



MASsoft

Reference Manual

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Certificate 6738

This manual aims to provide a comprehensive reference to the MASsoft application.

Information in this manual is presented as a series of topics arranged in alphabetical order.

This manual serves a source document for on-screen help and as such the format differs from other Hiden manuals. The intention is for the user to refer to this manual for specific information rather than to read it from cover to cover.

Hiden Analytical Limited try to ensure the information presented in this manual is comprehensive, relevant and accurate. If the reader thinks there is a mistake, requires some clarification or needs further information please do not hesitate to contact us, we are always happy to provide assistance.

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3D Graphical view

A 3D Graphical View can be created from a Bar or Profile Scan, which has historical data (more than 1 cycle) or has multi-variant inputs.

Alternatively a 3D Graphical View can be created from a MID scan if it has at least 2 has multi-variant inputs.



Selecting the **3D Graphical View** option from the **Views** menu or clicking on the button creates the view.

The convention used for the 3D view is that the X and Z axes lie in the 2D plane, and the Y axis is the vertical axis.

The plot can be rotated and its angle of view adjusted by using either the scroll bars or by left-clicking and dragging with the left-mouse button down.

The Y axis is plotted on Linear scale. There is no option to plot on a log scale on a 3D plot

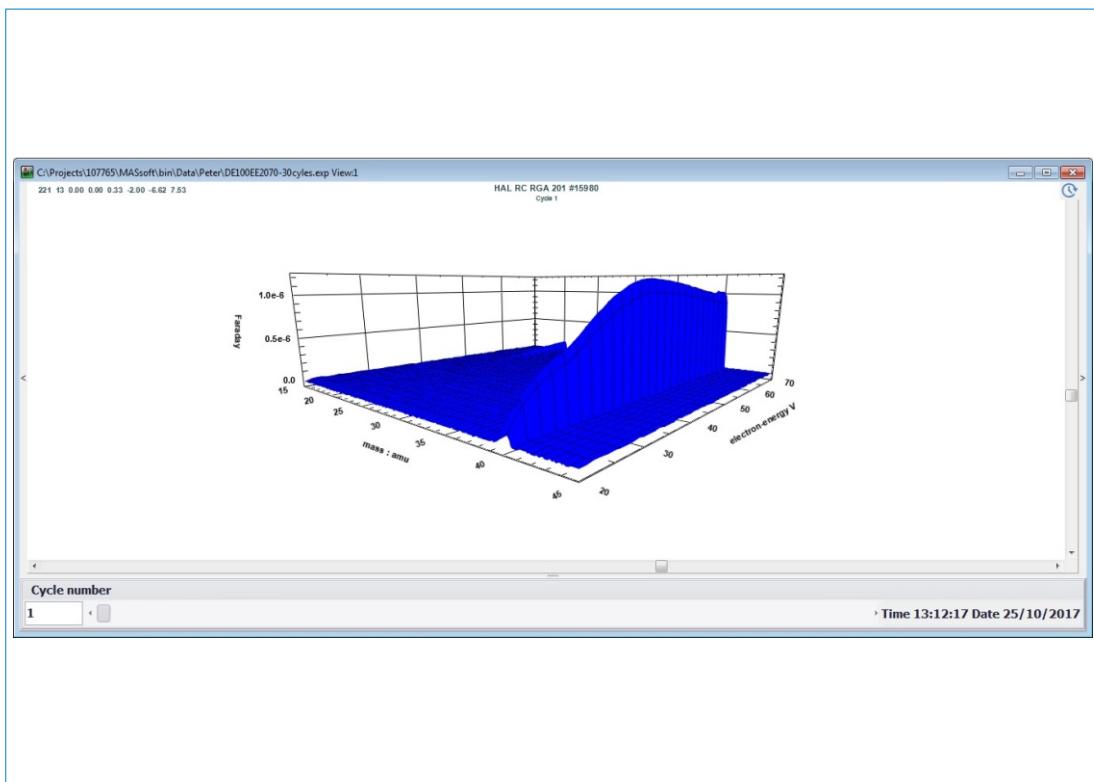
The 3D Graphical View can be viewed while collecting data, in which case the plot is updated at the end of every scan. Alternatively it can be used to display historical data.

3D Graphical Profile View

If a Bar or Profile Scan has more than 1 cycle of data (historical data) then a 3D view is possible. For such a 3D view the X axis will display the variable which is being scanned, which is typically mass. The Z axis displays the number of cycles and the Y axis the reading from the input device, for example Faraday.

By default, the 3D plot does not display every cycle if there are more than 20 cycles of data. In this case the total number of cycles is divided by approximately 10 to determine the interval at which cycles of data are displayed. If every cycle of data was plotted it would be extremely slow to display.

If a Bar or Profile Scan has at least one multi-variant input, then the Z axis will default to display the first multi-variant value over the range of values for which the data has been collected. An example is given below for a system containing Argon which has been scanned across mass range 15 to 45. The multi-variant input is electron energy which has been increased from 20 to 70 in increments of 1.

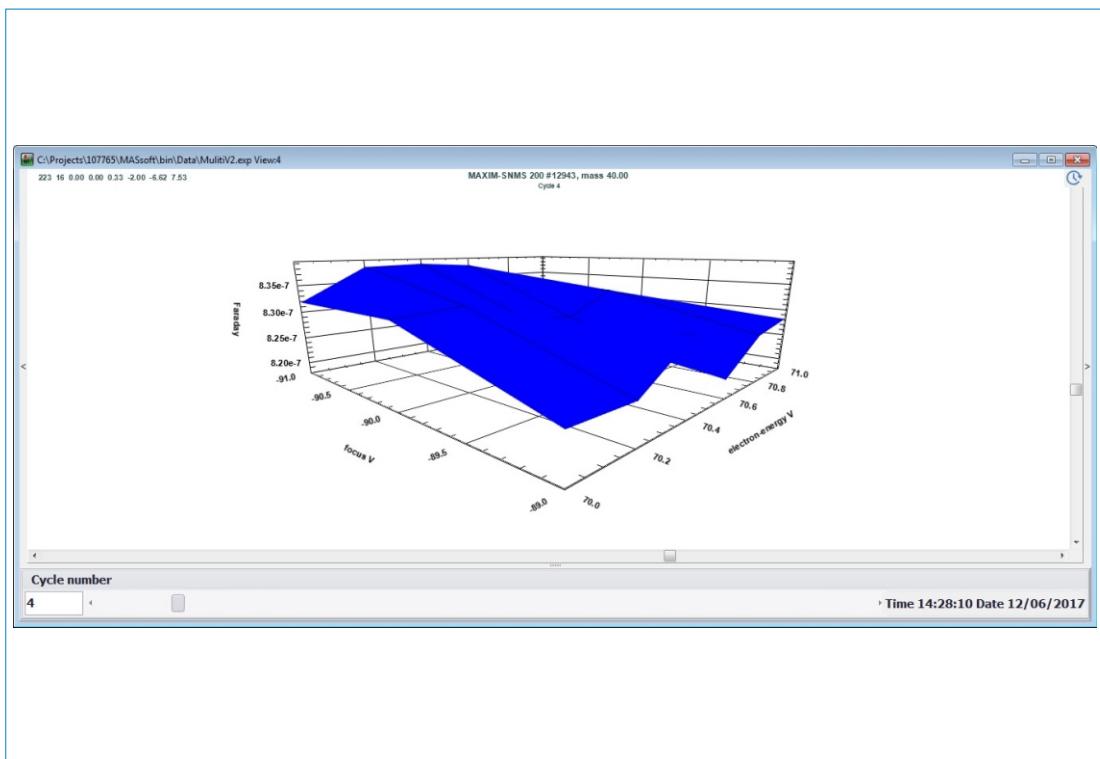


3D Graphical MID View

At least 2 multi-variant inputs must exist in order to create a **3D Graphical MID View**. For such a 3D view the X and Z axes display the multi-variant values, and the Y axis displays the reading from the input device at the given MID scan value. This creates a 3D surface at the MID value, where the input value will change depending on the values of the multi-variant inputs.

Note that unlike the 2D Graphical Trend View and Tabular View only one MID value can be displayed on a single plot, as only one surface can be displayed at a time. Different 3D plots are required to display data at different MID values.

An example is shown below.



Plot Mode and Sliders

Mode is a sub menu of the **3D Graphical Views** menu containing the **Historical** and **Update every cycle / iteration** options. These options determine whether the 3D plot is updated while scanning or whether historical data is displayed.

The mode can also be changed using the icon in the top right hand corner of the 3D Graphical View.



Switches to **Historical**



Switches to **Update every cycle / iteration**

Historical (Sliders)

When displaying in **Historical** mode the sliders are displayed.

For multi-variant values (including Cycles) which are not displayed on the plot, a scroll bar is added below the 3D plot. These sliders allow the multi-variant values which are not displayed on the plot (including Cycles) to be changed. Moving these sliders backwards and forwards will update the display of data. Alternatively, a specific cycle number can be typed in the text box. These sliders operate like those when historical data is viewed in 2D profile

plots. The Cycles slider bar also displays the time and date for the currently selected cycle number.

If the **Historical** mode is viewed while scanning the plot will not be updated. The plot will display the 3D plot at the given slider positions and determined by the plot axes. The data displayed will be that which was available at the point the plot was created, or at the point the plot was switched from update to historical mode.

Update every cycle / iteration

When displaying in **Update every cycle / iteration** mode, no sliders are displayed. The 3D plot data displayed will be for the currently selected axes. The data displayed in the plot will update each time a newcycle or iteration of scan data is obtained. The option will be labelled either **Update every cycle** or **Update every iteration**.

How data is updated depends on what kind of 3D plot is displayed.

If displaying a 3D plot where cycles is displayed on one of the axes, the plot will automatically adjust the interval between cycles to display a maximum of 10 historical cycles of the data on the plot. Data displayed across the whole plot may be updated when a new iteration of data is added to the plot. The update menu option will be given as **Update every cycle**.

When displaying a plot with axes which are multi-variants, the size of the surface grid plot is already known. Values of 0 are displayed where data has yet to be added to the plot. When a new iteration is added, the 3D plot will be update with a new row of data on the surface. The 3D surface will build up until complete, then when a new cycle of data occurs the plot will clear and the surface will once again be constructed line by line as new data is added. The update menu option will be given as **Update every iteration**.

When displaying a scan with multiple multi-variants, the surface is updated as the values of hidden multi-variants (which are not displayed on the plot axes) change. The update menu option will be given as **Update every iteration**.

When displaying a 3D plot of a MID Surface, the size of the surface grid plot is already known. In this case the 3D plot is only updated when all data points for the new surface have been collected.

See also:

[3D Graphical View](#)

[3D Graphical view menu](#)

[Views menu](#)

[Scan Tree](#)

3D Graphical view menu options

When a **3D Graphical View** is created or while it is the active window, the **Views** menu options change to include these options.

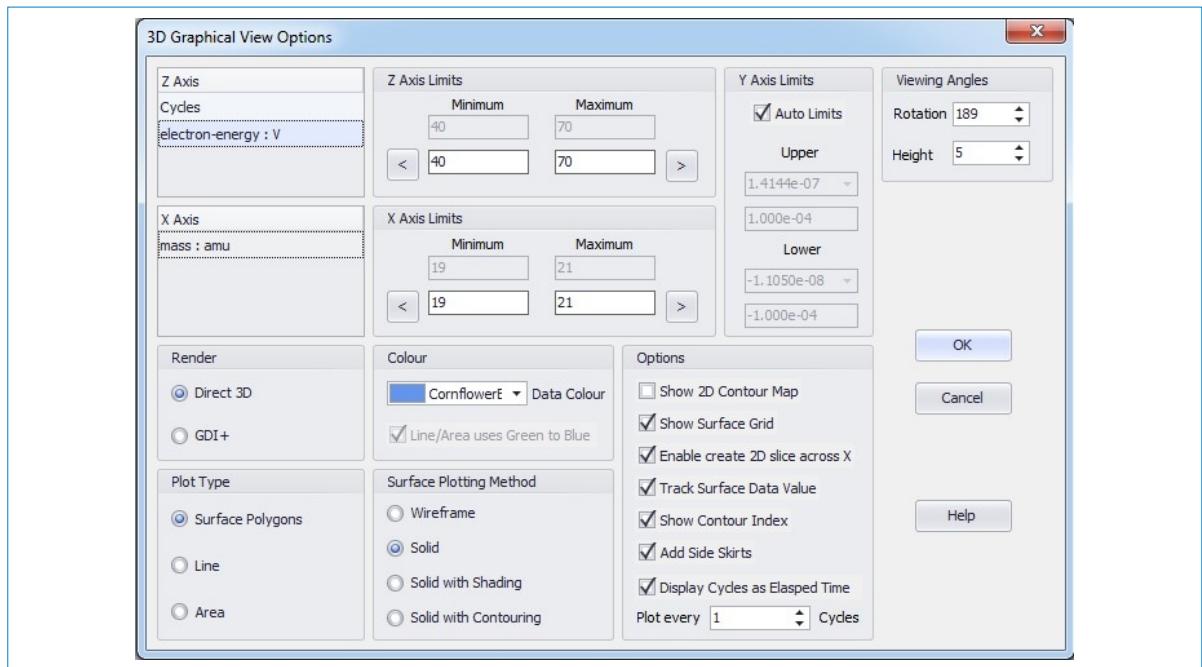
Title	Opens a dialog to edit the title in the 3D view. By default, the view's title is the name of the currently connected mass spectrometer. The title is shown immediately below the view's title bar.
3D Display As	Offers four options for quick selection of default configurations for displaying the 3D plot as a Surface , Contour , Area and Lines display types.
Mode	The Historical and Update every iteration options determine whether the 3D plot is updated while scanning or whether historical data is displayed.
3D Graph Options...	Displays the 3D Graphical View Options dialog to control what is plotted on each axis, the plot ranges and how the 3D surface is displayed.
Create a 2D plot along data line	This option is only available when a data line across a surface has been set (available for Direct 3D only) and when in Historical mode . It is used to create a 2D plot of a data slice through the 3D plot data. A new 2D Graphical View profile plot will be created, with sliders set to the values to match the selected line of data in the 3D plot.
Copy	This option only appears on the right-click popup menu. It copies the 3D plot as a graphic image.

See also:

[3D Graphical View](#)

3D Graphical View Options

By default a 3D plot will be displayed as a solid surface. This together with what variables are plotted on the axes can be changed using the **3D Plot Options...** on the **Views** menu. The option can also be obtained by right-clicking on the plot to display a popup menu.



Z Axis

The Z Axis box lists the multi-variant variables which can be viewed on the Z-axis. The selected variable is highlighted. Choosing a new Z axis variable updates the **Z Axis Limits** to the minimum and maximum values of the chosen variable.

For a 3D view of a bar or profile Scan, this including Cycles as well as any multi-variant input variables.

For a 3D view of a MID scan then this lists all the multi-variant input variables.

Z Axis Limits

The Z axis limits can be adjusted to any values within their possible range. The Z axis of the plot will be updated to display the given range.

Clicking the < or > restore values to their minimum and maximum values.

X-Axis

For 3D views of bar or profile Scans the X axis always displays the scanned variable. The **X Axis Limits** default to display the start (minimum) and stop (maximum) values of the scan.

For a 3D view of a MID scan then this lists the same multi-variant input variables as displayed in the **Z Axis** box. The same variable cannot be displayed on the X and Z axis.

X Axis Limits	The X axis limits can be adjusted to any values within their possible range. The X axis of the plot will be updated to display the given range. Clicking the < or > restore values to their minimum and maximum values.
Y Axis Limits	If the Auto Limits check box option is checked on then the Y limits are automatically determined from the data values displayed on the plot. This means that the y axis always spans the full range of the Y data within the X and Z axes ranges. If the Auto Limits option is not enabled, then manual Upper and Lower limits are used. These values can be changed using the pull down choices or entering values into the text fields. When these limits cut though the surface Y values then the data which is above or below the limits is displayed plateaued at the limits.
Render	The plot can be rendered with either Direct 3D or GDI+ . The use of Direct 3D allows for features not available for GDI+ , however the rendering may be slower if your PC has not got a dedicated graphic card. When using the Direct 3D render the middle mouse scrolling button can be used to zoom in and out of the plot.
Plot Type	Plot type options are listed below.
Surface Polygons	The data is displayed as a solid surface of polygons. How the polygons are coloured and shaded is determined by the Surface Plotting Method .
Line	Lines of data are displayed across the X axis, at each Z axis value. If the Line / Area uses Blue to Green option is checked on then the lines are shaded from green to blue.
Area	A series of area plots of data are displayed across the X axis, at each Z axis value. If the Line / Area uses Blue to Green option is checked on then the areas are translucently shaded from green to blue.
Surface Plotting Method	The Surface Plotting Method only affects the display when the Surface Polygons plot type is selected. The options are
Wireframe	The polygons are drawn in wire frame, which can be seen through.
Solid	The polygons are drawn in solid colour. The colour is determined by preferences.
Solid with Shading	The polygons are 3D shaded.

