sequence.* If the user does not check the box, then the software will interpret the *Run At* field as a time specification during the day and will run the event at the time.

Ex: If the user specified the *Run At* field as 02:00:00, the system would interpret that as either 'Run this step after two hours of running this sequence' or as 'Run this step at 2:00 am local time' depending on whether the box is checked.



If the user checks the *Repeat At* box, the software will create a new set of fields for the user. The software will create fields for the user to specify how often the event should be repeated once triggered, as well as assigning an event priority like in the *Alarm Events* section.



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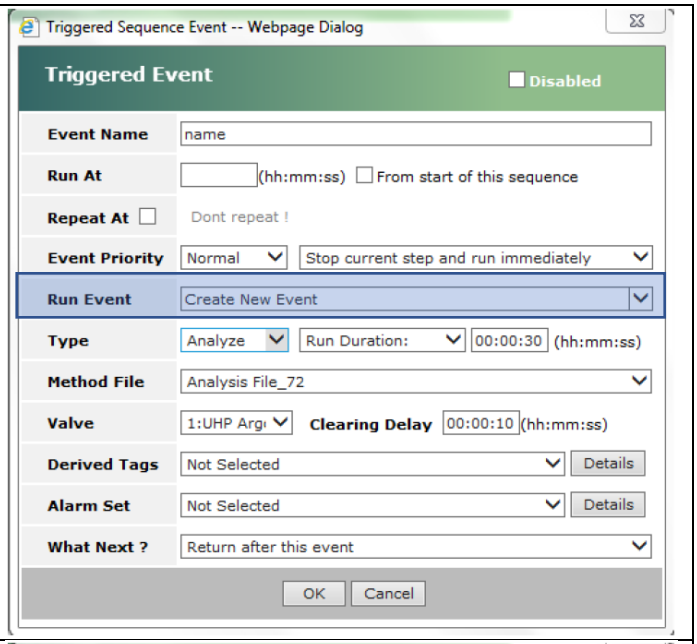
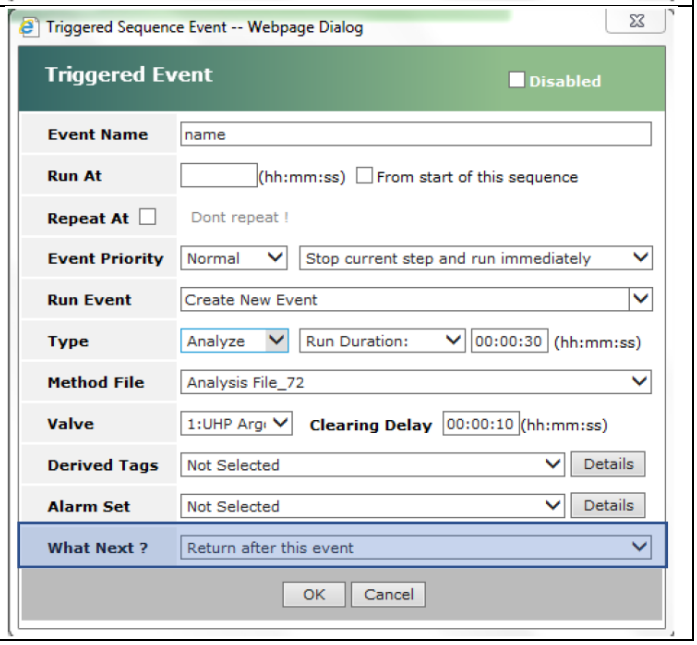
The user must specify the *Run Event* field with the same options as those found in the *Alarm Events* section. The software will trigger the designated *Event* once the time trigger has been reached. **Note:** The user can specify preexisting events as well as creating new ones in the *Run Event* field.	
The user must specify the *What's Next?* field with the same options and conditions as those found in the *Alarm Events* section.	

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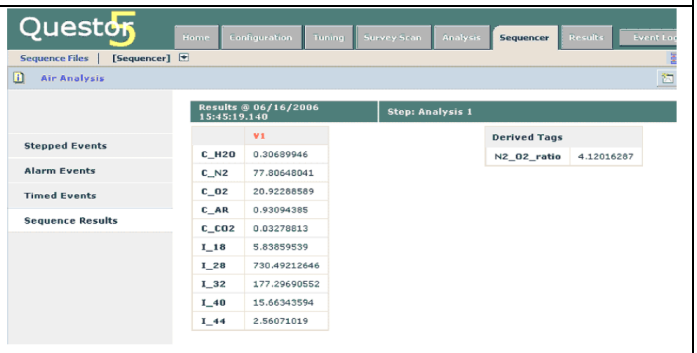
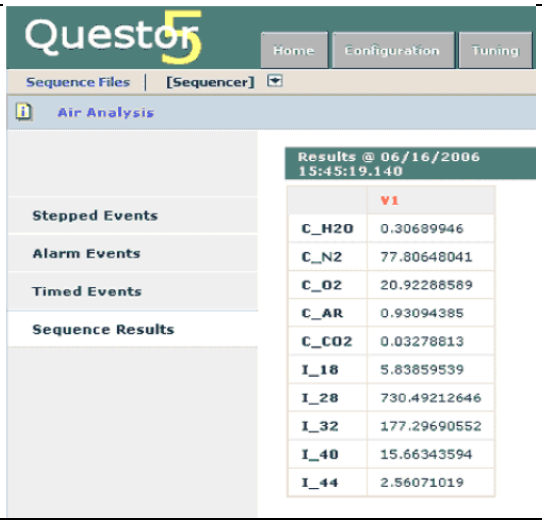
7.3 Sequence Results

The Sequence Results *selection on the* Sequencer Tab *allows the user to view the data gathered and generated from the user-defined and created sequences.*

The user must start a *Sequence* to have the software execute it and acquire and record the specified data. The user must select the *Run Sequence* button from the *Sequencer* tool bar at the top-right of the tab.	
When the user has started the *Sequence*, the software will shift the display to the *Sequence Results* section of the *Sequencer Tab.* The spectrometer will display the generated data in a table. The default format of the table allows the user to view the date and time of the acquired data, as well as the name of the ran *Sequence* file.	
The software automatically populates the left table with the generated concentration and intensity tags from the user-specified method file from the *Sequence.* **Note:** The *Concentration Tags* report percentages normalized to 100%. The *Intensity Tags* report in arbitrary units with a maximum value of 10,000.	

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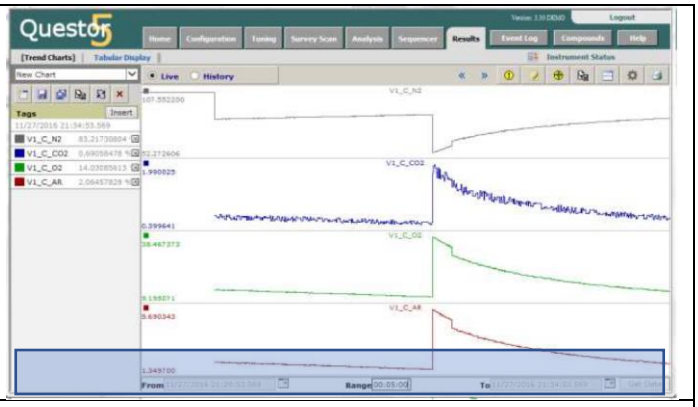
8.0 The Results Tab

The Results Tab *allows the user to view real-time and historical data generated from an* Analysis Method *or an automatic* Sequence. *The user can also export the acquired and recorded data from the* Results Tab.

NOTE: All data displayed in the *Results Tab* is dependent on the running method from either the *Sequencer* or *Analysis* tabs.