Solid with Contouring

The polygons are drawn in a colour determined by the height of the polygon on the Y axis from the lowest value (blue) to highest value (red).

Options

Data Colour

This controls the colour preference for the 3D Surface / Data. The preference can also be set in the Views tab of the Preferences. This colour will be used to display the surface or data lines if other options such as contouring are not used.

Line / Area uses Blue to Green

If this is checked on then when displaying 3D plot as a series of Lines or Areas, then green to blue colour graduation is used. Otherwise the 3D Surface / Data colour is used for Line and Area plots.

Show 2D Contour Map

If displaying **Surface Polygons** then a 2D contour map (contours are projected onto the 2D surface below the data surface) can be displayed by enabling this option.

Show Surface Grid

Applies a grid to the **Surface Polygons**

Enable create 2d slice across X

This is only available for **Direct3D**. When clicking on the 3D plot surface, a red line with a transparent area under it is displayed along the line of X values of data at the closest Z point clicked on the plot. Typically this is along the mass in a conventional scan.

The **Create a 2D plot along data line** option of the menu produces a new **2D Graphical View** profile along the highlighted data line.

Track Surface Data Value

This is only available for **Direct3D**. When enabled, the interpolated value of the 3D surface coordinates (X, Z) and data values (Y) at the surface point under the currently mouse cursor is displayed in a grey box. Moving the mouse over the surface will update the values of the data surface at the point the mouse pointer is located.

Show Contour Index

When checked on, if the **Surface Polygons** plot is displayed as **Solid with Contouring** then an index of the contour colours and their associated value is displayed to the right.

Add Side Skirts

When plotting with the **Surface Plotting Method**, this option determines if the skirts are added to the plot edges. The side skirts add polygons around the edge of the plot from the data minimum to the data value of each edge point.

Display Cycles as Elapsed Time	When this is checked on, if Cycles are being displayed on the Z Axis, then the cycle is displayed by its elapsed time on the plot Z-axis, rather than cycle number.
Plot every N Cycles.	This manually controls the interval between cycles displayed on the plot. By default the total number of cycles is divided by 10 rounded up, which determines the interval between displayed cycles. If there are a large number of cycles you should not choose to reduce the interval at which cycles of data are displayed because there would be a large amount of data which would be extremely slow to display.
Viewing Angles	The Rotation and Height angles can be specified. The 3D view will orient to the entered values allowing the user to set a consistent known point of reference for plot orientation, allowing for easier comparison of plots.

See also:

[3D Graphical View](#)

[3D Graphical view menu](#)

Accessing the web interface

Some models of Interface Unit also provide a web-based user interface. This allows the configuration of certain the aspects of Interface Unit to be changed, for example communication settings, auxiliary inputs and firmware. This user interface can be accessed using a web browser.

To access the Web Interface:

1. Open a web browser
2. In the address bar type
`http://HIDEN-WR<works-ref>`

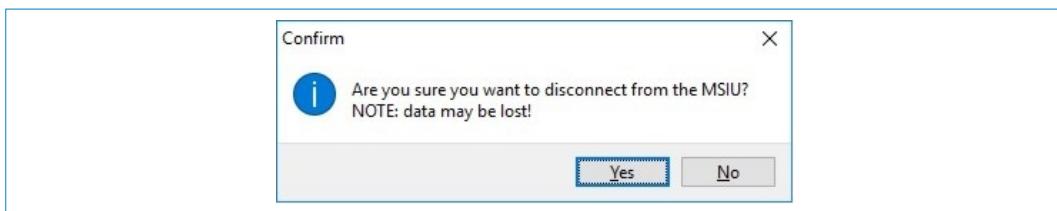
Where <works-ref> is the Works Reference Number of the Instrument
 Eg. for Work Reference 12345, type
`http://HIDEN-WR12345`
3. Press Enter and if supported, the Web Interface login page will be displayed

If the Interface Unit does not support the Web Interface then communication settings and auxiliary inputs must be configured using MASsoft while the Firmware Upgrade utility must be used for firmware changes.

Acquisition menu

Items on the Acquisition menu are described below.

Setup	Prepares the current instrument for data acquisition by downloading the data from its scan tree window. It does not start the data acquisition. This command is grayed out if the current instrument is unavailable.
Shutdown	Stops any data acquisition on the current instrument and loads the shutdown settings into the instrument. This command is grayed out if the current instrument is unavailable.
Activate	Puts the instrument into a powered-up ('ready') state using the device values from the file settings. This command is grayed out if the current mass spectrometer is unavailable.
Start	Starts data acquisition. This command is grayed out if the current mass spectrometer is unavailable.
Stop	Stops data acquisition at the end of the current cycle. This command is grayed out if the current instrument is unavailable or if not scanning.
Abort	Stops data acquisition as quickly as possible. This command is grayed out if the current instrument is unavailable or if not scanning.
Disconnect	The Acquisition, Disconnect command is used to run the control unit in a stand-alone monitor mode; MASsoft stops retrieving data from the control unit and storing it to disk. The control unit continues to acquire data, store it internally and compare it with trip limits. The appropriate mass spectrometer control window must be selected before selecting the command. The warning message shown in the figure below appears when the Acquisition, Disconnect command is selected.



The filaments and Secondary Electron Multiplier (SEM) detector may be left switched on after MASsoft has been disconnected.

The control unit can store approximately 9626 MID channels or 760 BAR cycles of 1 to 100 amu. If the buffer becomes full, acquisition will not stop and data may be lost.

The **Instrument, Connect State, Connected** command must be used for MASsoft to regain control of the mass spectrometer and recover data automatically.

Event sequences may be set up to suspend monitoring (rather than aborting monitoring) by external or over pressure trips. Event sequences may also be used to restart monitoring after a power failure; contact Hiden Analytical Limited for further information.

Reconnect

The **Acquisition, Reconnect** command is used to regain control of the control unit after it has been disconnected using the **Acquisition, Disconnect** command.

The appropriate mass spectrometer control window must be selected before selecting the **Acquisition, Reconnect** command.

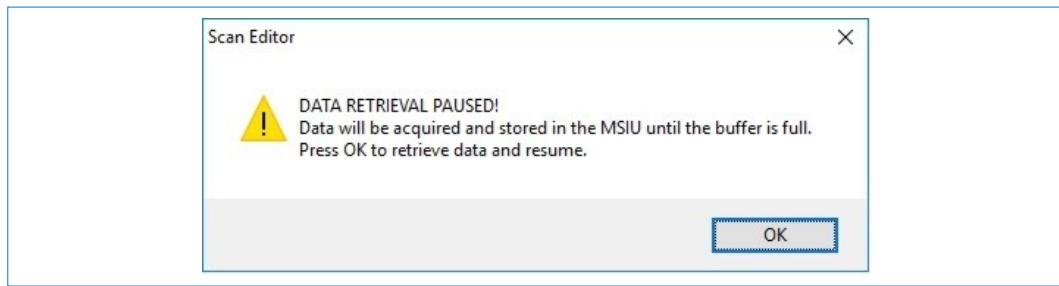
Data stored in the control unit is retrieved, but data may be lost, depending on the data acquisition rate and how long the control unit was disconnected. Because MASsoft can take quite a long time to catch up with the control unit, the scan can be aborted, and retrieval stopped, by using the **Abort** button (red), **Stop** button (amber), stops acquisition but retrieves all the stored data. Any event sequences started prior to disconnection are stopped on stopping or aborting the scan.

Stop Data Retrieval

The **Acquisition, Stop Data Retrieval** command stops MASsoft retrieving data from the control unit to the PC when scanning, thus speeding up data acquisition.

The appropriate mass spectrometer control window must be selected before selecting the **Acquisition, Stop Data Retrieval** command.

The **Scan Editor** data retrieval paused message box will appear when the scan is started.



Data will only be retrieved to the PC when the **OK** button is clicked. This option can also be accessed via the **Edit Start Options** dialog box.

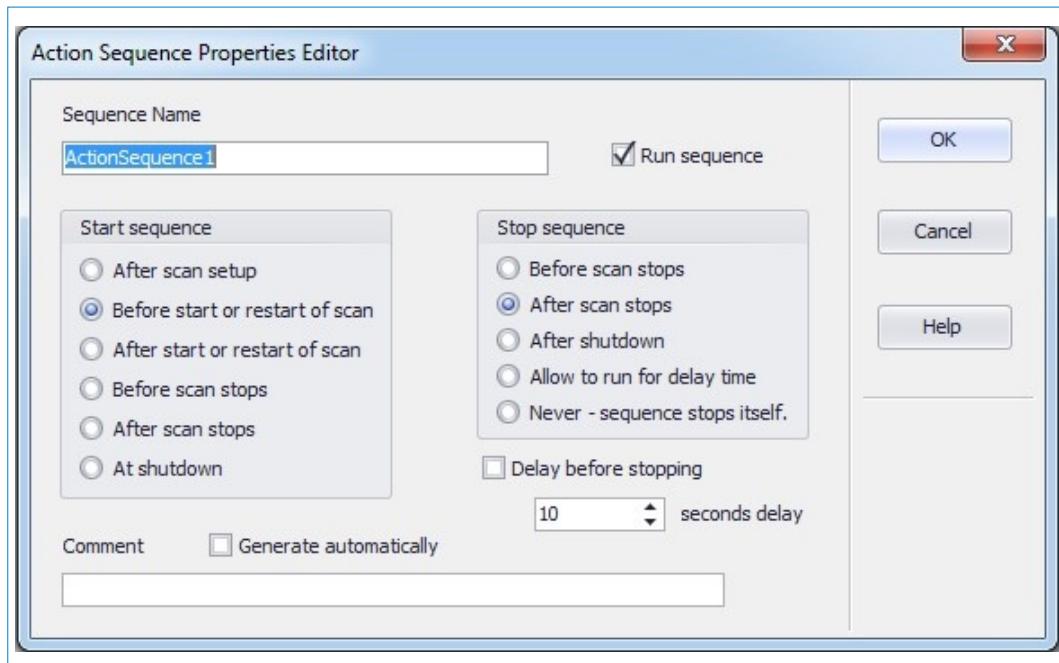
Data acquisition is stopped if the control unit data buffers become full.

Action Sequence Editor

The action sequence marker  identifies the start of an action sequence. If any actions are programmed in this sequence, they appear directly underneath the marker.

Several sequences may be programmed as required. Action sequences can contain functions in any order. Functions are executed in order from top to bottom unless a branch is taken.

The **Action Sequence Editor** is displayed when editing the action sequence marker by using double-click on action sequence marking the beginning of an action sequence.



Fields in the **Action Sequence Editor** are:

Sequence Name	The marker name can be typed in this text box.
Run sequence	If this option is checked, the trip list starts at the same time as data acquisition. If this option is not checked, the sequence does not start unless run by another trip or event.
Start sequence	Specifies the point at which to run the event sequence.
Options	
After scan setup	The sequence is started as soon as the scan and Action Sequence have been downloaded to the IU. If Automatic scan restart is enabled the sequence is only started before the first run starts. If the stop option is Allow to run for delay time then the sequence will run until completion or until the delay time expires, whichever is sooner, before the scan starts.
Before start or restart of scan	The sequence is started immediately before data acquisition starts on every run. If the stop option is Allow to run for delay time then the sequence will run until completion or until the delay time expires, whichever is sooner, before the scan starts.

After start or restart of scan	The sequence is started immediately after data acquisition starts on every run. If the stop option Allow to run for delay time then the sequence will run until completion or until the delay time expires, whichever is sooner, before MASsoft starts to display data; to avoid the instrument's data buffer becoming full the delay time should be kept short.
Before scan stops	The sequence is run before stopping the scan. If the stop option is Allow to run for delay time then the sequence will run until completion or until the delay time expires, whichever is sooner, before MASsoft stops the scan. During this time data is not displayed; to avoid the instrument's data buffer becoming full the delay time should be kept short.
After scan stops	The sequence is run after the scan has stopped, but before switching to shutdown. This option should be used to write a sequence to return IO devices to a known state at the end of a run. If the stop option is Allow to run for delay time then the sequence will run until completion or until the delay time expires, whichever is sooner, before proceeding.
At shutdown	The sequence runs when the mode changes to Shutdown. Note if the file is closed before switching to shutdown then the sequence will not be run. If the stop option is Allow to run for delay time then the sequence will run until completion or until the delay time expires, whichever is sooner, before proceeding.
Stop sequence	Specifies when to stop the sequence
Options	

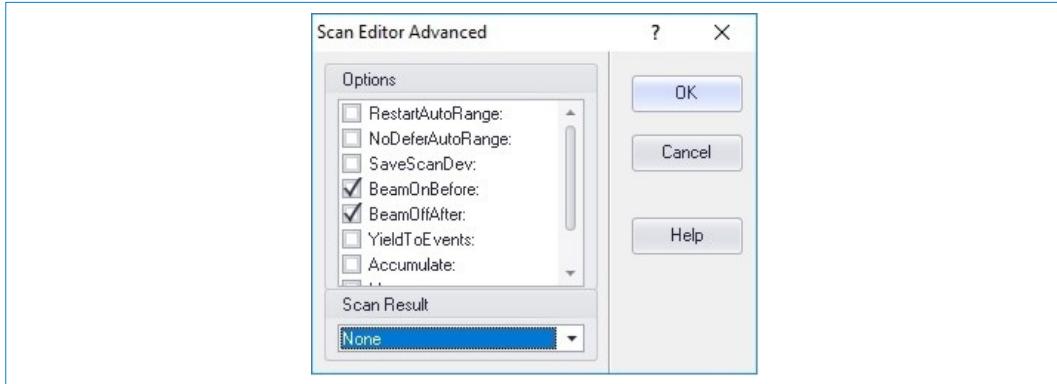
Before scan stops	The sequence is stopped before stopping the scan. If the Delay before stopping check box is selected MASsoft will wait until the sequence self-terminates or until the delay time expires, whichever is sooner, before MASsoft stops the sequence. During this time data is not displayed; to avoid the instrument's data buffer becoming full the delay time should be kept short.
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After scan stops	The sequence is stopped after stopping the scan but before switching to Shutdown. If the Delay before stopping check box is selected MASsoft will wait until the sequence self-terminates or until the delay time expires, whichever is sooner, before MASsoft stops the sequence.
After shutdown	The sequence is stopped after switching to Shutdown. If the Delay before stopping check box is selected MASsoft will wait until the sequence self-terminates or until the delay time expires, whichever is sooner, before MASsoft stops the sequence.
Allow to run for delay time	<p>When MASsoft starts the sequence it performs the following actions:</p> <p>Start sequence – delay – Stop sequence</p> <p>The delay should be long enough to allow the sequence to complete. If the sequence completes before the delay expires the delay is terminated and the Stop sequence action is omitted.</p> <p>If two sequences with this option have the same Start sequence option then one will run to completion before the other starts, but the order in which they run can not be relied on.</p> <p>The delay time is always used with this option even if Delay before stopping is not selected.</p>
Never – sequence stops itself	MASsoft does not stop the sequence, it must self terminate (end on an End marker). If sequences are left running various errors may be encountered such as:
	<ul style="list-style-type: none"> No free task. Illegal trip type. Programme stopped. Device in use Scan not initialized
Delay before stopping	Allows time for an event sequence to run to completion before trying to stop it. The delay time can be specified. If the sequence does not stop within the delay time then MASsoft will send the command to force it to stop. The delay time starts at point specified by the chosen Stop sequence option.
Comment	<p>The comment associated with the Action Sequence.</p> <p>If Generate automatically is selected, the comment is generated by the selections made within the dialog.</p>

See also:

[Automation page](#)

Advanced scan options



The Advanced scan options are set in the Scan Editor Advanced dialog opened by clicking the **Advanced** button in any of the Scan Editor dialogs.

The Advanced scan options allow control of the way scans interact with the system; it may also be used to perform mass alignment and automatic tuning when the automatic options are not sufficiently flexible.

Click on the item in the **Options** frame to selected it. A check mark is shown in the item's check box when it is selected. To deselect an item click it's check box. More than one option can be selected at a time.

Only one function can be selected at a time in the **Scan Result** frame. A function can be deselected by selecting **None**.

RestartAutoRange: This option forces the scan to restart on a new range as soon as an over-range value is detected, without waiting for the scan to complete. Values are not reported until an in-range scan has been acquired. This option defaults to Off.

NoDeferAutoRange: This option completes the scan, before examining the data. If out of range values are detected, the scan will be restarted on a different range setting. Values are not reported until an in-range scan has been acquired. This option defaults to Off.