8.1 Trend Charts

The Trend Charts *allow the user to view the real-time and historical data presented in a graphical format presented as continuously recorded data. The user can change the format of the graphs, how it can be exported, and the desired time span of the data being displayed.*

The user can view the data generated by the mass spec from the *Trend Charts* window of the *Results Tab.*	
The user can search for previously recorded data in the *History* designation of the *Trend Charts.* The user can define a time range to view the currently generated data, as well as a date range. The formatting for the time fields is the same as those previously described. **Note:** The user must click the *Apply* button for the selected dates and time to become the active time ranges, and the user must click the *Get Data* button to retrieve the data from the specified times.	

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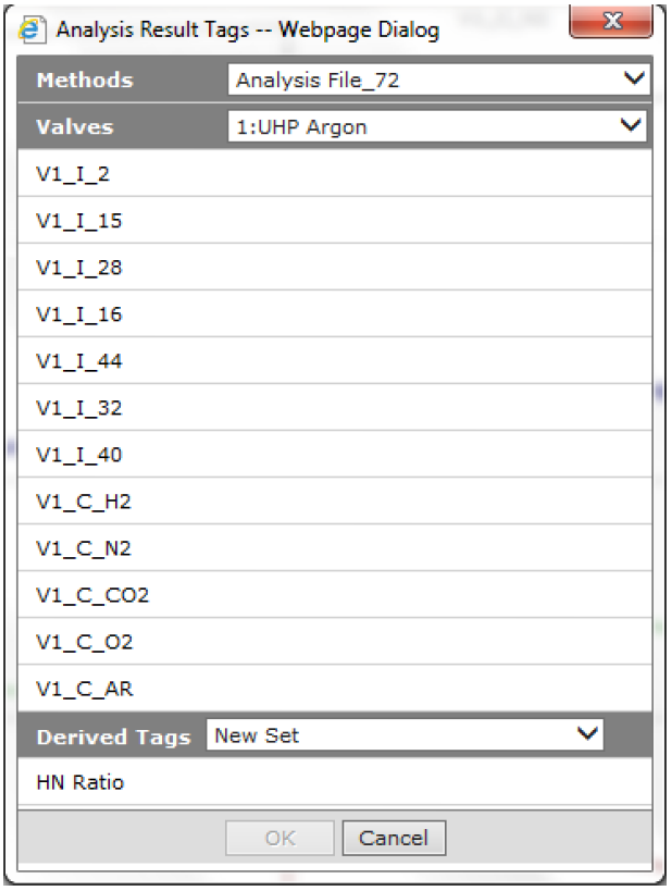
The user can select the data being displayed by selecting the desired *Data Tags* associated with the running analysis method. The user can add data tags being displayed by clicking the *Insert* button on the left of the *Trend Charts* screen. The software will create a new window where the user can add or create data tags to be monitored and recorded in the graphs.	
The user can select new data to be displayed in the *Trend Chart* by selecting a tag from the displayed list and clicking the *Ok* button at the bottom of the screen. The user can also select a different *Valve* by clicking the name field and selecting one of the available options from the drop-down menu. If the user selects a new *Valve*, the available data tags will change to reflect the new selection. The user can also select a different *Method* by clicking the named drop-down menu. If the user selects a new *Method*, then the list of available data tags will change to reflect the new selection. The user can also select a different *Derived Tags* set by clicking the named drop-down menu. If the user selects a new *Derived Tags* set, then the list of available tags will change to reflect the new selection.	
Once the user has made the new selections and clicked the *Ok* button on the bottom of the new window, the *Trend Charts* will need to be updated by clicking the *Apply* button on and load the new tags and their data.	

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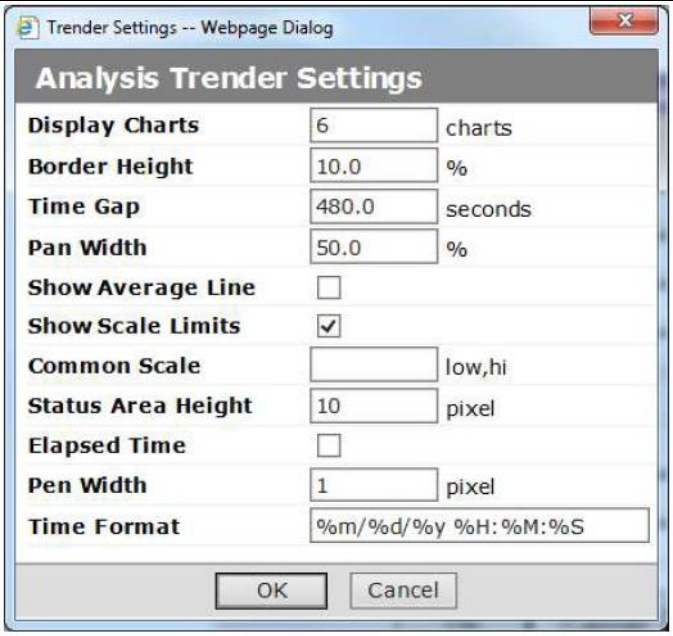
The data tags selected will be compiled in a chart to the left of the screen. The chart displaying the tags allows the user to see the time and date of the last data received for the specified time range. The software automatically displays the tags by name order, with the last data point displayed alongside the name. The user can save the current tag configurations by selecting the *Save* icon at the top of the tags chart.	
Along with editing the tags being used, the user can change how the data in the graphs can be displayed as well. The user can click the *Settings* button in the top right of the *Trend Charts* window.	

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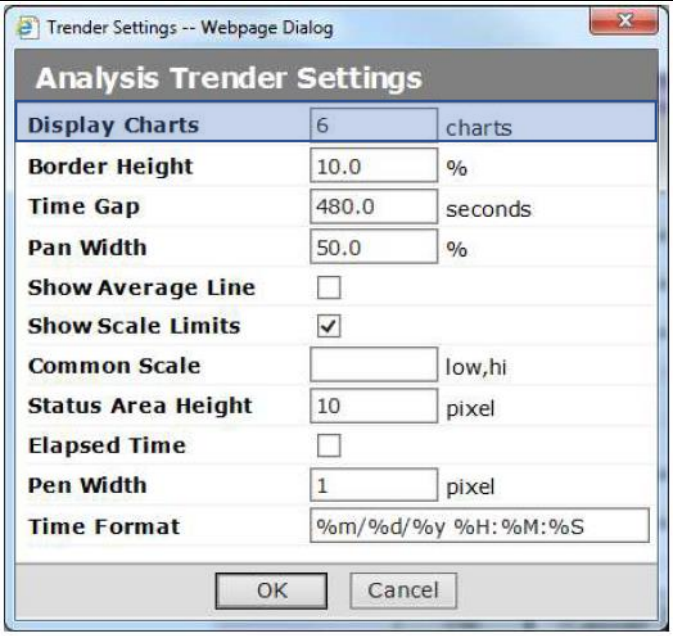
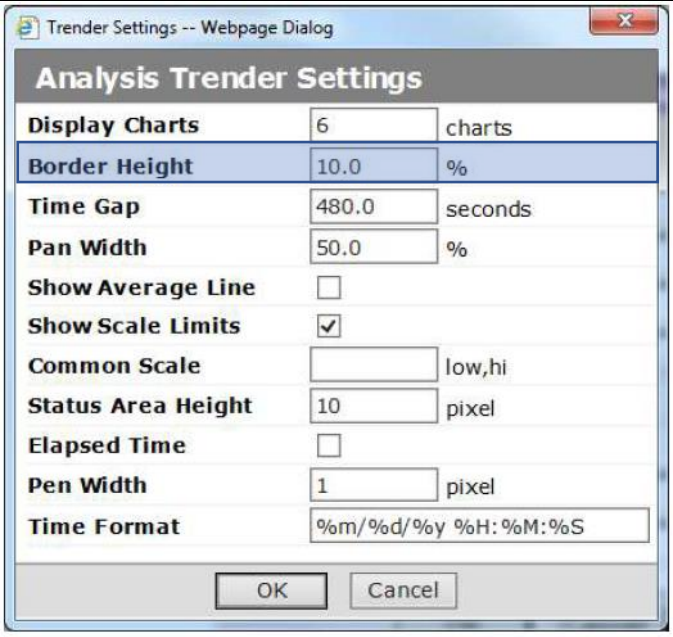
The *Display Charts* option allows the user to designate the number of charts visible on the screen at a time.	
The *Boarder Height* option allows the user to select an area on the top and bottom of the chart to never be occupied by data, to keep the data easily readable.	