SaveScanDev: This option is selected by default; at the end of a scan the scanned variable value is reset to what it was on entry to the scan. This option should, therefore, be left selected for every variable in a scan set where it is important to preserve the value of the scanned variable at scan exit (e.g. for subsequent scans). When the **Easy Scans** are used to set up a complex scan this is done automatically.

If **SaveScanDev:** is deselected, the value of the scanned variable is left at its **Stop value** when the scan ends.

SaveScanDev: should be deselected for co-varient scans.

There is a small time penalty in using **SaveScanDev:**; so, for maximum cycling speed, it should be avoided; for example, this option can be turned off if only one mass is scanned.

BeamOnBefore: Turns the ion beam On before a scan starts. It defaults to On.

BeamOffAfter: Turns the ion beam Off after a scan ends. It is selected by default.

BeamOnBefore: and **BeamOffAfter:** may be used to maximise scan speeds (especially **MID** speeds) by not switching the beam off between scans. When operating in this manner care must be taken to ensure that the mass jumps between scans do not include a large partial pressure peak; this can lead to a large momentary signal in the detector.

These options are valid only if operating in RGA mode where the instrument has control of the source of ions.

YieldToEvents: Should be set if the auxiliary inputs are to be read by an event sequence during scanning.

Accumulate Allows multi-channel data acquisition; it is useful for dealing with low signal levels from the detector. Normal single-scan acquisition collects data over one scan only. For a low signal level, a **Dwell Time** of one second may be required to achieve a reasonable signal-to-noise ratio; this leads to a very long scan time and unrepresentative relative mass intensities if there is a time variation of the spectrum.

Multi-channel acquisition uses a relatively short **Dwell Time** and accumulates the signal for each mass so that the spectrum builds-up over successive scans. As the same total time is spent collecting data there is no loss in signal-to-noise ratio, but the rapid scanning minimises any errors in relative mass intensity due to time variation of the spectrum.

When using the **Accumulate:** option, select a relatively short **Dwell Time**, e.g. 10 ms, in the **Input selection** dialog.

The number of **Cycles** for which the scan is to be repeated must be entered into the **Duration settings** dialog.

If required, a trip may be used to stop scanning should any channel reach a maximum. Alternatively, the number of **Cycles** should be chosen so that no channel overflows, or the scan should be manually stopped before this occurs.

Accumulate: should not be used with multi-variant scans.

Accumulate: may be used with the **Raw counts** input device to accumulate the total count rather than the sum of the counts per second values.

Mean: Is similar to the **Accumulate:** option; the mean data value for all the scans acquired is stored for each mass channel.

When using the **Mean:** option, select a relatively short **Dwell Time**, e.g. 10 ms, in the **Input selection** dialog box.

The number of **Cycles** for which the scan is to be repeated must be entered into the **Duration settings** dialog.

See also: [Duration settings dialog](#)

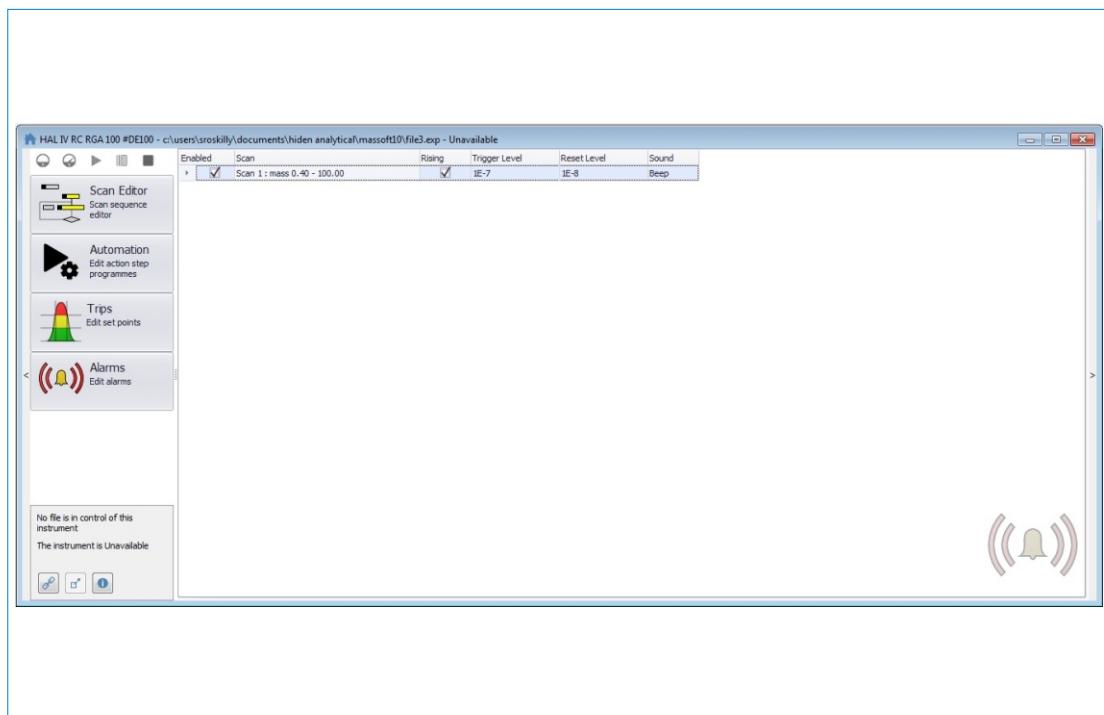
Mean: should not be used with multi-variant scans.

Scan Result functions define what a scan does with its result. This is not the same as the data acquired during a scan, but is a single value associated with how the scan operates. At present, the main uses are for automatic mass alignment and tuning.

None	No result is generated. This is the default setting.
Align	Uses a Savitzky-Golay filter to find the effective maximum value of a peak, ignoring any “noise” effects (i.e. returns the value of the scanned variable which is the effective maximum of a peak in the input device readings). This is used for automatic mass alignment. See also: Auto mass align
AutoTune	Finds the value of the scanned variable at which the input device reading is a maximum and saves it for automatic tuning in the global run environment. This is used for automatic tuning. See also: Auto tune
Max	Returns the maximum value of the input device.
Sum	Returns the integral of the input device readings over the range of the scanned variable.
Top	The same as Align but uses the point of the true maximum value instead of the effective maximum value.
XvalAtMaxY	Returns the value of the X (scanned) device at the point of maximum Y (input).

Alarms Page

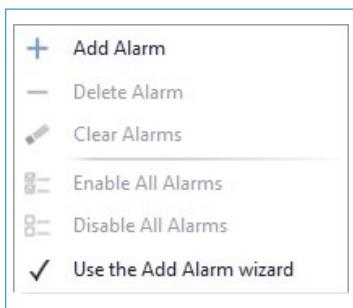
The **Alarms** page of the Home Window of a MASSoft experiment file allows an audible and text based alarm to be added to a scan. The Alarms page is displayed when the **Alarms** button is pressed. Initially this page is displayed empty. Otherwise if an alarm has previously been created then it is displayed as a row in the alarms table on the page. An example where an alarm has been created is shown below.



A new alarm can be added to the **Alarms** page using a popup menu or the Tool bar shown below



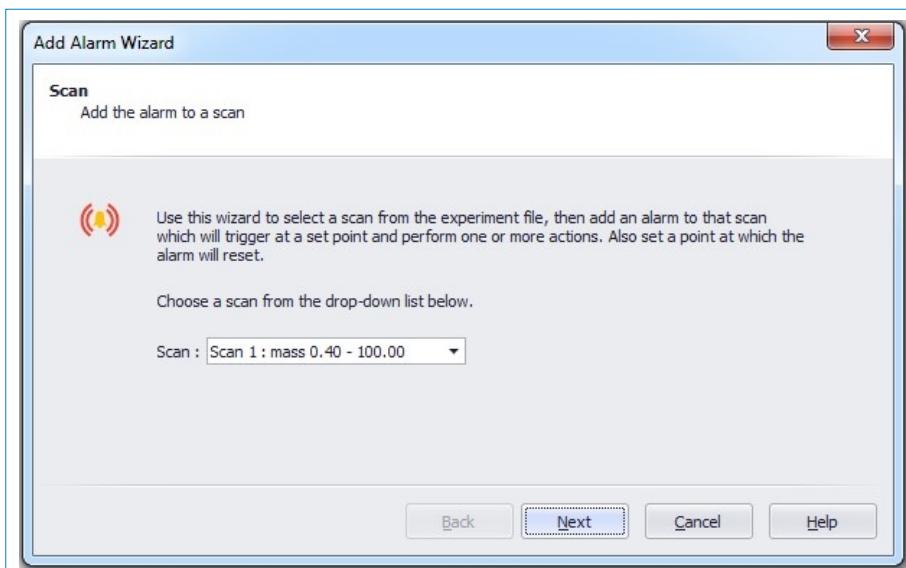
Right-clicking on the Alarms page brings up the Alarms popup menu.



Add Alarm

If the option to use it is enabled, then this opens the **Add Alarm Wizard**. Otherwise a row is added to the table displayed on the Alarms page. The values entered in the table can be edited.

The first page of the **Add Alarm Wizard** is shown below.



The following controls are found on the pages of the wizard

Scan

The scan to be monitored is selected from this list box.

Trigger alarm on rising signal (uncheck to trigger on falling signal)

When checked on, the alarm is triggered on a rising signal level, otherwise when unchecked it is triggered on a falling level.

Trigger Level

Specifies the data value at which an alarm is triggered.

Trigger Reset Level	Specifies the data value at which an alarm resets switching off.
Create event log entries	When checked on, a message is added to the Event Log .
On Triggered	Specifies the message to be displayed when an alarm is triggered. This message is auto generated, but can be edited.
On Reset	Specifies the message to be displayed when an alarm is reset. This message is auto, but can be edited.
Show a message box	When checked on, MASsoft displays a message box. The On Triggered and On Reset specify the message to be displayed when an alarm is triggered and reset.
Create Tag and Value	When checked on a tag and value is created. The Tag and Value for the On Triggered and On Reset alarms are specified.
Include Time Stamp	Determines if a time stamp is added to the alarm text.
Do not display the wizard again	When enabled the Add Alarm Wizard is not displayed the next time Add Alarm is selected.
	When the Finish button is pressed a row is added to the list of alarms displayed on the Alarms page.
Delete Alarm	Delete the highlighted alarm in the list of trips on the Alarms page.
Clear Alarms	Clear all alarms in the Alarms page. A warning message is displayed asking if you wish to carry this action.
Enable All Alarms	Ticks on the Enabled field of all alarms in the alarms table, enabling them all.
Disable All Alarms	Ticks off the Enabled field of all alarms in the alarms table, disabling them all.
Use Add Alarm Wizard	Ticks on or off, whether the Add Alarm Wizard will be used when Add Alarm is selected, or if alarms are added directly to the alarms table.

See also:

[Home Window](#)

Applications menu

The **Applications** menu contains applications dependant on information stored in the Hiden.ini file. The Hiden.ini file is configured automatically during the MASsoft installation process.

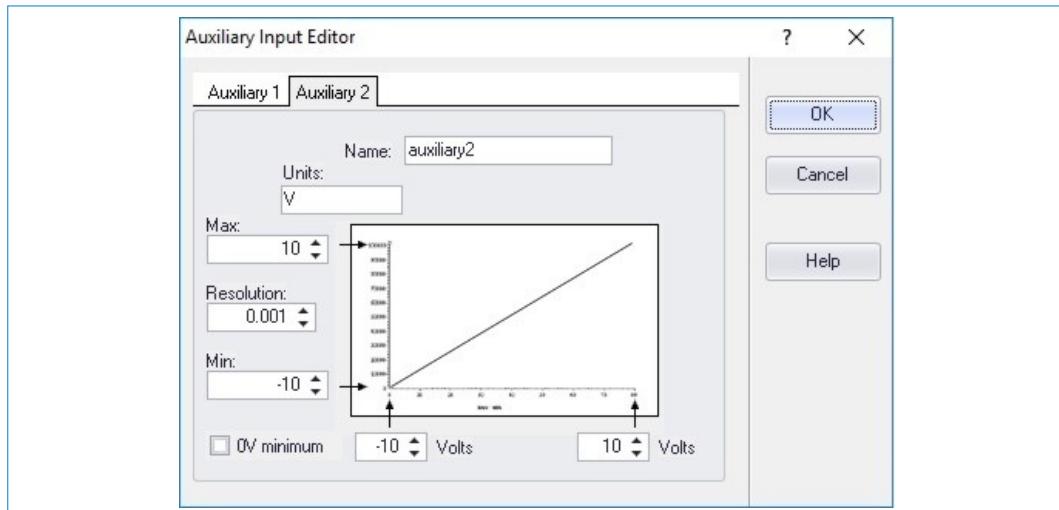
Analogue inputs

The mass spectrometer control unit is equipped with two auxiliary analogue inputs for user parameter monitoring. These may be used to acquire data from external equipment and store it with mass spectral data. Typical uses of the auxiliary analogue inputs are for thermocouples, Pirani gauges, etc.

The auxiliary analogue inputs, auxiliary1 and auxiliary2 may be configured by the user so that, for example, instead of reading auxiliary1 with a range of 10 V, the input could be named Temperature with a range of 0 °C, at 0 V input, to 1000 °C, at 10 V output.

The analogue inputs are configured in the **Auxiliary Input Editor** opened by selecting **Configure Auxiliary Inputs..** on the **Instrument** menu.

Alternatively, select the **Status** control tab and double click on **Auxiliary Inputs**.

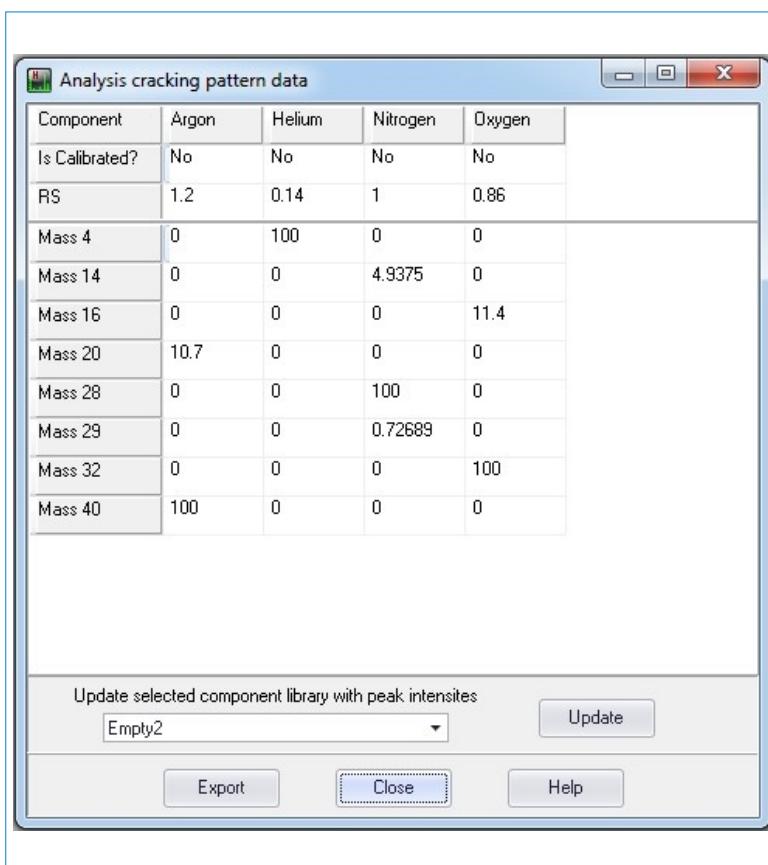


The **Auxiliary Input Editor** is only available if an instrument is connected.

The auxiliary inputs can only be configured when there are no files open. If there are any files open then the controls in the dialog will be disabled.

Analysis Cracking Pattern Dialog

The **Analysis cracking pattern data** dialog displays the cracking pattern for the current analysis in the form of a table. The table shows each of the components in analysis, and all of the contributing masses from the chosen components. This also displays the relative sensitivities and whether the components have been calibrated.



Update

Selecting a field in the spreadsheet, and then pressing the **Update** button updates the cracking pattern for the selected component to the library specified in the **Update selected component library with peak intensities** pulldown list.

Export

Pressing the **Export** button opens a dialog allowing you to choose to save the cracking pattern data to a .csv file which can be read in by Microsoft Excel.

Close

Closes this dialog.