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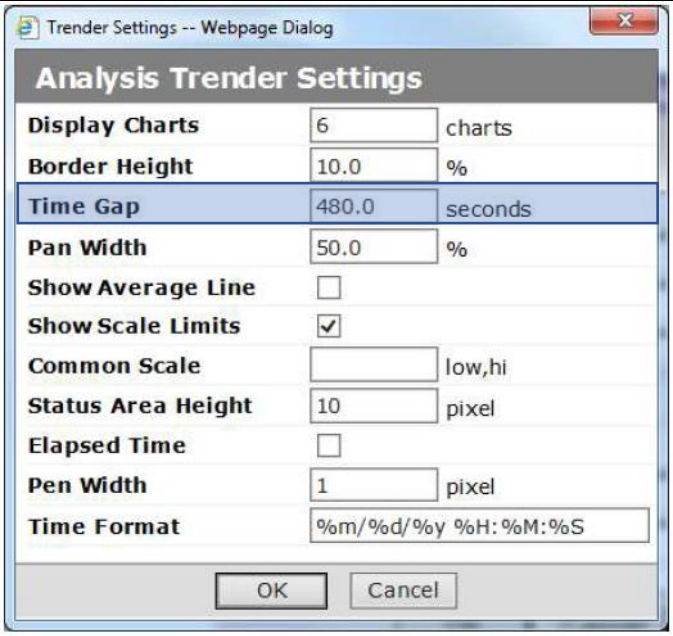
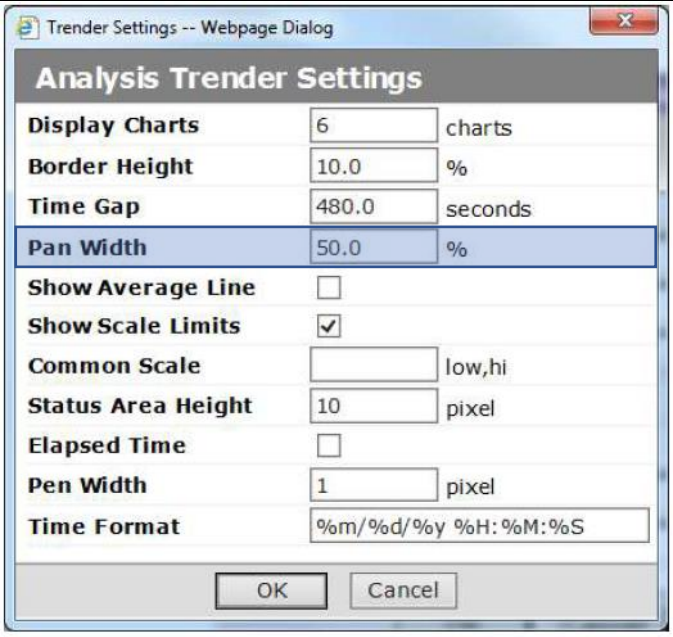
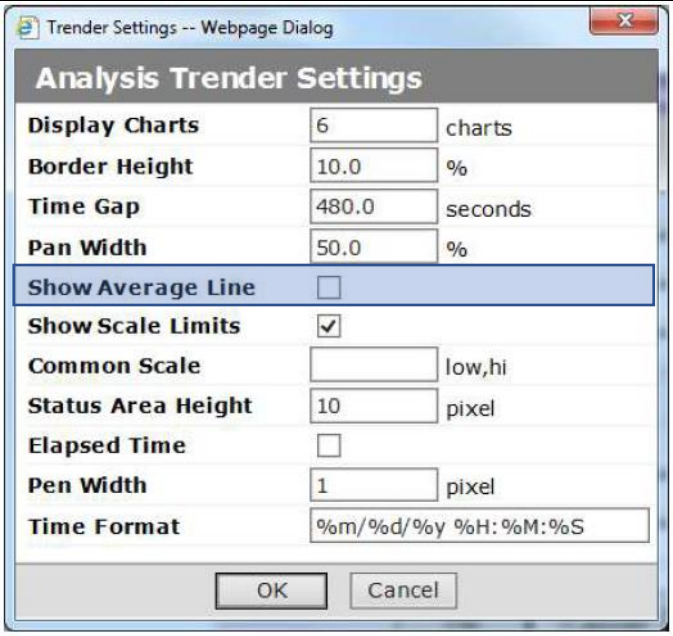
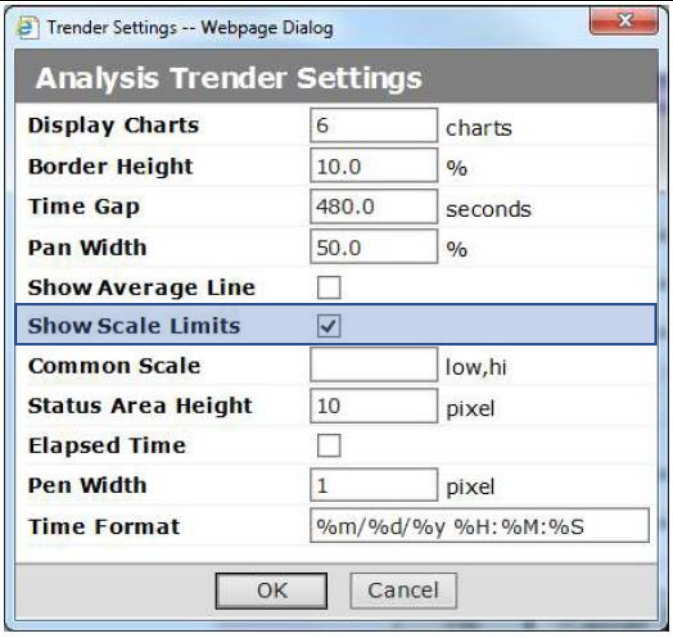
The *Time Gap* option allows the user to specify the length of time between when data points are considered continuous for graphing purposes.	
The *Pan Width* allows the user to determine the action of the *Pan* buttons. The default setting is 50%, meaning the user can pan across the displayed data in increments of one half of the currently time selected to display data.	

The *Show Average Line* box allows the user to display a horizontal dashed line on each chart that corresponds to the average value of eth currently displayed data.	
The *Show Scale Limits* option allows the user to display the scale limit values at the top and bottom the data charts. **Note:** The values displayed are the maximum and minimum values of the data window, not the maximum and minimum of the data being displayed.	

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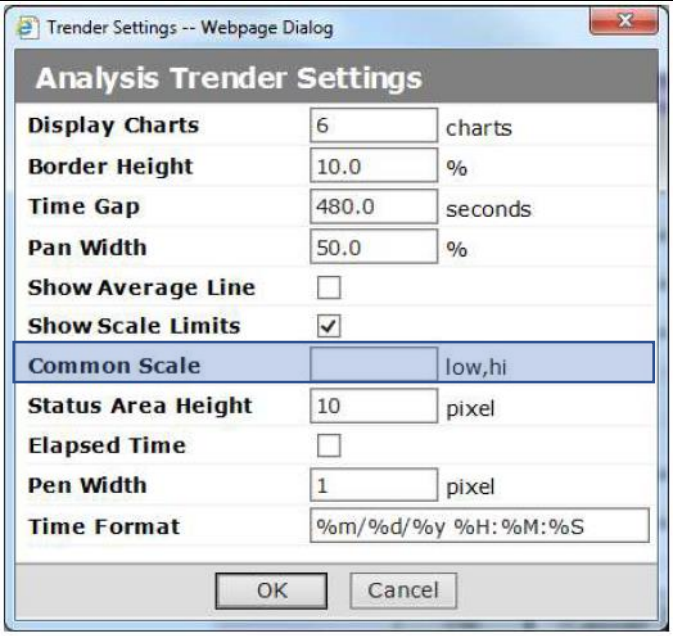
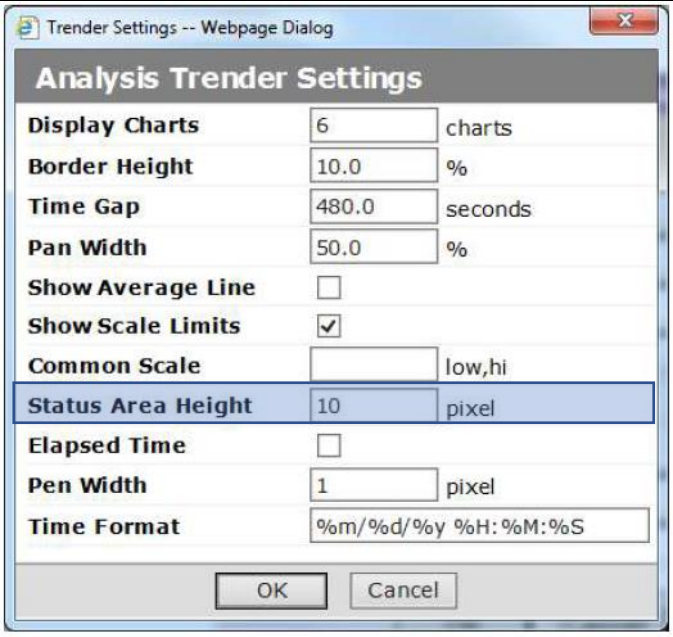
The *Common Scale* option allows the user to specify a common scale for all charts to follow. If the user sets values in this field, all the displayed charts will shift their maximum and minimum values to the defined values.	
The *Status Area Height* option allows the user to specify the number of pixels used to display the auxiliary charts for *Alarms, Annotations,* and *Calibrations.*	

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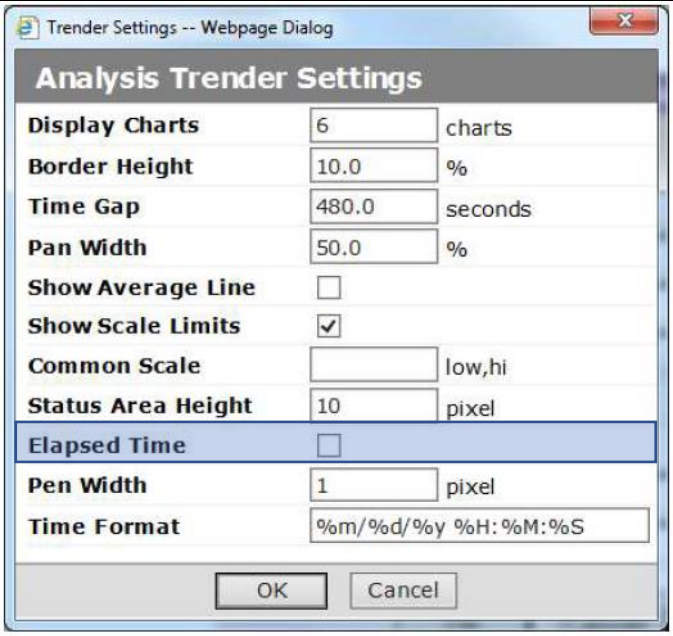
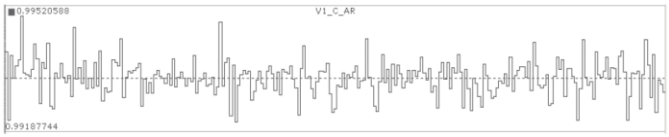
The *Elapsed Time* option allows the user to change the time display to show the time elapsed since the beginning of the current *Analysis*. **Note:** The last options for *Pen Width* and *Time Format* are unused. Altering the *Time Format* will not allow the software to understand time inputs and the *Pen Width* has no meaningful function.	

NOTE: The user must click the *Save* button for any of the changes made in the *Settings* to become active.

The user can also view more specific settings in each of the graphs. The software automatically displays a center line running horizontally through the window that sits at the middle point of the scale for the graph. The line generated is to allow the user to view the changes in the data over time relative to a controlled point.	
The user can view the data being displayed within each graph through a label at the top-center of each graph.	

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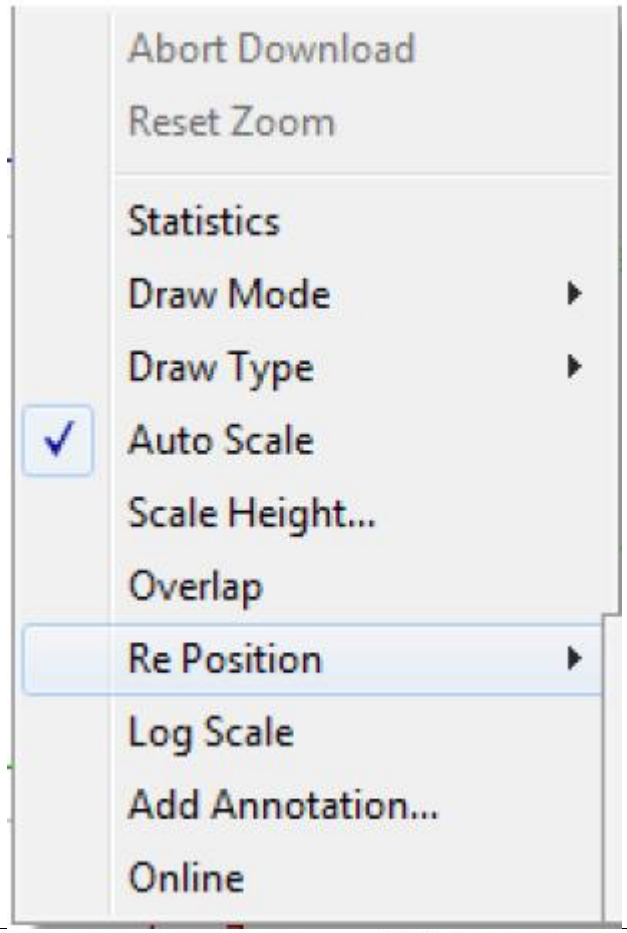
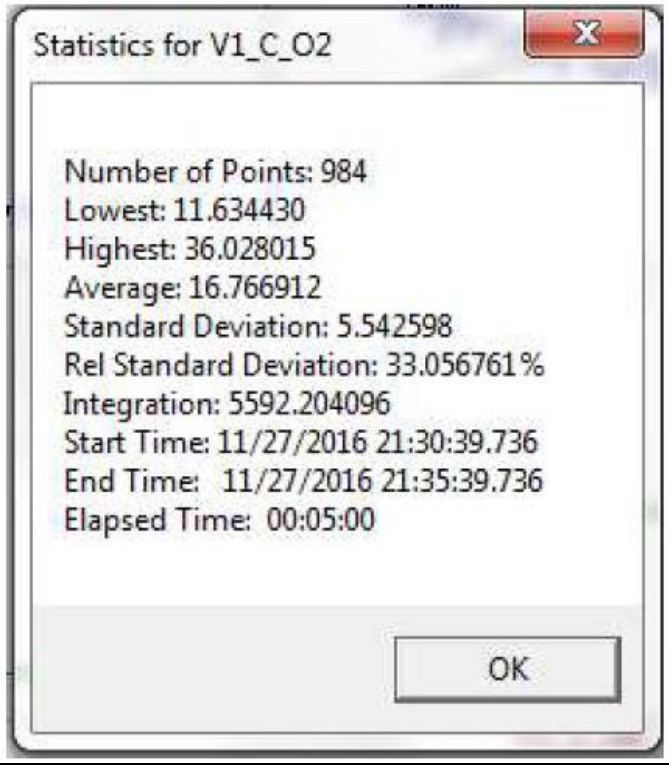
The user can alter the graphs even further through right-clicking on the desired graph and interacting with the generated window.	
The *Statistics* option allows the user to see statistical data relating to the selected graph.	