See also:

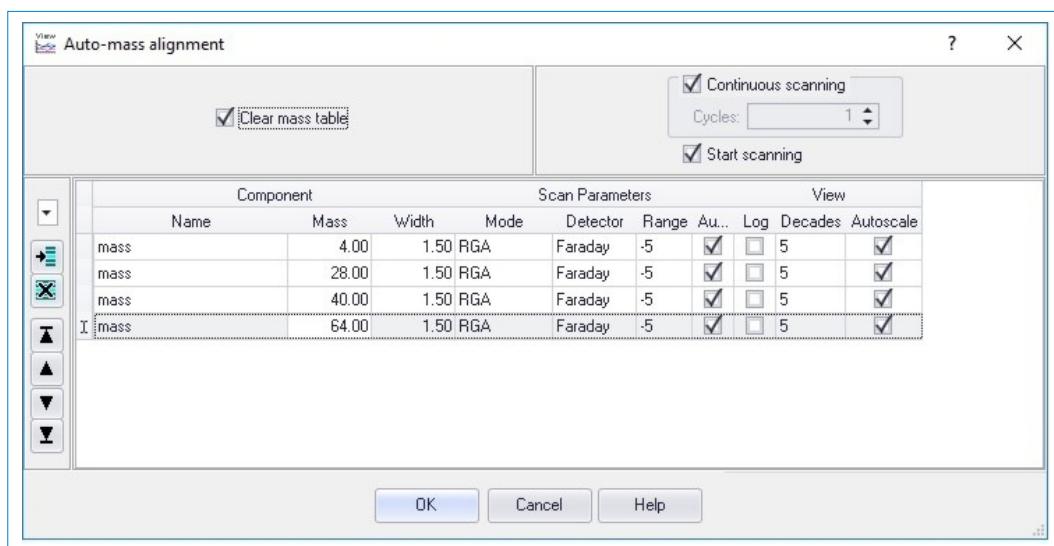
[Quantitative Analysis](#)

[Quantitative Analysis Template Wizard](#)

[Quantitative Analysis Menu](#)

Auto mass align

Selecting **Instrument, Maintain, Auto mass align** from the Menu Bar opens the **Auto-mass alignment** dialog to allow easy calibration of the instrument's mass scale. It automatically creates a view for each monitored mass, and is similar to the **MID** scan tree except that a maximum of eight masses may be used for mass calibration. The scans produced are **Profile** scans centred on each mass. The apex of each mass is determined and its position entered into the mass table.



For general purpose mass alignment, masses evenly distributed across the instrument's mass range should be used where possible, and the closer the highest mass is to the instrument's top mass, the more accurate is the last (top) segment of the calibration scale.

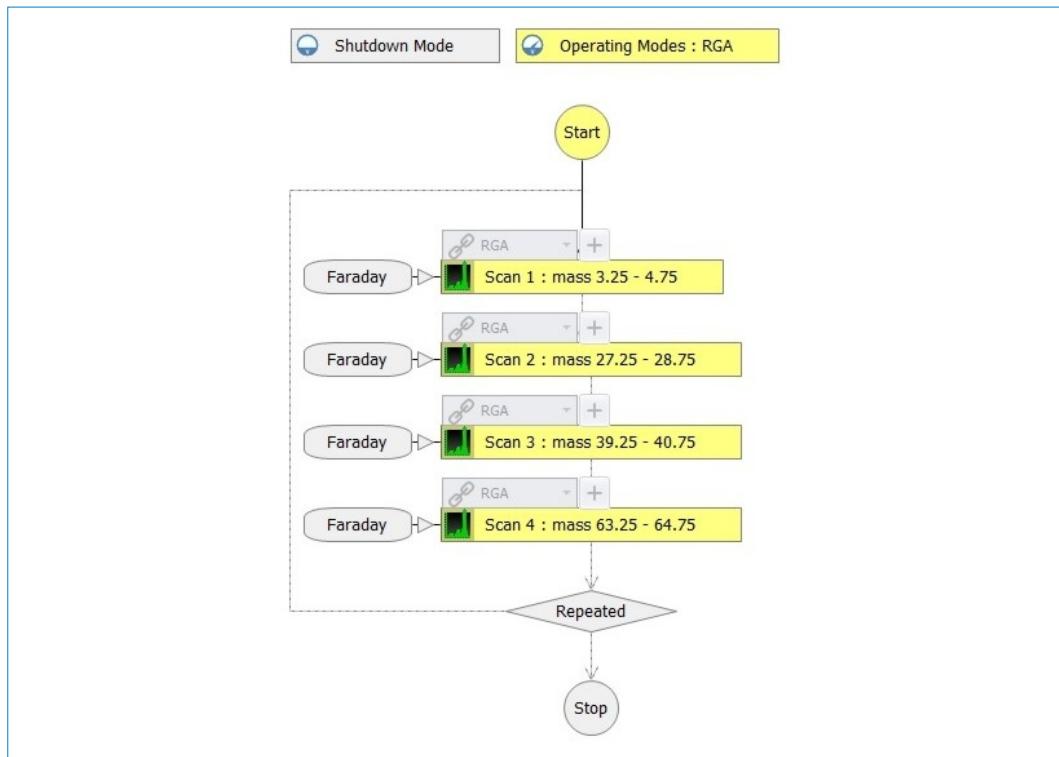
If a new set of masses is selected and these are to be used instead of, rather than as well as, the existing masses, the **Clear mass table** check box must be selected. Unless the user is familiar with the existing mass table, or needs to align gases one at a time, it is advisable to select this option.

Where a specific set of masses is to be monitored, these peaks may be used to set the instrument up as precisely as possible.

Once alignment is complete, the resulting mass table is used until such time as the **System, Maintain, Auto mass align** command is used again.

The dialog shown above produces the scan tree shown in below with a view created for each scan. All the required **Scan Advanced** options are selected automatically.

An alternative to using the **Instrument, Maintain, Auto mass align** command is to use the **File, Open** command to read an existing mass alignment experiment. One example file is included with each instrument.

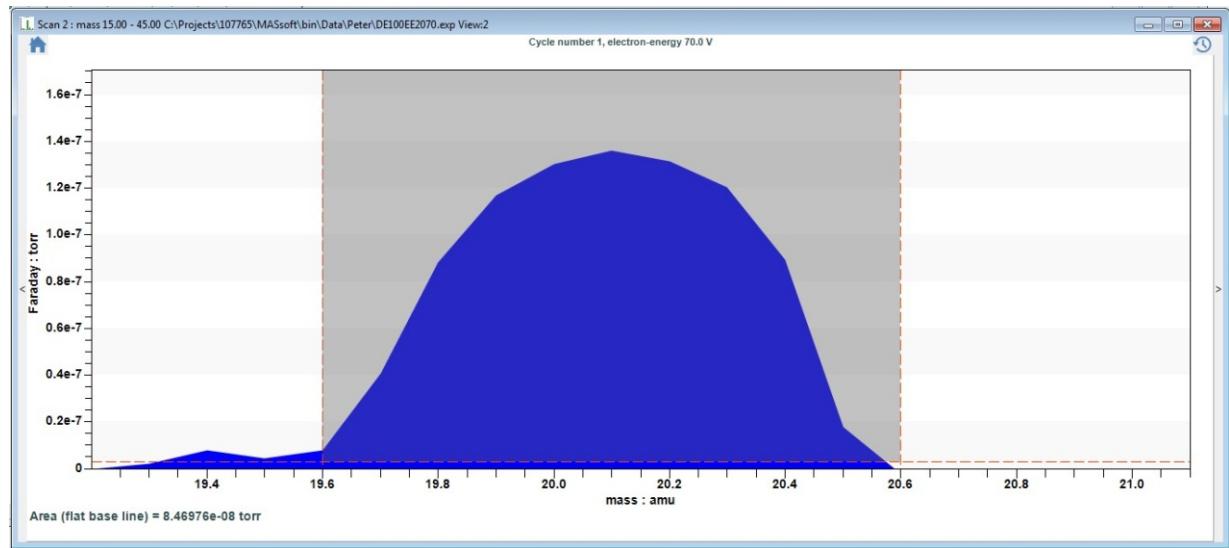


See also: [Mass alignment](#)

Area Calculation

How the area under a peak in a **Bar/Profile Graphical View** is determined, is controlled by the **Area** submenu options.

An example is shown below where the area of the peak between 19.6 to 20.6 is calculated using the initial position of a moveable baseline.



Note that the colour of the lines defining the bounds of the area is determined by the **Graph Cursor** colour in the preferences.

The area is calculated by dividing the selected X range into slices defined by the scan increment size, and summing the Y data value minus the baseline multiplied by the X value at centre of each area slice in the selected region.

The user is required to select a sensible range of X data, i.e. to have selected the X range across a peak in order to calculate a sensible value for the peaks area.

If the **Convert C/S to Counts via Dwell Time** option has been selected then when the units of the Y axis are in **Counts Per Second (c/s)** and a value in ms (not %) has been entered for the **Dwell Time**, the area is calculated in **Counts** by taking into account the **Dwell Time** of the scan.

The area is reset when the **Clear Area Selection** option is selected, or when the SHIFT button is pressed. It is also reset when the plot data is cleared.

See also:

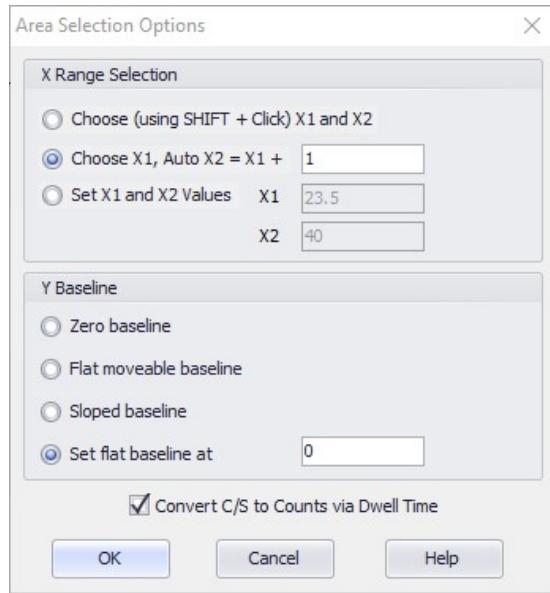
[Area Selection](#)

[Highest Peak Value](#)

[Bar/Profile plot view](#)

Area Selection

The new **Area Selection Options** dialog has options to determine how the X range is set and how the Y data baseline is determined when calculating the area under a peak in a **Bar/Profile Graphical View**.



X Range Selection

There are 3 methods for setting the X range.

Choose (using SHIFT + Click) X1 and X2

When displaying the Y data cursor line (SHIFT is pressed and the mouse is moved), the first left mouse button click sets the X1 point (while keeping SHIFT pressed), and the second left mouse button click (while keeping SHIFT pressed) sets the X2 point. If the SHIFT button is released the X1 and X2 selections are cleared.

Choose X1 , Auto X2 = X1 + (a value, default 1)

When displaying the Y data cursor line (SHIFT is pressed and the mouse is moved), the first left mouse button click sets the X1 point. The X2 point is automatically determined as the X1 value plus the given value entered. By default the increment value is 1.0, hence if mass is on the X axis the peak X range can be determined from the first click

Choose X1 and X2 (as values entered)

Enter the values of X1 and X2 into the two input boxes. Selecting **OK** on the dialog the area is then calculated using the entered values. Pressing SHIFT is not required.

Y baseline options

There are 4 methods for setting the Y data baseline used in the area calculation

Zero baseline

A zero baseline is used.

Flat moveable baseline	A flat moveable baseline is used. This baseline is initially set as the averaged value of the Y data point located at the X1 and X2 position. The position of the baseline can be adjusted, by left-clicking with mouse on the plot after the X1 and X2 points have been set. The new position of the Y baseline is then used in the area calculation.
Sloped baseline	A sloped baseline is used. The value of Y1 at X1 is determined, and the value of Y2 at X2 is determined. A linear gradient is then applied between these two points, as displayed on the plot. The calculation of the area under the peak data takes into account the gradient of this sloped baseline.
Set flat baseline at	A flat baseline is set at the given Y value.
Convert C/S to Counts via Dwell Time	If this option is selected, then if the units of the input device are in counts per second (c/s) and the dwell time has been entered in mS (not %) via the Input Editor then the area is converted into Counts.

See also;

[Area Calculation](#)

[Highest Peak Value](#)

[Bar/Profile plot view](#)

Automation

MASsoft provides trip and event facilities which allow actions to be taken based on the data acquired, and allow the mass spectrometer to be controlled by external signals. Trips and events may be defined for any mass spectrometer, and are saved in the experiment file.

Trip lists and action sequences run as independent tasks under the Interface Unit's multi-tasking operating system, and action sequences can be started and stopped as required. The action sequence(s) are generally started and stopped at the same time as the data acquisition task.

A trip is the simplest object, and allows output devices to be set/reset depending on the data acquired. Its functions are limited to comparing data with fixed levels and deciding whether to set or reset an attached output device. Trips may be attached to a scan (i.e. local) or may be assigned to monitor a particular mass independently (i.e. global, taking data from all scans). Several trips may be defined for a particular scan tree, but each is stand-alone and cannot take data from other trips. The Secondary Electron Multiplier (SEM) protection in Hiden Analytical Limited mass spectrometers is an example of the global use of a trip.

The event or action object is more versatile; it can take data from a number of sources, manipulate it, and signal its decisions in a number of ways. Events may be built into a sequence which can call-up other sequences, branch on the results of decisions, etc. and may

be considered a high-level mass spectrometer macro language. Inhibit protection and emission lamp control are examples of action sequences.

Trips

Trips check the data as it is acquired and perform actions should limits be exceeded. They may be tied to a specific scan or may be global. If global, the input device to which the trip applies may be specified and, optionally, the output device (e.g. mass) values between which the trip applies.

Each trip has an upper and a lower limit value, and decisions may be taken in a variety of ways: between limits, outside limits, equal to either limit, above upper limit or less than lower limit. These last two comparisons may incorporate hysteresis. When data exceeds the limits, the trip becomes active, and the defined output action is executed.

When a trip changes between active and inactive states, it can perform one of three types of action:

Write a value to an output device.

Enable or disable another trip.

Run an action sequence.

Events and Action Sequences

Events and actions can be used to manipulate data, calculate ratios, restore values to the event log, control a scan from an external input and for many other purposes. Actions can extract values from data already acquired and stored in the Interface Unit (IU), or direct from a device, manipulate the data using simple calculations, evaluate the results, print messages, execute commands or call-up other sequences as a result of the evaluation. A number of action functions are available, and these can be built into an action sequence:

Data Action	Used to fetch data from a scan.
Evaluate Action	Performs simple calculations on fetched data.
Limit Action	Checks data against limit values.
Timer Action	Perform actions periodically.
Set Action	Unconditionally sets an output device.
Command Action	Executes an internal mass spectrometer command.
Task Action	Similar to Command event , the specified command is executed as a task by the IU, running in the background.

Print Text Action Sends a text string to an output device.

Print Number Action Converts a number to text and sends it to an output device.

Events are described in the Hiden Analytical manual “MASsoft Event Sequences Guide” reference HA-085-660. This guide uses MASsoft 7 so the interface is different, but the principals applied in creating event sequences remain the same.

See also:

[Automation Page](#)

[Trips Page](#)

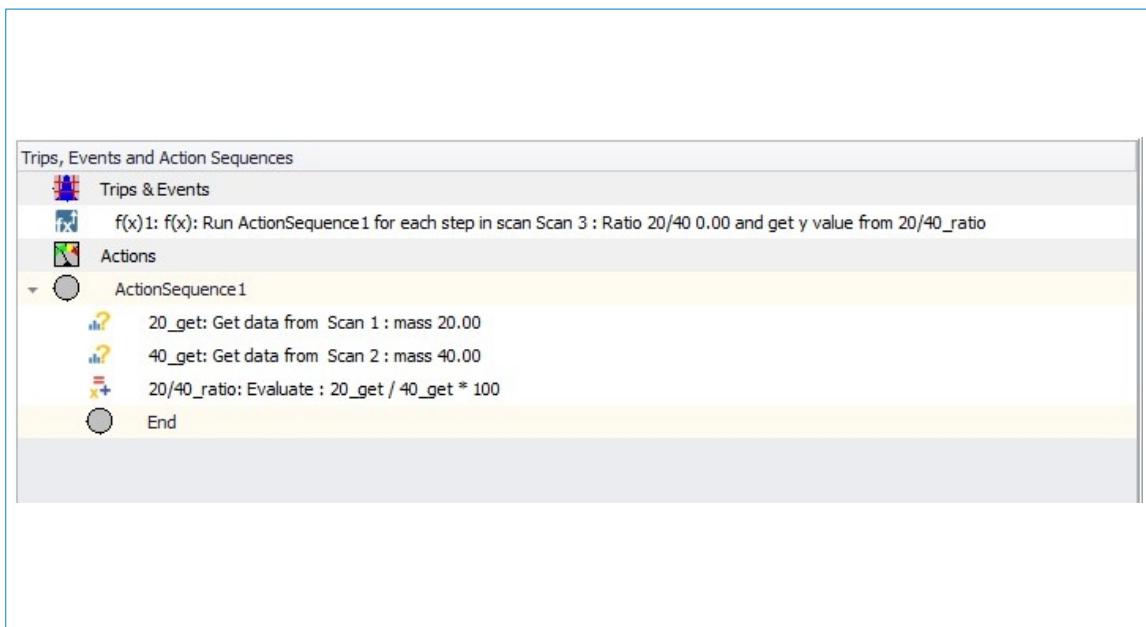
Automation Comments Panel

Displaying the Comments Panel is optional. The Automation page right click popup menu includes the sub menu **Comments panel** with the options **Hide Panel**, **Show Vertical** and **Show Horizontal**.

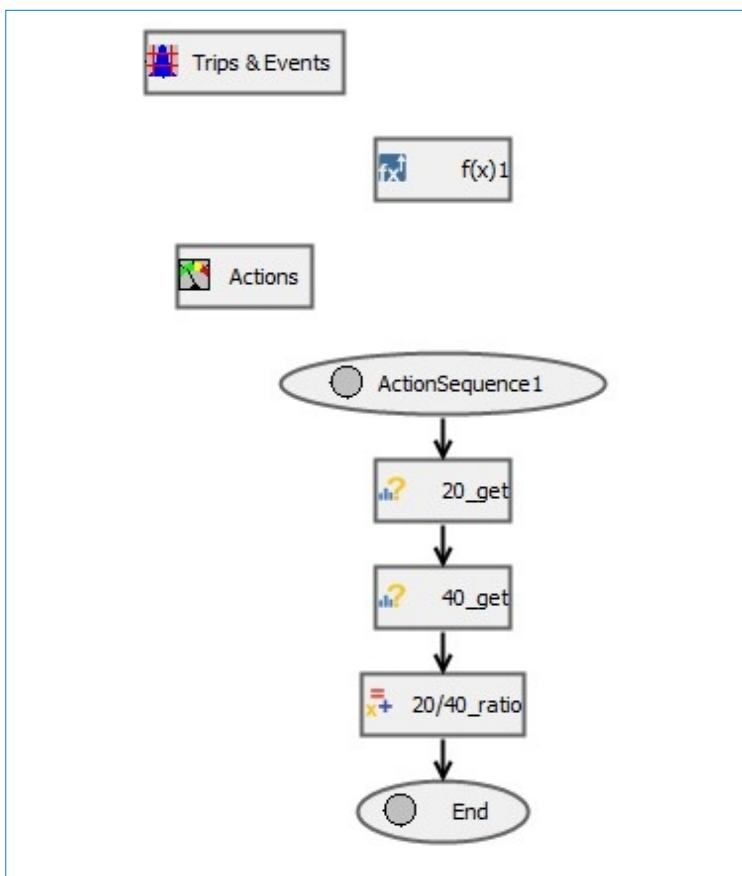
When the **Show Vertical** or **Show Horizontal** option is selected a panel is displayed either above or to the right of the flow chart. This panel displays a list of each event name and the comment associated with the trip, event or action. Clicking the **Hide Panel** option hides the panel from view.

Any changes to the flow chart are mirrored in the comments panel, and vice versa. Therefore Trips and Actions can be added to the via the comments panel list using the right-click popup menu. Items can be edited by double clicking the comment within panel, which opens the associated dialog for that action. Likewise items can be deleted from within the comments panel.

Example of the vertical comments panel is shown below



For the following flow chart



How the comments panel is displayed, and its width or height are restored when a new Automation page is viewed. When comments are viewed as a vertical panel the flowchart controls are shifted to the left.

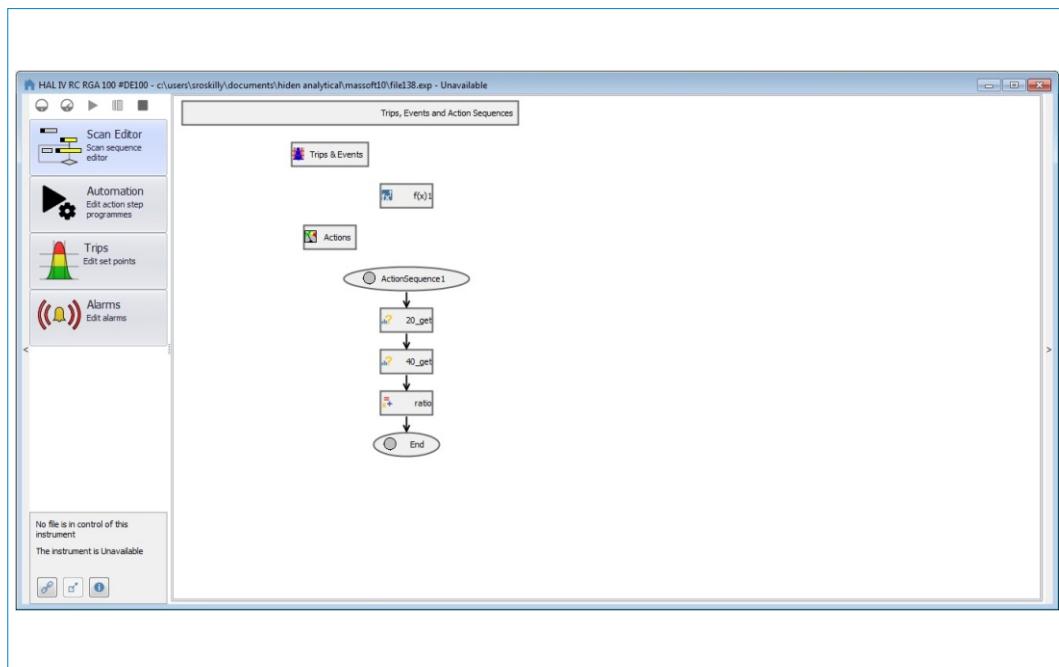
The comments panel size can be changed by left clicking and dragging the splitter control which separates the comments from the flow chart. Left clicking on the splitter without dragging will hide the panel.

See also:

[Automation Page](#)

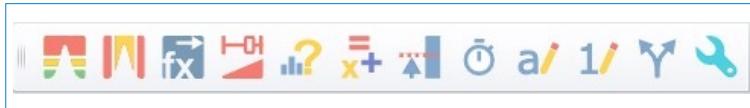
Automation Page

Trip, Events and Action sequences are entered on the **Automation** page of the Home Window of a MASsoft experiment file. The Automation page is displayed when pressing the **Automation** button is pressed. For a new structure, the **Trips, Events and Action Sequences** header box is the only object displayed on the page. Otherwise if an automation structure has been previously entered then the objects associated with the automation sequence are displayed on the page. An example with an automation structure displayed in a flow chart is shown below.

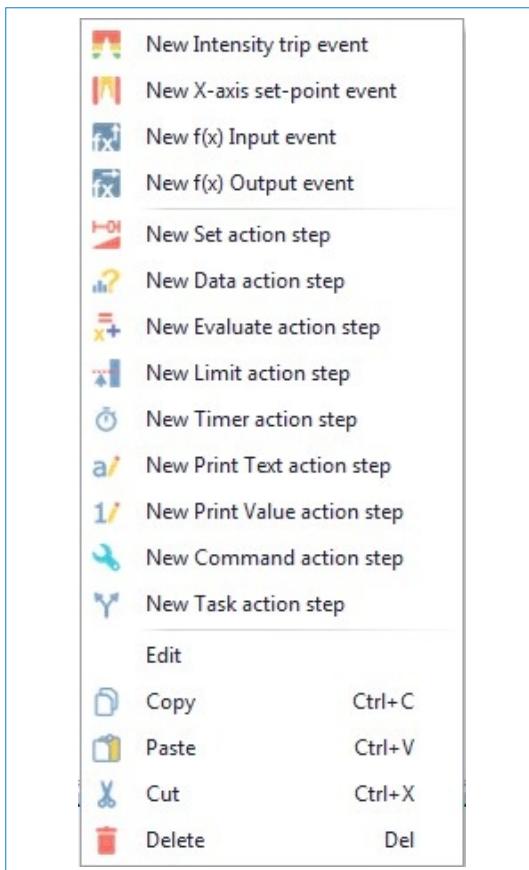


Under the **Trips & Events** object box are listed all the trips and events. Under the **Actions** object box are listed all the action sequences added as elements of a flowchart. Multiple action sequences can be created.

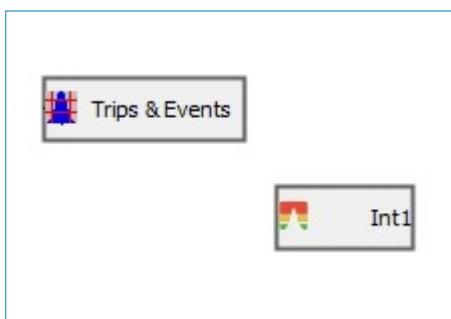
A new Trip, Event or Action Sequence can be added to the Automation page using the Automation popup menu or Tool bar as shown below



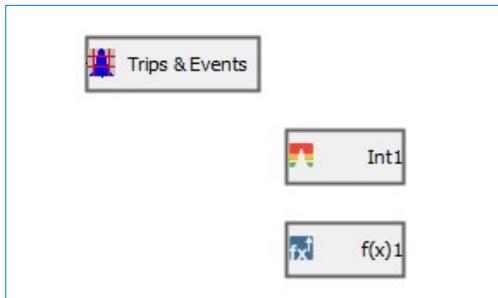
Right-clicking on the Automation page brings up the Automation popup menu.



Choosing one of the new event options from the menu will create an object box in the Automation page under the Trips & Events box. An example is shown below when the **New Intensity trip event** option is selected when starting a new structure

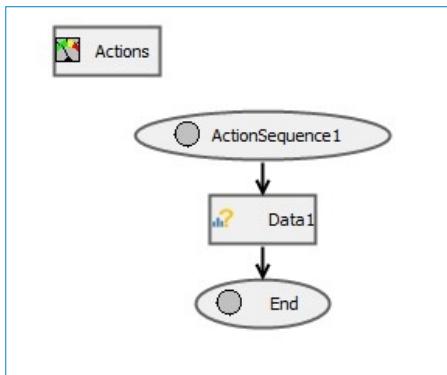


Addition new event options will add further elements listed under **Trips &Events**. For example when the **New f(x) Input event** option is selected from the menu a new box is added



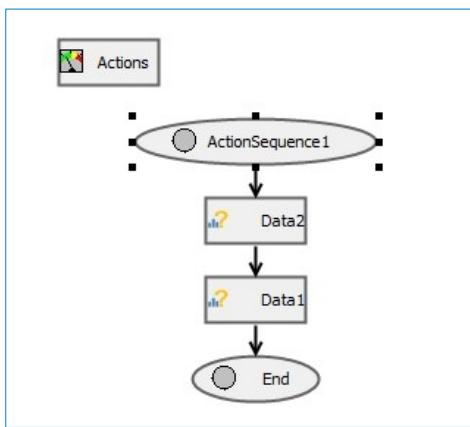
Choosing a new action step from the window will either add a new step to an existing action sequence or create a new action sequence including the selected step.

If no action sequence object box is selected in the Automation page then a new action sequence is added to the page including the selected step. For example if **New Data action step** was selected then the **ActionSequence1** object box would be created including a **Data1** action step, as shown below.

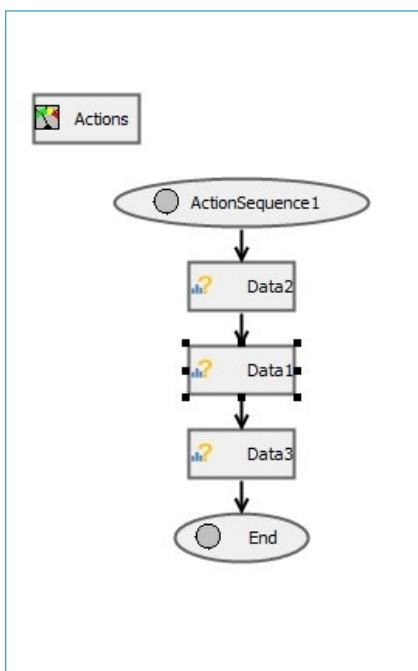


ActionSequence1 denotes the beginning of a new action sequence, which is followed by the elements of the action sequence. The end of the action sequence is denoted by an **End** object box.

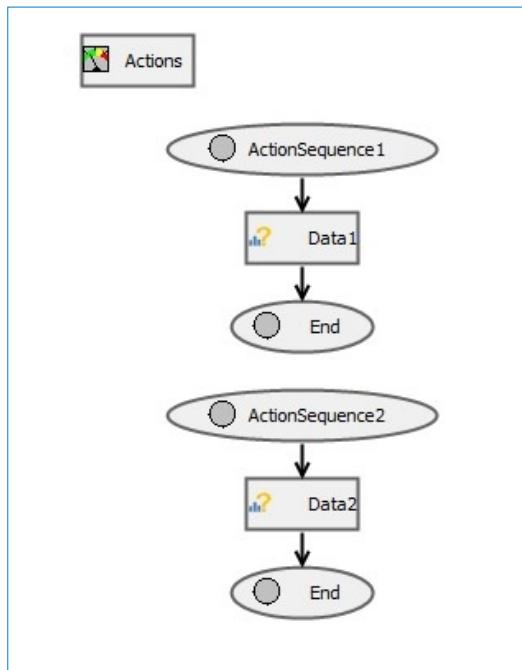
When adding a new data action if the box of an existing action sequence has been selected then the new data action is inserted at the point in the sequence after the selected component. For example if the **ActionSequence1** object box was selected (it is highlighted with black squares when selected). Then if the **New Data action step** was selected then the new step **Data2** is inserted before **Data1** as shown below



Whereas if we now select the **Data1** object box then choose **New Data action step** then **Data3** is appended to sequence after **Data1**



If no element of an existing Action Sequence is selected, then choosing **New Data action step** will create a new action sequence including the selected step. An example is given below on adding a second new data action after then first.



The **Edit**, **Copy**, **Paste**, **Cut** and **Delete** options of the Automation popup menu, allow for editing of the trips, events and action sequences.

Edit	Edits the currently selected object. The appropriate edit dialog box is displayed. An edit dialog box can be opened for any trip, event or action sequence object. The Trips , Events and Action Sequences , the Trips & Events and Actions object boxes cannot be edited. Alternatively, double-clicking on the object on the Automation page will open the editor.
Comments Panel	The Comments Panel submenu contains options to determine how the optional comment panel is displayed.
Hide Panel	The comments panel is hidden from view. Only the flow chart is displayed.
Show Vertical	The Comments Panel is shown in a panel on the right of the flow chart.
Show Horizontal	The Comments Panel is shown in a panel above the flow chart.
Copy	Copies the currently selected object to Windows clipboard.
Paste	Pastes a copy of a previously copied object from Windows clipboard.

- Cut** Cut the object.
- Delete** Delete the selected object. A warning message, to confirm deletion, will appear for an Action sequence marker or a limit event object.

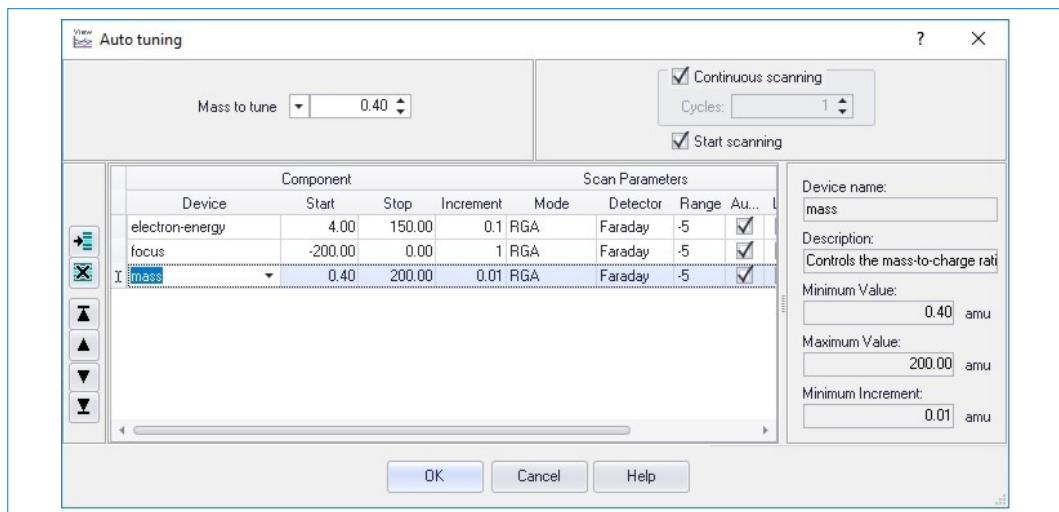
Normally a new trip and action structure is created by inserting trip or action objects on an individual basis, however, a trip and action structure containing an **Intensity** trip and **Print text** function can be automatically generated from the Trips page of the Home Window.