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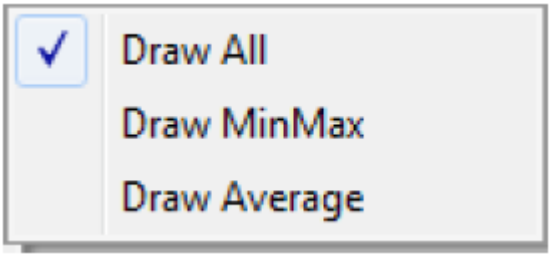
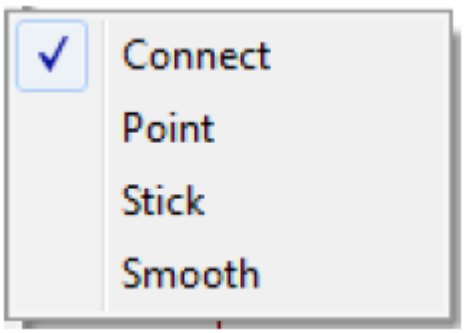
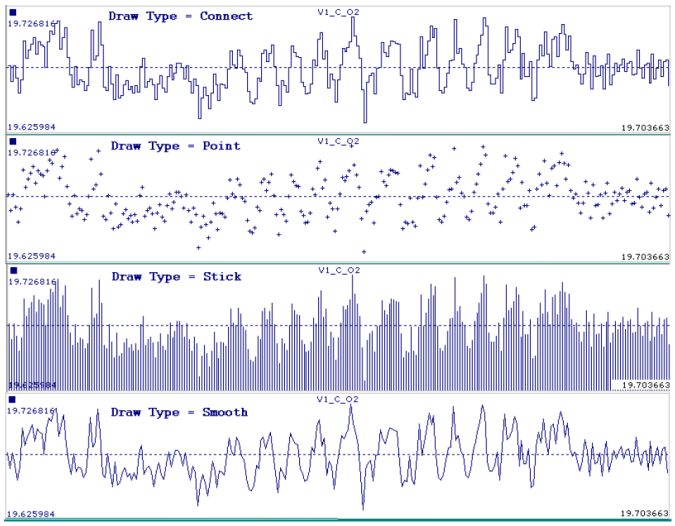
The *Draw Mode* allows the user to access a sub-set of additional options. The selections allow the user to determine how the software displays a se of data that contains more datapoints than there are pixels in the screen. The user's selection will not have a large effect on smaller data sets but changing the *Draw Mode* for larger data sets could help visualize and interpret the data.	
The *Draw Type* allows the user to specify how the data will be displayed in the windows. The user can select from four different draw types: • *Connect* gives the standard display that plots the points collected and connects them to create the peaks. • *Point* shows the individual data points as "+", without continuity between points. • *Stick* creates a bar graph with each point acquired being represented by its own line. • *Smooth* displays the data in a similar manor to the *Connect* type, however it combines the time and data components to allow the user to view a single line for a smoother display at higher magnifications.	 

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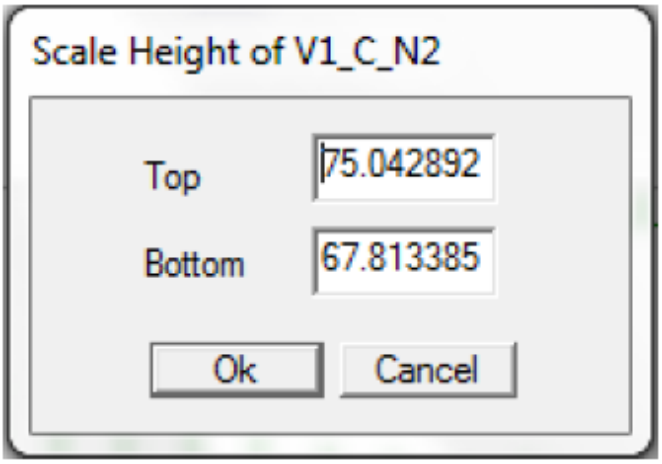
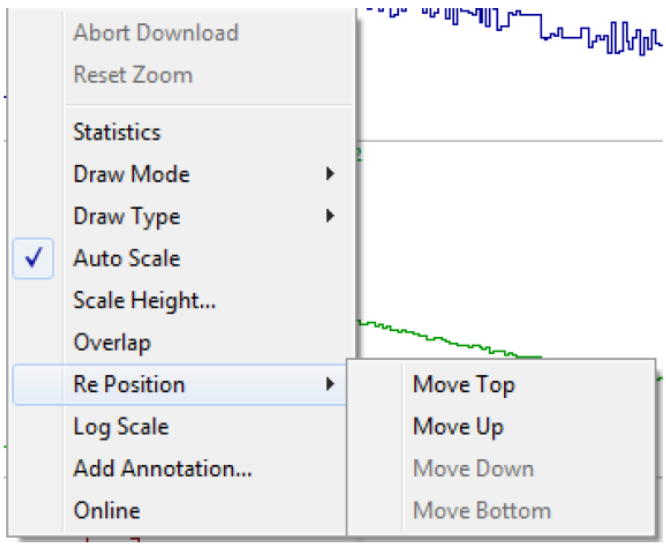
The user can use the *Auto Scale* and *Scale Height* selections from the right-click menu to alter the height of the display window. The *Auto Scale* selection allows the software to set the data window to display the most amount of data with the least amount of unused space. The *Scale Height* section allows the user to manually select the data window maxima. The selected values will not become active until the user clocks the *OK* button in the *Scale Height* window.	
The user can use the *Overlap* selection to command the software to display the data from the currently selected chart overlapped onto the graph above it. **Note:** If the user selects *Overlap* while selecting the top chart in the display, the software will overlap the top chart with the chart below it rather than attempt to overlap it with a nonexistent chart above it.	
The user can move where the charts are within the *Trend Charts* screen. If the user selects the *Re Position* option, they will be presented with four options. The user can move the charts up or down by one position with the *Move Up* and *Move Down* selections. The user can also command a chart to move to the top or bottom of the list by selecting the *Move Top* or *Move Bottom* option.	