See also:

- | | |
|---|--|
| Automation Comments Panel | Home Window |
| Automation | FofX Input Device Event Editor |
| Intensity Trip Editor | Set Action Step Device Event |
| FofX Output Device Event Editor | Timer Action Step Editor |
| Limit Action Step Editor | Print Text Action Step Editor |
| Evaluate Action Step Editor | Command Action Step Editor |
| Print Number Action Step Editor | X Axis Set Point Editor |
| Data Action Step Editor | Task Action Step Editor |
| Trips page | Branch Editor |
| Action Sequence Editor | |

Auto tune

Selecting the **Instrument, Maintain, Auto tune** opens the **Auto-tuning** dialog box which allows easy loading of variables for automatic tuning of the instrument.



The borders of the dialog may be dragged to make the dialog larger. The column borders may also be dragged to make the columns wider giving more space for the column titles.

Select the mass for tuning in the **Mass to tune** box. Use the spin buttons or type the required value.

If **Continuous scanning** is checked scanning will repeat until it is stopped manually. If **Continuous scanning** is not checked the number a scan cycles can be entered in the **Cycles:** box. On completion scanning will automatically stop.

If **Start scanning** is selected the scan will begin as soon as the dialog is closed by clicking on the **OK** button. Otherwise the scan must be started manually.



Click the  Add component button to add a device to the scan list. A device can be



removed from the list by clicking the  Delete component button. Once some devices have been added to the components list the order can be change by using the arrow buttons found below the Add and Delete components buttons. The Devices will be scanned in the order they appear in this table.

Click in each device box to display a drop down list of available devices to tune.

The available devices are instrument dependant.

In the drop down list click on the device to select it. Click in the **Start**, **Stop** and **Increment** boxes to adjust the values using the spin button or by typing the required value. Parameters may be scanned from high to low values (i.e. **Start** value higher than the **Stop** value) if this aids the auto-tune process.

Mode Sets the acquisition mode. The same mode should be used for all components.

Detector Selects the detector (input device) to be used.

Range Sets the acquisition range. The value entered directly is a power of ten; e.g. if 7 is entered, the range set is 10^7 .

Autorange When selected, the analyser automatically changes the range and follows changes in the input signal.

Log When selected, the display's Y-axis is logarithmic, otherwise it is linear.

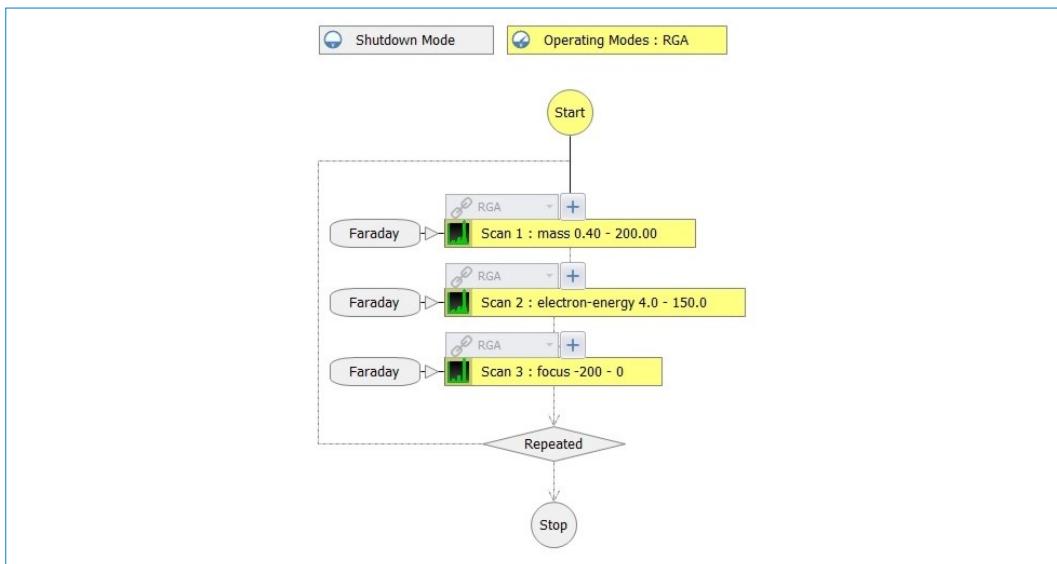
Decades Sets the number of decades on the log Y-axis.

Autoscale When selected, the Y-axis is forced to fit the largest peak. When not selected, the Y-axis maximum will be set to suit the selected range.

To the right of the dialog helpful information is displayed for the selected device.

After each scan, the system notes the scanned device value which produces the largest signal intensity and loads it into the device, so that after the first pass through the scan tree each device has a new value loaded into the global environment. The next pass through the scan tree uses these values to produce a new set, which is again stored in the global environment. At the end of the process, the optimised values are stored in the global environment and may be saved to file for later use.

The **Auto-tuning** dialog box shown in above produces the scan tree shown below with a view created for each scan. Optimised values for **electron energy** and **focus** are stored in the **Global: RGA** environment box at the end of the auto-tune operation. All the required **Scan Advanced** options are automatically selected.



This system may not be optimum for tuning the **energy** variable. In some circumstances the integral of the **energy** scan should be maximised instead of the absolute signal. MASsoft cannot offer this option at present.

When the instrument has been tuned, the tuned global environment variable values should be saved in a file, TUNE.EXP, for future reference.

Background subtraction

Background Subtraction allows data from one view to be subtracted from data in another view. The two views should be of a compatible type. You cannot subtract data from a Profile Plot view from a MID View

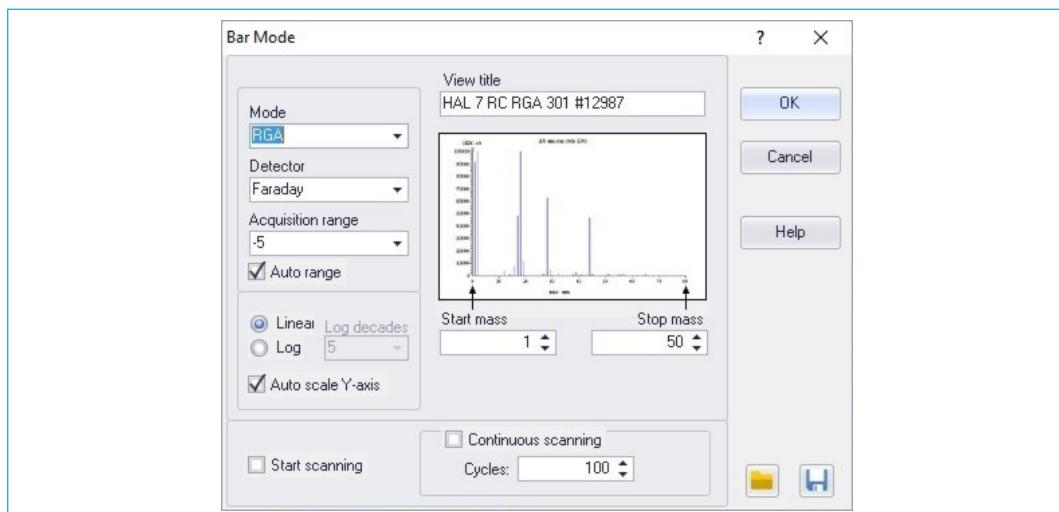
The first step in carrying out a background subtraction is to choose one of the views as the “source” view. Then select a different view as the “target” view. This subtracts the data

values in the “source” view from the data values in a selected “target” view. The subtraction is then automatically performed and the result displayed in the “target” view. An operations window, describing the operation that has been performed, is displayed by default in the “target” view.

For MID Tabular and Graphical views a dialog is displayed giving options for which cycle of data is going to be source. In the case of the tabular view this includes the possibility of using values determined from the statistics

Background subtract works on both graphical and tabular views. This command is grayed out if no “source” view has been selected, or if the view selected as the “target” has already been designated as the “source” view.

Bar Mode dialog



Clicking the Bar Scan button on the Easy Scans tab opens the **Bar Mode** dialog box for a simple linear mass scan. Parameters for the scan such as **Start mass** and **Stop mass** are defined in the Bar Mode dialog box.

All the dialog items in the **Bar Mode** dialog are common to other scan mode dialogs.

See also: [Common dialog items](#)

Bar/Profile plot menu options

Trend View Setup... Opens the **Tabular View Editor** allowing new data trends to be created from data within the current Profile plot.

Plotting Types Displays a sub-menu of Plotting Types. Data may be plotted on a Linear or Log (Log10) scale.

Grid Options Displays a sub-menu of Grid options.

Mode	Determines the Plot Mode and whether real time or historical data are displayed.
Title	Opens a dialog to edit the title in the graph area of a view. By default, the view's title is the name of the currently connected mass spectrometer. The title is shown immediately below the view's title bar.
Configure X Axis	Opens the X Axis Properties dialog for a Bar/Profile plot.
Configure Y Axis	Opens the Y Axis Properties dialog for an Bar/Profile plot.
Graph Cursor	When acquiring data, the graphics cursor can be switched on or off using this command.
Blank Ahead of Cursor	When this option is enabled an area just ahead of the Graph Cursor is blanked of data.
Area	The Area submenu contains the options Area Selection Options... and Clear Area Selection . Area Selection Options... displays a dialog with options as to how the X range is set and the Y data baseline is determined when calculating the area under a peak. Clear Area Selection clears a selected area.
Points	The Points submenu contains the options Mark Points and Track Cursor When selected the Mark Points option displays the position of data points on the plot. When Track Cursor is selected the plot X and Y coordinate values at the current mouse coordinates, as well as the Y-Peak value at the X coordinate are displayed in a line under plot. A cross hair tracks the current position of the mouse coordinate. Selecting the Track Points option when it is enabled will disable it.
Overlay Data	The Overlay Data submenu contains options for adding or removing an overlay of a previous iteration of data. Options are for Previous Iteration , Fix Iteration and Clear Overlay . The Previous Cycle / Iteration option is only available when scanning. When this option is selected, the plot will overlay the previous cycle or iteration of data behind the Graph Cursor . When the Fix Cycle / Iteration option is selected then the current displayed iteration of the data is used as the overlay. Clear Overlay will remove the overlay from the plot.

Source View	Designates the Bar/Profile View as the “source” view for the Background subtract function. If the source is plotting historical data the currently visible cycle of data is used as the source. A tick mark beside Source view indicates whether a selected view is the source view.
Background Subtract	Designates the Bar/Profile view as the “target” view for the Background subtract function, then subtracts the data values in the “source” view from the data values in the selected “target” view. The result displayed in the “target” view. An operations window, describing the operation that has been performed, is displayed by default in the “target” view.
Show Operations	If this view has been a target for Background subtract , then this toggles the operations panel on and off.
Copy	This option only appears on the right-click popup menu. It copies the Bar/Profile plot as a graphic image.

See also:

Background subtraction	Graphical/Tabular view editor	Grid options
Plot mode	Plotting types	X Axis properties dialog
Y Axis properties dialog	Area Selection	Area Calculation
Data Overlay		

Bar/Profile plot view

The Bar and Profile Plot Views share the same functionality. The only difference is in the default Plotting Types with which they are assigned.

A Bar plot is created from a non-MID Scan in the Scan Tree, where it has been set as a Bar type or the Increment value between data points is 1. Selecting the **Graphical View** option



from the **Views** menu or clicking on the Bar Plot View, button creates the view. The View is assigned the Bar plotting type by default, although it is possible to change the Plotting Type.

A Profile plot is created from a non-MID Scan in the Scan Tree where it has been set as a Profile type and has a Increment value other than 1. Selecting the **Graphical View** option

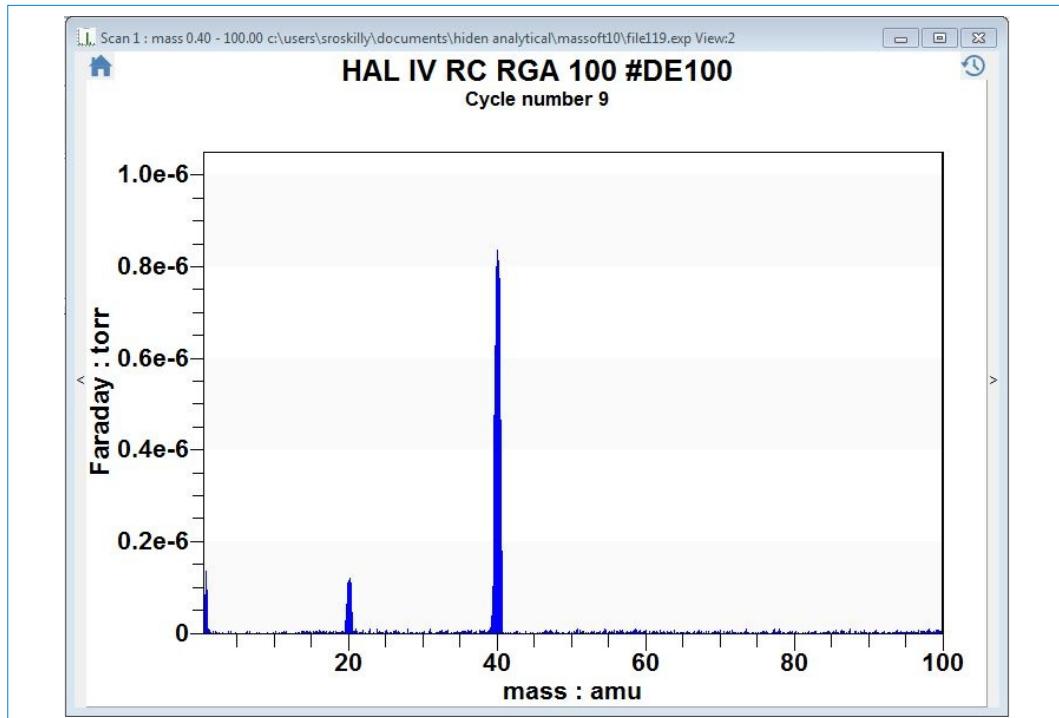


from the Views menu or clicking on the Profile Plot View, button creates the view. The plot is assigned the Area plotting type by default, although it is possible to change the Plotting Type.

The Bar / Profile view plot displays one cycle of data (which may be real-time or historical), which by default starts at the Start Value and ends at the End Value, as entered in the Scan Editor for the given Bar or Profile scan.

When a Bar/Profile View is created or while it is the active window, the **Views** menu options change to include options applicable to the Bar/Profile View.

An example is given below for Cycle number 9 of a Profile scan where the data have been collected over the range 0.4 to 100amu, and has a mass 40 peak and smaller mass 20 peak.



The icon in the top right hand corner of the view determines the Mode in which the plot is displayed.

Area Selection

Pressing the SHIFT button and moving the mouse while the cursor is over a Bar / Profile plot will display a vertical line and below the plot the X coordinate value and highest peak value of the data displayed at that point in the plot.

The SHIFT button may also be used when setting the X range for the **Area Calculation** in a Bar / Profile plot, depending on the **X Range Selection** type in the **Area Selection Options** dialog. The first left mouse button click sets the X1 point, which may automatically set the X2 point, or it may require a second left mouse button click to set the X2 point. If the SHIFT button is released and the mouse moved the X1 and X2 selections are cleared.

Also see:

[Plot mode](#)

[Highest Peak Value](#)

[Plotting types](#)

[Scan Editor](#)

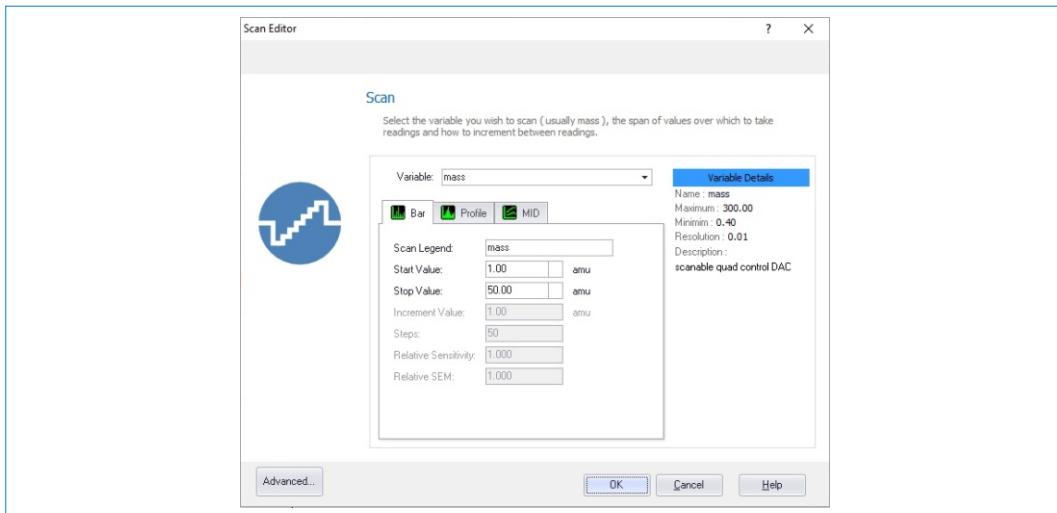
[Scan tree](#)

[Views menu](#)

Bar Scans

A Bar Scan is a simple linear mass scan with a non-equal **Start mass** and **Stop mass**, and an increment of one amu producing a histogram style display. MASsoft allows a simple Bar Scan to be generated quickly using the Easy Scan Bar Scan button. More complex series of Bar Scans covering different ranges of masses are also possible.

Bar tab



The Bar tab creates a scan which takes a measurement at all integer values from the Start value: to the Stop value: The default view created for this type of scan is a "2D Bar Graph".

Typically, this type of scan is used to survey a range of masses to identify which masses are present. Mass alignment ensures that each reading is taken close to the maximum of each individual mass peak.

- Scan Legend:** Allows the scan legend name on views to be edited; the required name is typed into this box; up to 32 characters (including spaces) may be used. This name also appears on the **Scan** box. The scan legend defaults to the contents of the **Variable:** box.
- Start Value:** The scan start value for the variable selected in the **Available to Scan:** list box. This must be within the **Minimum Value** and **Maximum Value** range for the variable.
- Stop Value:** The scan stop value for the variable selected in the **Available to Scan:** list box. This must be within the **Minimum Value** and **Maximum Value** range for the variable.
- Increment Value:** Defines the increment value for the scan. For a BAR scan, by definition, this is 1 and cannot be edited.

- Steps:** Defines the total number of steps during the scan, for the defined **Start value**, **Stop value** and **Increment** is calculated and displayed in this box. This cannot be edited as the Increment Value is fixed at 1 due to the type of scan.
- Relative Sensitivity:** This is only available for MID scans.
- Relative SEM:** This is only available for MID scans.

Branch Editor



The action sequence end marker , marks the end of an action sequence. It is used either to end that particular event task or to branch to another event or sequence.

Double-clicking the End marker opens the **Branch Editor**.



Branch to

Choose a previously created action sequence from the pulldown box to branch to. The type of actions listed can be filtered using the **Show sequences**, **Show all actions** and **Sort** options.

If no action is entered then the sequence is terminated.

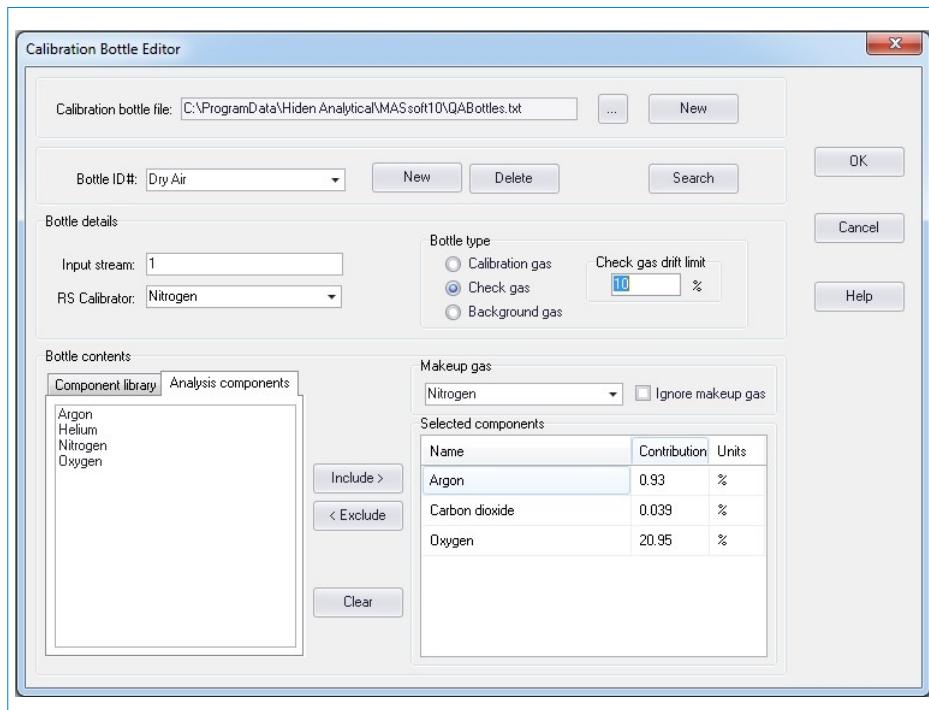
See also:

[Automation page](#)

Calibrate Bottle Editor

The **Calibration Bottle Editor** is accessed from the **Calibration bottles...** option of the **Edit** menu. It provides an interface for adding, deleting and modifying entries in the calibration bottle library. The library is used by the optional **Quantitative Analysis** module,

to store details of each of the bottles used in the calibration process. Bottles can contain either calibration gases or check gases. A calibration bottle must not contain gases with coincident peaks to allow for accurate calibration of the cracking pattern library. A check bottle may contain coincident peaks and is used to determine whether changes to the instrument sensitivity have occurred since calibration. If changes have been detected the process will apply the appropriate correction factors.



Calibration bottle file: The current default calibration bottles file name is shown here. The name is not editable in this field. Press the ... button to open a file browser to select an existing calibration bottle file or press **New** to create a new bottle file. The selected calibration bottle library is used by

Quantitative Analysis.

Creating a new bottles library requires a name for the file to be entered in the displayed dialog box and then clears all the bottles entries. New bottles must then be entered into the library following the procedure below.

BottleID#

Shows the bottle identifier given to the entry in the library. The drop down list shows all the bottles in the library. The **Bottle details** change when a bottle is chosen from the list.

New	Pressing the New button to the left of the BottleID# field clears that field and clears all the Bottle details , allowing a new bottle to be created and added to the library. The Add and Abort Add buttons become active. Enter the new bottle name into the BottleID# field and all required details in the Bottle details section. Then press the Add button, to add that bottle to the list of bottles. A new bottle entry is automatically placed in alphabetical order. If any required fields are missing a warning message is displayed. Press Abort Add to cancel the addition of the new bottle. After adding the bottle or aborting the addition of the bottle the New and Delete buttons are once again enabled.
Delete	Deletes the current bottle entry from the library
Search	A dialog box is displayed which enables the bottles in the current library to be located by name. If the required name is located in the current library it will be selected in BottleID# list.
Bottle details	
Input stream	Shows the valve to which the current library entry is attached.
RS Calibrator	Choose from the pull down list, the component in the bottle whose relative sensitivity is already known and will be used to determine the RS of the other components. Note that a component must be in the Selected components list or the Makeup gas before it can be assigned to the RS Calibrator field.
Bottle type	The bottle type is chosen from one of the three options: Calibration gas , Check gas and Background gas . A Calibration gas is used to measure peak ratios the cracking pattern of its components. Calibration gases contained in the current library entry must not have overlapping cracking patterns. A Check gas is used to check and revise the RS of a component in a mixture. Check gas permits overlapping peaks. A Background gas is used when measuring the system background. It should contain a gas that is not in the analysis and that does not have any peaks that contribute to the analysis.

Check gas drift limit When a **Check gas** bottle is measured the Relative Sensitivity values are adjusted for each component in the bottle so that the measured concentrations match the known concentration in the bottle. If the adjustment, when expressed as a percentage of the old RS value, is less than the “Check gas drift limit” then the RS of the component is revised. The check will fail if any adjustment exceeds the limit.

Bottle contents

Component library	Displays a list of all the species contained within all the component libraries which are being used with MASSsoft. A default RGA library is supplied with MASSsoft. The libraries contain the cracking patterns which are used by Quantitative Analysis . Because all the libraries are merged into this list, it can contain duplicate entries with the same name, although the cracking patterns of those entries may be different.
Analysis components	The Analysis components tab is only visible when a Quantitative Analysis Template is currently open. It displays a list of the components selected for the current analysis.
Selected components	Displays the list of selected components. The contribution for each component needs to be entered into the table in the Contribution column. Clicking on the entry in the Units column for a particular component will toggle the Units between % and PPM. If no makeup gas is specified then the contributions for all components must equal 100%. A bottle must contain at least one component.
Include >	The component(s) highlighted in the component library/current analysis will be added to the list of selected components with zero contribution. The contribution should be entered after including all components.
< Exclude	The component(s) highlighted in the list of selected components will be removed.
Clear	Removes all entries from the list of selected components.
Makeup gas	Shows, if present, the makeup gas used in the current library entry. Makeup gas is also known as bulk or balance gas.

Ignore makeup gas

If a Makeup gas has been specified then selecting this item will exclude that component from the calibration process.

Pressing the **Cancel** button will close the dialog without making any changes to the bottles library.

Pressing the **OK** button displays a dialog asking if you wish to **Save the changes to the bottle library?** **Cancel** will return to the dialog. **No** will close the dialog without making changes to the bottles library. **Yes** will close the dialog and update the bottles library file with any changes made.

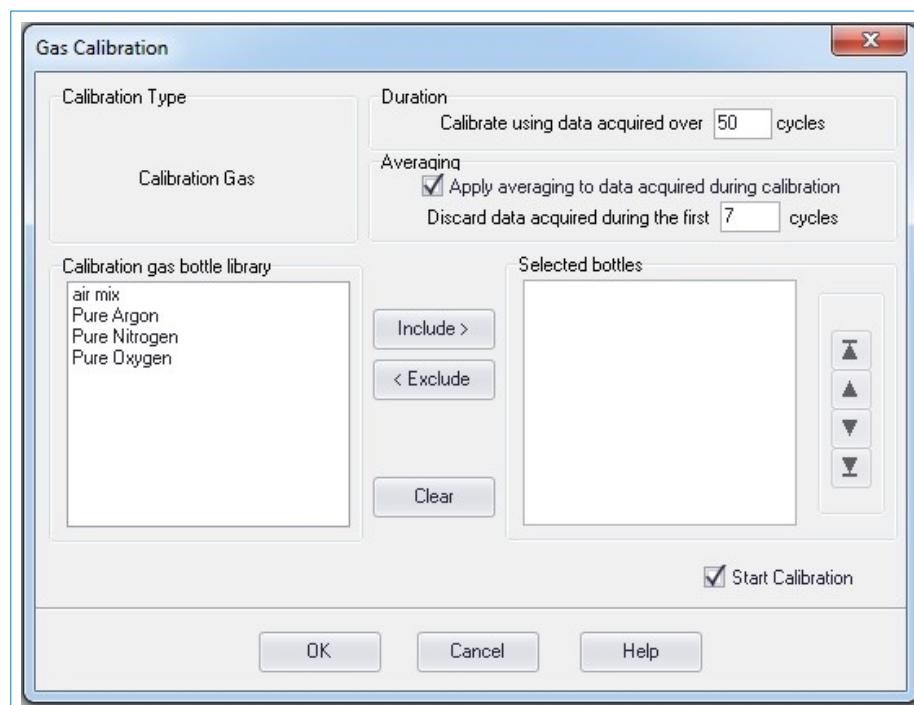
See also:

[Library](#)

[Quantitative Analysis](#)

Calibration Editor

The **Calibration Editor** is displayed when starting a calibration by selecting **Background Calibrate**, **Calibrate** or **Gas Check** from the **Calibration** submenu of the **Quantitative Analysis** menu. This allows components of the analysis to be calibrated.



Calibration Type	This box displays the calibration type, either a Background Gas , Calibration Gas and Check Gas calibration.
	The type of calibration depends on the selection made on the Quantitative Analysis menu.
Background Gas	Performs an analysis to obtain levels for background subtraction. The background gas should contain a gas that is not in the analysis and does not have peaks that contribute to the analysis.
Calibration Gas	Measures the contributions for each mass of a component. The calibration gas should have none overlapping cracking patterns.
Check gas	Calculates correction factors that ensure the calculated results match the actual concentrations in the check gas bottle. Depending on the calibration type the bottles available in the gas bottle library list will differ.
Include >	Pressing the Include > button adds bottles(s) from the gas bottle library list appropriate for the current calibration to the Selected bottles list.
<Exclude	Pressing the <Exclude button removes bottles from the Selected bottles list.
Clear	Pressing the Clear button removes all the bottles from the Selected bottles list.
Duration	Determines for how many cycles MASsoft should acquire data during the calibration.
Averaging	Check the Apply averaging to data acquired during calibration to average the data. If this is not enabled then only data from the last cycle is used in the calibration. A number of cycles of data may be discarded in order to allow the readings to settle. Discard data acquired during the first n cycles determines the number of cycles of data which are ignored before using it in the calibration.
Start Calibration	If Start Calibration is enabled then the calibration is started when the OK button is pressed, otherwise it is not.

See also:

[Quantitative Analysis](#)

[Quantitative Analysis Template Wizard](#)

Clear mass table

When a mass is aligned, either by the **Instrument, Maintain, Auto mass align** command or by means of the **Scan Advanced** dialog, the peak positions measured are saved in the control unit and the HIDEN.INI file. As new masses are measured they are added to those saved. The **Instrument, Maintain, Clear mass table** command is used to delete the mass table; this is used to start with a new set of masses, to return to the default mass alignment or to stop the mass table filling up. A total of eight masses can be stored.

It is advisable to select this option in most cases. An exception would be if the calibration gases could only be admitted one at a time.

Command Action Step Editor

CAUTION

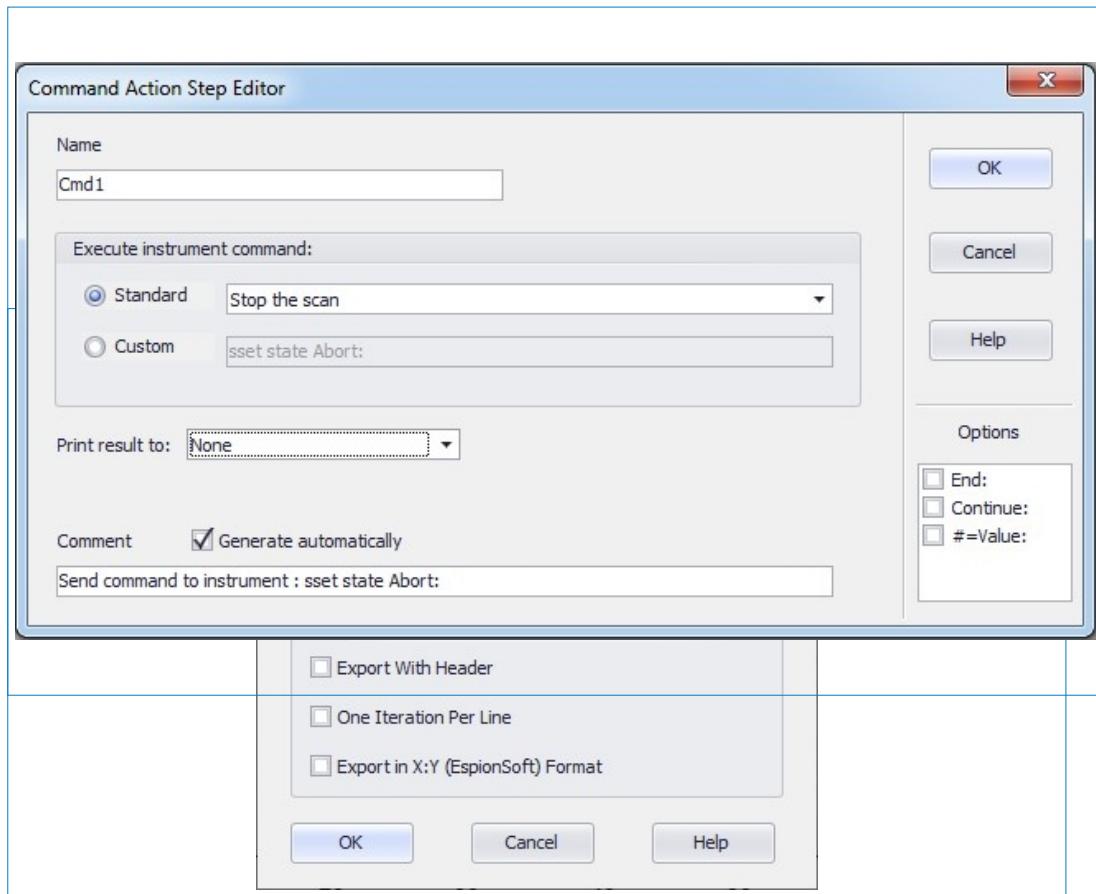
This function should be used under guidance from Hiden Analytical Limited and **with great care, as operation of the IU may be compromised by the use of an inappropriate command.**



The **Command Action** , function, provides access to the IU command language.