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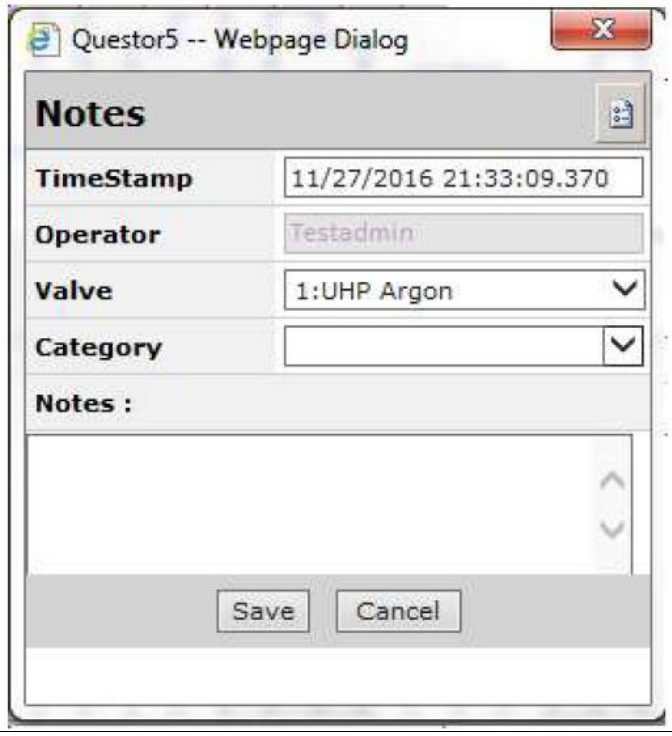
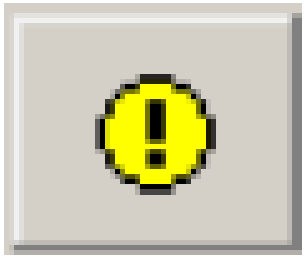
The user can select the *Log Scale* option for the data displayed as well. The software will set the chart maximum and minimum in much the same way as *Auto Scale*, but it will follow a logarithmic scale instead. This allows the user to view a dataset that has a large spread of values relative to each other in a more meaningful way.	
The user can add information to specific points in the chart that will be available when viewing any time range containing the annotated data point. The *Add Annotation* selection is the option that allows the user to add the additional specific information. The *Add Annotation* option allows the user to view the timestamp of the annotation. The user can also specify the valve of the gas being analyzed, specify a user defined category, and create notes for the annotation.	
The user has access to additional functions for the *Trend Chart* window of the *Results Tab.* The user has access to the standard functions of other tabs, but the *Results Tab* also allows the user to enable a view for any triggered alarms if any are specified in the running method. The user can activate the alarm view by selecting the yellow exclamation point button in the *Trend Chart* tool bar at the top of the window.	

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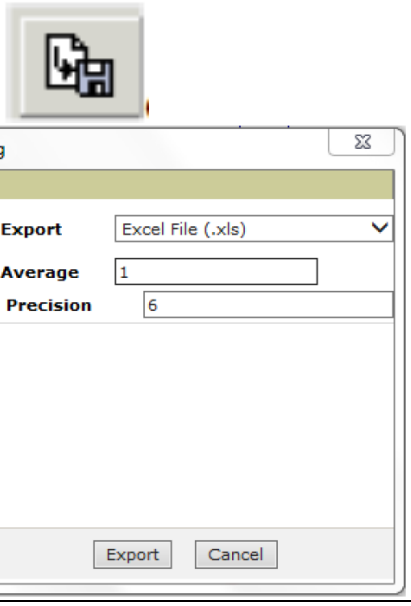
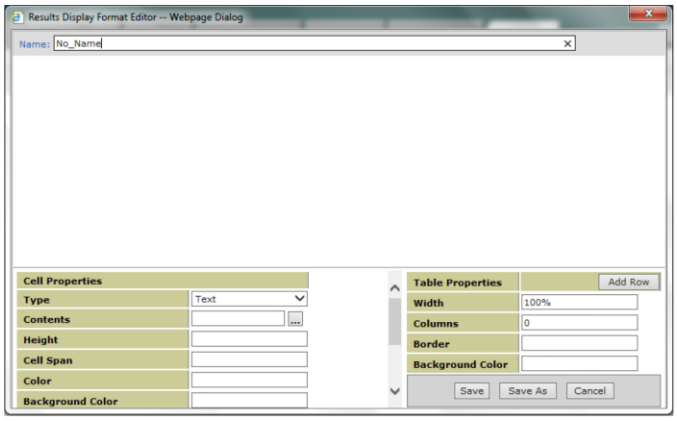
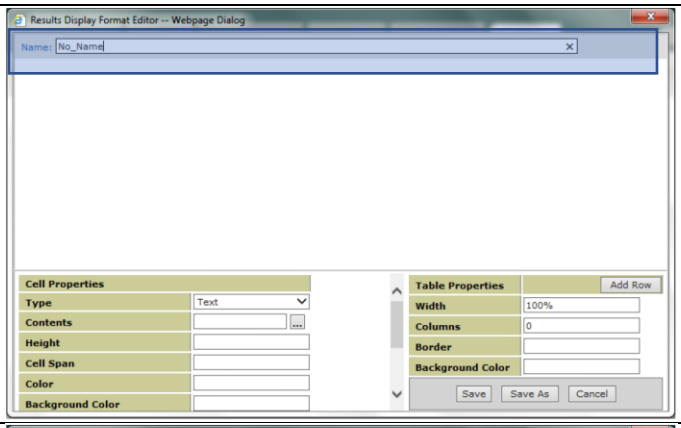
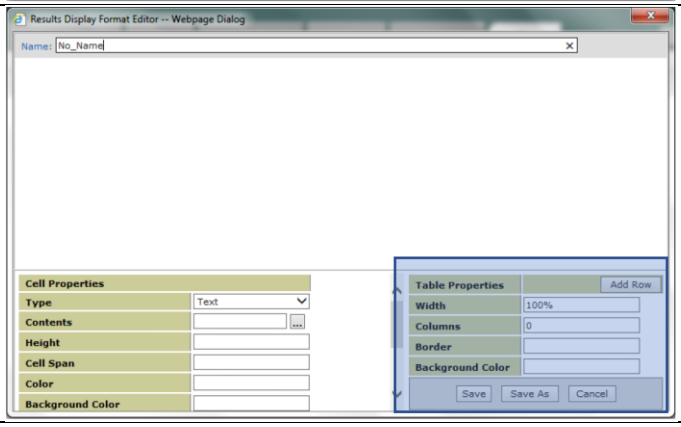
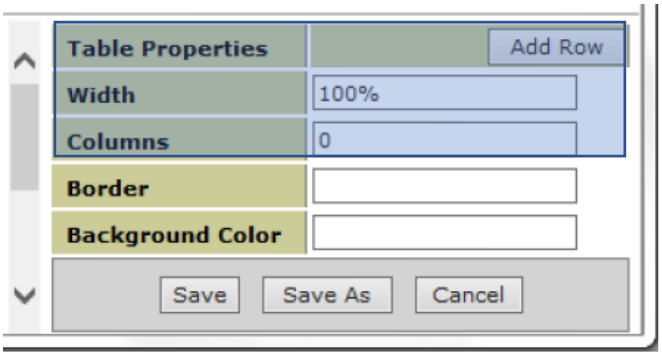
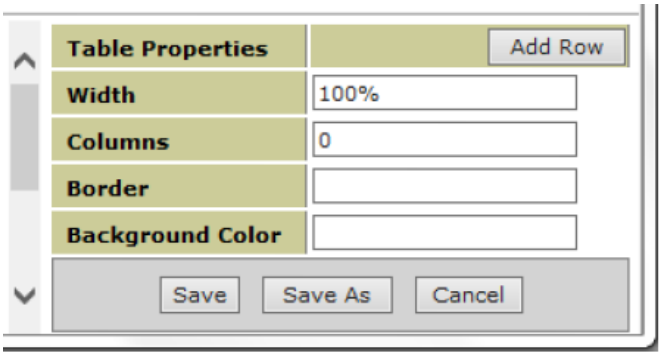
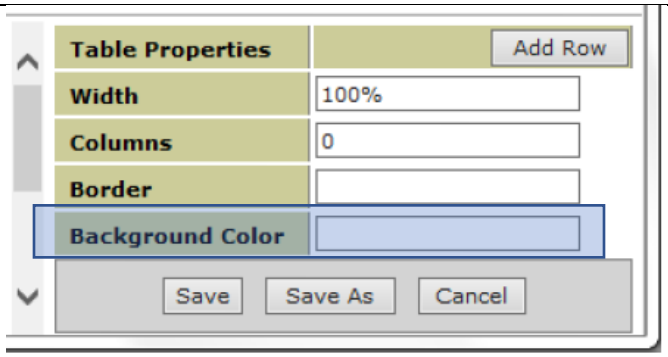
The user can view any triggered calibrations during data acquisition in a similar way to the alarms. The user can view the calibrations by selecting the yellow cross hair button in the tool bar.	
The user can export data from the *Trend Chart* window of the *Results Tab.* The user can export the data through the *Export Data* icon in the tool bar at the top of the screen. The user will be presented with multiple options for the data to export. The user can specify: • Which tags and related charts • File type to export into • The number of data points averaged together per exported data point • The quantity of numbers after the decimal point (precision.)	

8.1.1 Custom Tabular Display

The Custom Tabular Display *allows the user to format and customize the data display to allow for better analysis and visual interpretation.*

The user can customize the formats for the data displayed from *Analysis* or *Sequence* methods. The user can create or edit a custom format by clicking the *Tabular Display* text at the left edge of the *Results Tab.*	

The user can define many aspects of the data display through the *Results Display Format Editor* window created by the software. The user must first give the file a name. It is recommended the user create a name to indicate the purpose of the data display format.	
The *Results Display Format Editor* has a field for *Cell Properties* and *Table Properties.* The *Table Properties* allow the user to enact change on the entire table and the user should adjust these properties first.	
The *Table Properties* has multiple fields for the user to edit. The *Add Row* button allows the user to add a new row of cells to the display. The *Columns* field allows the user to specify the number of columns the software will divide the rows into. The *Width* field allows the user to specify the portion of the display area the custom format will use. The user can specify a quantity of pixels (units px) or a percentage of the screen (units %.)	

The user can specify the boarder properties as well with the *Boarder* field. The software has predefined style types to pick from. • *Dotted* will create a boarder with dotted lines. • *Dashed* will create a boarder with dashed lines. • *Solid* will creates a boarder with solid lines. • *Double* will create a boarder with double lines. • *Groove* will create a boarder that will look like a groove. • *Ridge* will create a boarder that will look like a ridge. • *Inset* will create a boarder with the line looking inset into the web page. • *Outset* will create a boarder with the line looking outset from the web page. The user must specify a quantity of pixels for the boarder to occupy, the style type, and a color. **Ex:** The user could specify a boarder that is 5 pixels wide, with a dashed style, and the color green. The use would populate the *Boarder* field with "5 dashed green" to create the desired boarder.	
The user can specify a color to occupy the background of the chart type. The colors can be instructed from the *Background Color* field and can be chosen from a list of colors and a list of modifiers. The user can find the list of colors and modifiers below: http://www.w3schools.com/html/html_colornames.asp http://www.oreilly.com/catalog/wdnut/excerpt/color_names.html	

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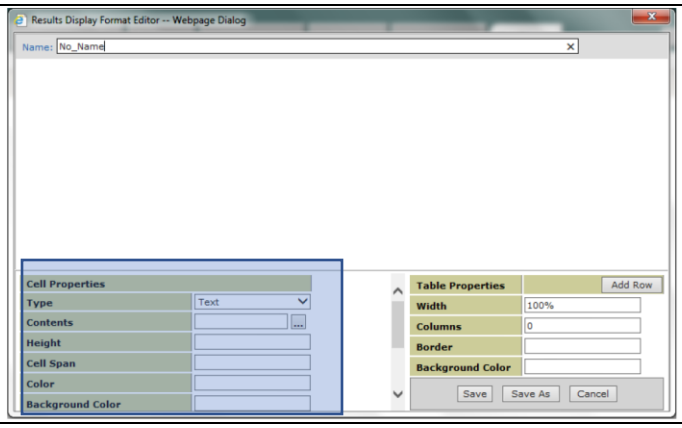
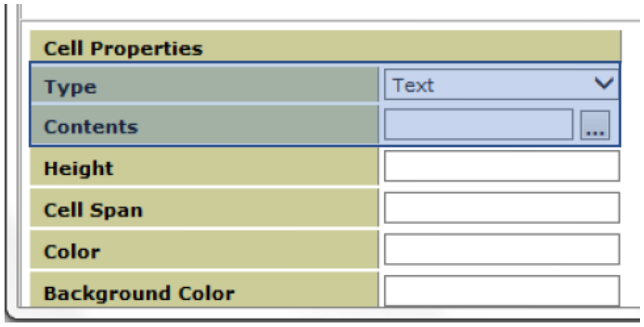
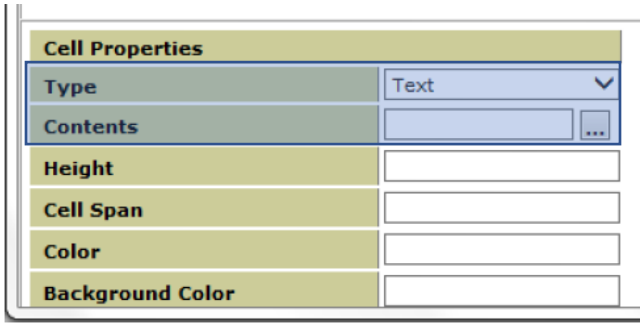
The user can specify properties to be used in specify cells through editing the *Cell Properties* section.	
The user can highlight a cell to select it and adjust its properties with the *Cell Properties* fields. The user must assign a cell type to each cell in the table from the *Type* field. The user can specify one of five options, *Text, Tag, Valve, Timestamp,* or *Status.*	
The cell type specified by the user will change what data that cell will display. If the user specifies the *Type* cell type the user must type text to be displayed in the cell in the *Contents* field. If the user specifies the *Tag* cell type the user must use the button next to the *Contents* field to specify a *Tag* type. The user must select from *Concentration, Intensity,* and *Derived Value* tags from the active method. If the user specifies the *Timestamp* or *Valve* options, the software will be instructed to populate the cells with the corresponding information. If the user specifies the *Status* option, the software will populate the cell with status information once the user enters the *Results* tab and specifies for a property or quality to be monitored.	

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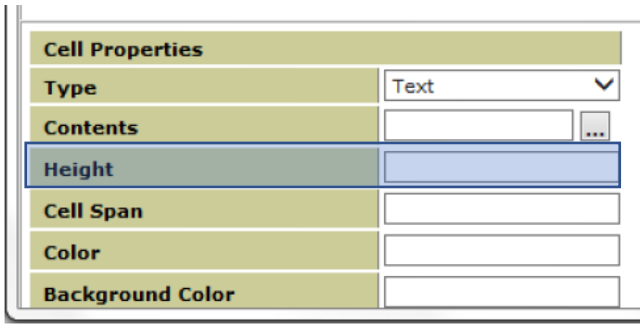
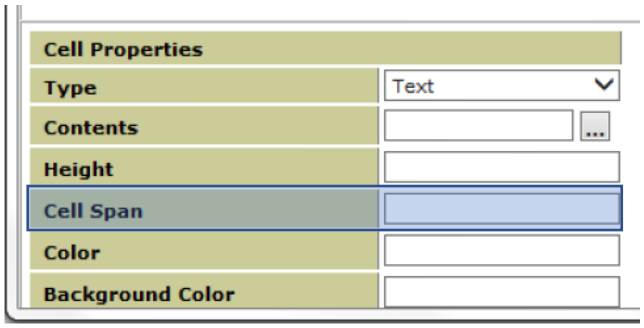
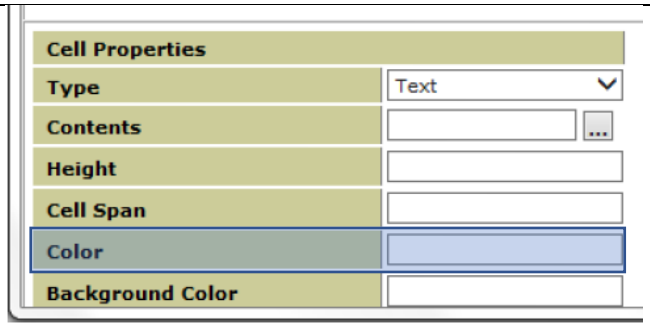
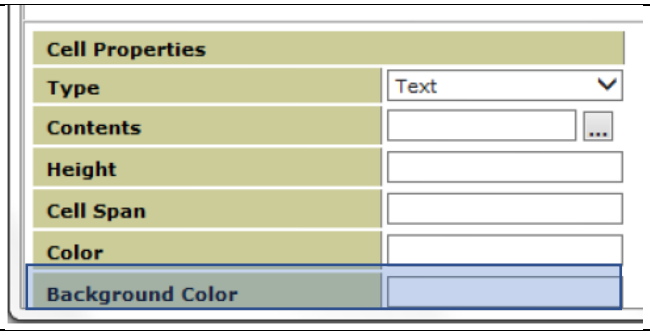
The *Height* field allows the user to specify the height of an entire row of cells in the table (in pixels.)	
The *Cell Span* field allows the user to define how many columns a select cell can span, up to the total number of columns specified under *Table Properties.*	
The *Color* field allows the user to specify the color of the contents of the cell, not the background color. The cell color options are the same as the color options found for the *Table Properties* selections.	
The *Background Color* field has the same functions for *Cell Properties* as *Table Properties.*	
The *Boarder* option allows the user to specify the boarder field with the same properties as those found in the *Table Properties* section.	

The *Alignment* option allows the user to select how the data will be displayed within the cell, from Left, Right, or Centered settings.	
The *Precision* field allows the user to specify how many digits will be displayed after the decimal point.	

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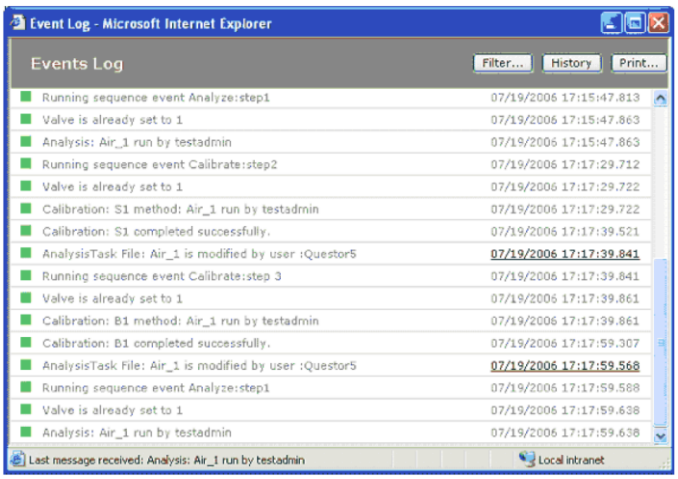
9.0 The Event Log

The Events Log *allows the user to view a window that records the last thirty events recorded by the system, as well as the ability to view more/older events recorded by the system.*

The *Event Log* is accessible from every screen from the button in the top right of the web paged labeled *Event Log.*	
The user can view the level of the event through the color of the square to the left of the entry. The user can hover the mouse cursor over the event color square to reveal a text description of the event level. The types of events are *Information, Warning*, and *Fatal.* • *Information* events are color tagged with green and are events indicate changes in instrument status as well as other general events. • *Warning* events are color tagged with yellow and are triggered by things that could interrupt the instrument function but do not immediately damage the instrument, but action should be taken. • *Fatal* events are color tagged with red and are events that will prevent the instrument from functioning properly and must be delt with as soon as possible.	

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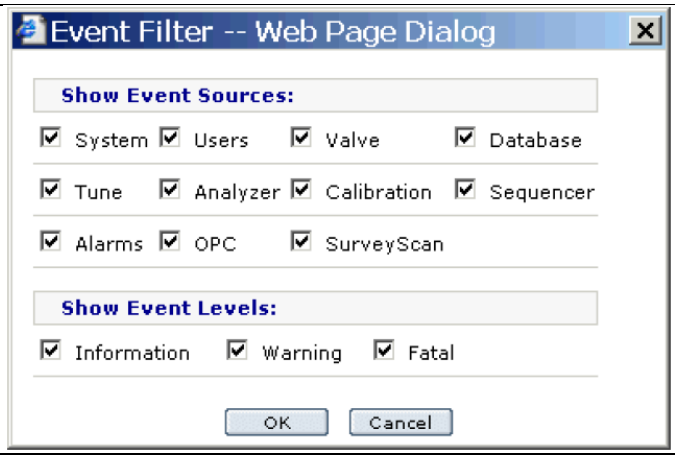
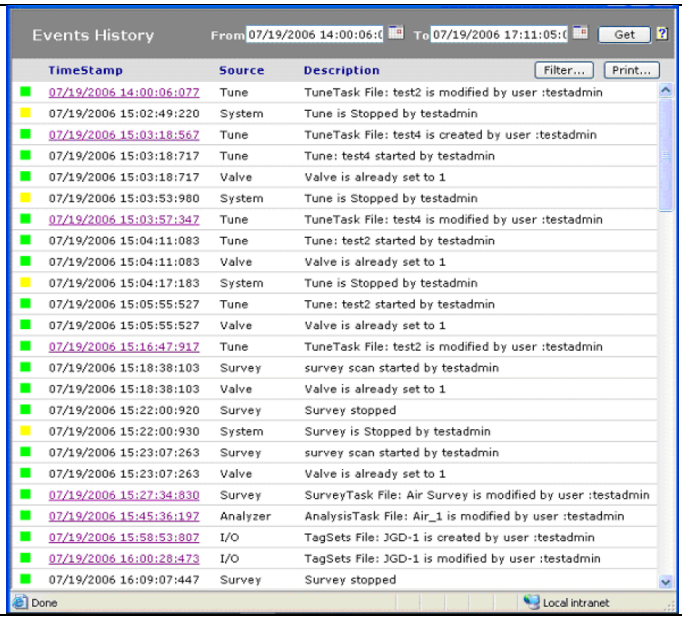
9.1 Event Log Filter

The Event Log Filter *allows the user to filter the event types being viewed in the* Event Log *window.*

The user can filter the events viewed in the *Event Log* window by clicking the *Filter…* button. The user can specify the source of the events, the level, or a combination of both. The user can specify the desired options through checking the box next to the desired types, with the default showing all available options.	

9.2 Event History

The Event History *allows the user to select and view events based on the time and date of the desired events. The user can view events from the last time the software database was backed up, through to the present.*

The user can access the *Event History* by clicking the *History* button at the top of the *Event Viewer.* The software will create a window where the user can define a date and time range to view desired events, as well as filtering the events with the *Filter…* button at the top of the screen. The *Filter…*button works in the same way as described in the previous section. The user will also be able to see the level of the events, their source, and a description of the event.	
The user must click the *Get* button after defining the date and time range of the desired events (time fields are the same here as previous sections.)	