The **Command Action Step Editor** is displayed when editing a **Command Action**.

An example of a Command Action is shown below.



Fields **Command Action Step Editor** are:

Name

The name assigned to the Command Action.

Execute instrument command

An IU command may be entered into this box; this is executed when the action executes.

Standard

commands are obtained from the file “msiu commands.txt” in the MASsoft program folder.

Custom commands may be any legal MSIU command.

Print result to

If required, any output generated as a result of the command execution can be directed to an output port using this control. Choose from the pulldown list.

This field depends on the **[STREAMS]** entries in the HIDEN.INI file; if this section is missing the field will be blank.

Options	A list of options supported by the firmware version of the instrument is displayed. Double click on an option to select or deselect it. A selected option is ticked.
End:	The message does not continue. The next message will start on a new line. This option is not required if printing results to None
Continue:	The message continues. The next message follows on the same line as the output from the command.
#=Value	A # character embedded in the message will be replaced with the event's value, using the value's associated device format. Use a Set event to store the value in the Command event. This option can be used to pass a value as an argument to a command.
	For backwards compatibility with old Action Sequences if neither End: nor Continue: are selected then the message continues; the Command event must be followed by a Print Text event which ends the message; failure to end the message will cause MASsoft to crash.
Comment	The comment associated with the Command Action.
	If Generate automatically is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation page](#)

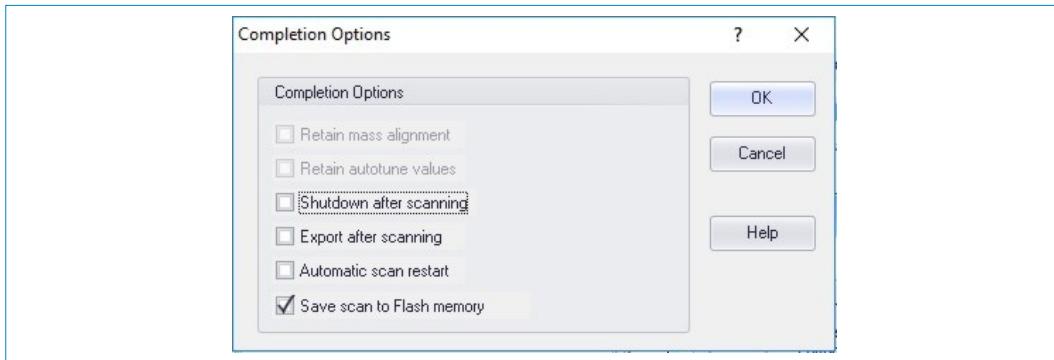
Common dialog items

Many of the dialog box items are common to a number of the scan modes, these items are described in this section. Unique dialog box items are described in the scan mode sections later in this chapter.

View title	The title for the resulting view is entered in this box. The default initially display is made from the instrument type and the WR number, this may be edited by the user.
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Mode	Sets the acquisition mode. This relates to the four operating modes; RGA, negative RGA, positive SIMS and negative SIMS not the scan modes. Depending on the instrument type and its options not all four operating modes may be available. For instance an RC RGA Analyser will only have the one RGA mode available.
Detector	Selects the detector (input device) to be used.
Acquisition range	Sets the acquisition range. The value entered directly is a power of ten; e.g. if -7 is entered, the range set is 10^{-7} .
Auto range	When selected, the analyser automatically changes the range and follows changes in the input signal.
Linear	When selected, the display's Y-axis is linear.
Log	When selected, the display's Y-axis is logarithmic.
Log decades	Sets the number of decades on the log Y-axis. This is grayed out if Linear is selected.
Start mass	Defines the scan start mass in amu.
Stop mass	Defines the scan stop mass in amu.
Auto scale Y-axis	When selected, the Y-axis is forced to fit the largest peak. When not selected, the Y-axis maximum will be set to suit the selected range.
Start scanning	If selected, scanning starts as soon as the OK button is clicked. If this option is not selected, the Tool Bar Go tool (green) can be used to start the scan.
Continuous scanning	Checking this box sets the instrument to scan continuously until it is stopped by the user.
Cycles:	Selects the number of times the scan will repeat until it stops automatically. This is grayed out if Continuous scanning is enabled.
	Click to load a previously saved Easy Scan setup. A standard Windows file open dialog will be displayed.
	Click to save the current Easy Scan setup so that it may be used again. A standard Windows file save dialog will be opened.

Completion options dialog



The Completion options dialog is displayed as a result of double clicking the Stop settings box in a scan tree.

Retain mass alignment

This box is normally grayed out. However, if mass alignment has already been selected, by using the Menu Bar **Instrument, Maintain, Auto mass align** command, the box will be ticked and, at the completion of scanning, the mass alignment information will be returned to the PC and stored to disk. This alignment information will be used until the mass table is cleared or another **Auto mass align** procedure is performed.

Retain autotune values

This box is normally grayed out. However, if autotuning has already been selected, by using the **Scan Editor** dialog box **Scan advanced** button, the box will be ticked and the tuned variable values will be stored in the scan tree global environment at the completion of scanning. They can then be stored in the experiment file and recalled or imported into a local environment later.

Shutdown after scanning

Selecting this option loads the variables from the **Shutdown** environment box into the mass spectrometer when scanning is stopped. This allows, for example, lower or zero ion source filament emission to be set and the SEM detector HT voltages to be reduced, or turned off, when the instrument is not in use.

If this option is not selected, the variables are left in the state they were in when scanning was stopped.

Export after scanning

Selecting this option causes data to be exported at the end of each scan. The file format is defined on **Edit, Preferences, User Options**. Data are exported from the first view attached to the scan tree.

Automatic scan restart	When this option is selected, MASsoft immediately tries to restart any scan stopped by a trip or event sequence. This option is intended for use with process automation controlled by event sequences.
Save scan to Flash memory	This option causes MASsoft to instruct the control unit to save its state information into flash memory when the experiment file has stopped running. This option is greyed out if the control unit does not support it. The default setting is OFF.

Configure Settings for an Instrument connected via a Network

This process required the Works Reference Number and Licence Key as shown on the Licence Certificate provided with the Instrument. If you do not have access to this information then please contact Hiden Analytical

Note: The appearance of the Network options in the Connection Settings dialog box depends upon the model of the Interface Unit. If no options are displayed after selecting Network then the Web Interface can be used to change the default configuration. The following instructions also include the extra steps that might be required

1. Navigate to the Control Tabs and right-click in the Status pane A context-sensitive popup menu will be displayed
2. Click the Add New Instrument... menu item The Instrument Connection Settings dialog box will be displayed
3. In the text box labelled Works Reference Number, type the WR number
4. In the text box labelled Licence Key, type the licence key
5. In the Communication Method drop-down list box, select Network (Ethernet-TCPIP)
6. In the IP Address Assignment drop-down list box, select the appropriate option If a static IP address has been assigned to the Interface Unit then enter the corresponding details
7. Click OK

Alternatively:

1. Click the Instrument->Add New Instrument... item from the MASsoft main menu
2. Continue with the instructions above from where the dialogue box is displayed

The Instrument Connection Settings dialog box will be displayed

Tip:

Use the Windows Device Manager to find more information about the PCs Network Adapters and Serial Ports. To open the Device Manager:

1. Press the Windows Key+R
2. In the text box labelled Open:, type devmgmt.msc
3. Click OK

The Device Manager window will be displayed

See also:

[Status Bar](#)

[Customise the status bar](#)

[Configure settings for an Instrument connected via USB](#)

[Configure settings for an Instrument connected via Serial](#)

[Access the Instrument's Web Interface](#)

Configure Settings for an Instrument connected via Serial

This process required the Works Reference Number and Licence Key as shown on the Licence Certificate provided with the Instrument. If you do not have access to this information then please contact Hiden Analytical

1. Navigate to the Control Tabs and right-click in the Status pane
2. Click the Add New Instrument... menu item
3. In the text box labelled Works Reference Number, type the WR number

A context-sensitive popup menu will be displayed

The Instrument Connection Settings dialog box will be displayed

4. In the text box labelled Licence Key, type the licence key
5. In the Communication Method drop-down list box, select Serial (ASCII)
6. In the list of Serial Ports, select the required port
7. Click OK

Alternatively:

1. Click the Instrument->Add New Instrument... item from the MASSsoft main menu
 2. Continue with the instructions above from where the dialogue box is displayed
- The Instrument Connection Settings dialog box will be displayed

Tip:

Use the Windows Device Manager to find more information about the PCs Network Adapters and Serial Ports. To open the Device Manager:

1. Press the Windows Key+R
 2. In the text box labelled Open:, type devmgmt.msc
 3. Click OK
- The Device Manager window will be displayed

See also:

[Status Tab](#)

[Customise the status bar](#)

[Configure settings for an instrument connected via a Network](#)

[Configure settings for an instrument connected via USB](#)

Configure Settings for an Instrument connected via USB

This process required the Works Reference Number and Licence Key as shown on the Licence Certificate provided with the Instrument. If you do not have access to this information then please contact Hiden Analytical

Note: The appearance of the USB options in the Connection Settings dialog box depends upon the model of the Interface Unit. The USB option may appear as USB (Ethernet-over-USB) or USB (ASCII). In the first instance there are no other properties to configue in MASsoft once USB (Ethernet-over-USB) has been selected. The Web Interface however, will provide some configuration options. The following instructions also include the extra steps associated with selecting a Port for USB (ASCII)

1. Navigate to the Control Tabs and right-click in the Status pane A context-sensitive popup menu will be displayed
2. Click the Add New Instrument... menu item The Instrument Connection Settings dialog box will be displayed
3. In the text box labelled Works Reference Number, type the WR number
4. In the text box labelled Licence Key, type the licence key
5. In the Communication Method drop-down list box, select USB (ASCII)
6. In the list of Serial Ports, select the required port
7. Click OK

Alternatively:

1. Click the Instrument->Add New Instrument... item from the MASsoft main menu The Instrument Connection Settings dialog box will be displayed
2. Continue with the instructions above from where the dialogue box is displayed

Tip:

Use the Windows Device Manager to find more information about the PCs Network Adapters and Serial Ports. To open the Device Manager:

1. Press the Windows Key+R
2. In the text box labelled Open:, type devmgmt.msc
3. Click OK The Device Manager window will be displayed

See also:

[Status Tab](#)

[Customise the status bar](#)

[Configure settings for an Instrument connected via a Network](#)

[Configure settings for an Instrument connected via Serial](#)

[Access the Instrument's Web Interface](#)

Connection settings dialog box

The Connection Settings dialog box is used to specify the method that should be used when attempting to communicate with the Instrument's Interface Unit. It also allows associated properties to be configured, if there are any.

The methods of communication that are available depend on model of Instrument Interface Unit. This information is deduced from the Works Reference (WR) Number of the Interface Unit and the associated Licence Key. A Licence Certificate document containing the WR Number and Licence Key is provided with the Instrument

Works Reference Number	Unique identifier associated with the Instrument's Interface Unit
Licence Key	Text string which encrypts information about the Hiden software that an Instrument can be used with
Communication Method	A list of the supported types of physical connection to the Interface Unit

The appearance of the dialog box and the displayed options may change depending up the Communication Method selected. The actual list will contain only a subset of the following, all methods are included for completeness

Network (Ethernet-TCP/IP)

The preferred communication method. If no properties are displayed and custom settings are required then the Web Interface should be used to specify them

IP Address assignment;

Automatic	Select this option if the Interface Unit should be left to attempt to obtain its IP address automatically from a DHCP server if connected to a network or, if connected directly to the PC, from the PC using APIPA
Static	Select this option if a static IP address has already been assigned to the Interface Unit using the Firmware Upgrade Utility or via a serial connection or if MASsoft itself should attempt to assign a specified IP address to the Interface Unit
Host Name	The unique identifier used to locate the Interface Unit by name on a network
MAC Address	The unique identifier associated with the Interface Unit's Network Adapter
Network Adapter	A list of the PCs installed Network Adapters
Adapter Subnet Mask	The subnet mask associated with the selected PC's Network Adapter
Interface Unit IP Address	The IP address that has already been assigned to the Interface Unit, or that MASsoft should attempt to assign to it.
Port	The number of the port that the Interface Unit listens on in order to accept TCP/IP connections

USB (Ethernet-over-USB)

MASsoft does not provide any properties to configure for this method of communication. If custom settings are required then the Web Interface should be used to specify them.

USB (ASCII)

It is recommended that the Ethernet communication method is used in preference to USB and Serial. Ethernet and USB provide more robust connections than Serial, while only Ethernet is suitable for a production environment.

Serial Ports	A list of the serial ports available on the PC.
Baud Rate	Speed of data transfer. For USB communication this should be 921600. The appropriate speed should be selected automatically.

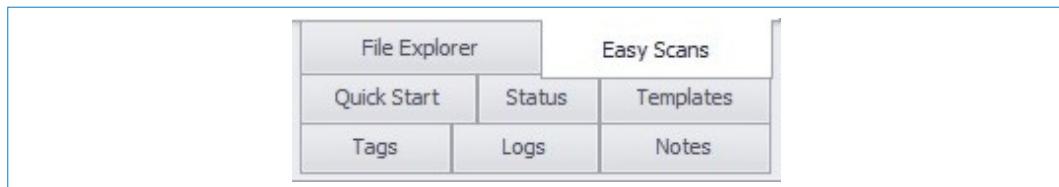
Serial (ASCII)

It is recommended that the Ethernet or, if not available then, USB communication method is used in preference to Serial. Ethernet and USB provide more robust connections than Serial, while only Ethernet is suitable for a production environment.

Serial Ports	A list of the serial ports available on the PC.
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Baud Rate Speed of data transfer. For Serial communication this should be 115200, however previous models of the Interface Unit have used 19200. The appropriate speed should be selected automatically.

Control tabs



In the bottom left of the MASsoft window are the eight Control Tabs the determine what is displayed in the Control Tabs frame.

See also:

[File explorer](#)

[Easy scans](#)

[Quick start tab](#)

[Status tab](#)

[Templates control tab](#)

[Tags](#)

[Logs](#)

[Notes](#)

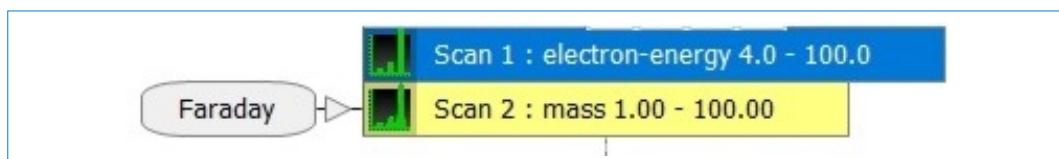
Control unit

In this document the term "control unit" is used to describe the electronics unit controlling the mass spectrometer. The control unit contains various power supplies, input/output circuits, the communications interfaces and microprocessor control board responsible for executing commands from MASsoft and reporting data back to the PC.

Hidden mass spectrometer instruments use one of two types of control unit. The Mass Spectrometer Interface Unit (MSIU) is a 7U high unit which forms part of EQP, EQS, PSM003 and EPIC instruments. The RC Interface is a 2U high unit used in RGA instruments and gas analysis systems such as the HPR20 and QGA. Both units may be either rack or benchtop mounted.

In some Hidden Analytical documentation MSIU is used as a generic term for either the RC Interface or Mass Spectrometer Interface Unit.

Co-varient scan



A co-varient scan sets the output variable in Scan 1 (electron energy in the above case) to its Start value; sets the output variable in **Scan 2** (in this case mass) to its Start value and then reads the input device (Faraday detector). It then steps each output variable by its Increment value and reads the input again (only the bottom scan of the structure allows the Increment to be set; this determines the number of steps for all the scans). This is repeated until both Stop values are reached. If one scan requires fewer steps than the other to reach its Stop value it repeats the measurement at its Stop value; the Stop value is not exceeded.

As many output devices as are required can be scanned in step together.

Note that the co-varient scan has several Scan boxes but only one input device, attached to the scan containing the last output device set. This is because the input is only read when all the outputs have been set.

To create a Co-varient scan click on the appropriate scan box to select it then click the Insert Co-varient Scan button or press **Ctrl+Ins** or right click on the Scan settings box and select **Insert Co-varient** from the pop-up menu.

Customise the Status Bar

To create a Status Bar ;

1. Navigate to the Status pane in the Control Tabs
2. For the required Instrument, right-click the sub-item in the tree labelled Status Bar A context-sensitive popup menu will be displayed
3. Click the Show Status Bar menu item A new Status Bar will appear at the top of the Status pane in the Control Tabs

Alternatively:

1. From the MASsoft main menu - make the required Instrument active by clicking it's name in the Instrument menu
2. Click the Instrument->Show Status Bar menu item A new Status Bar will appear at the top of the Status pane in the Control Tabs

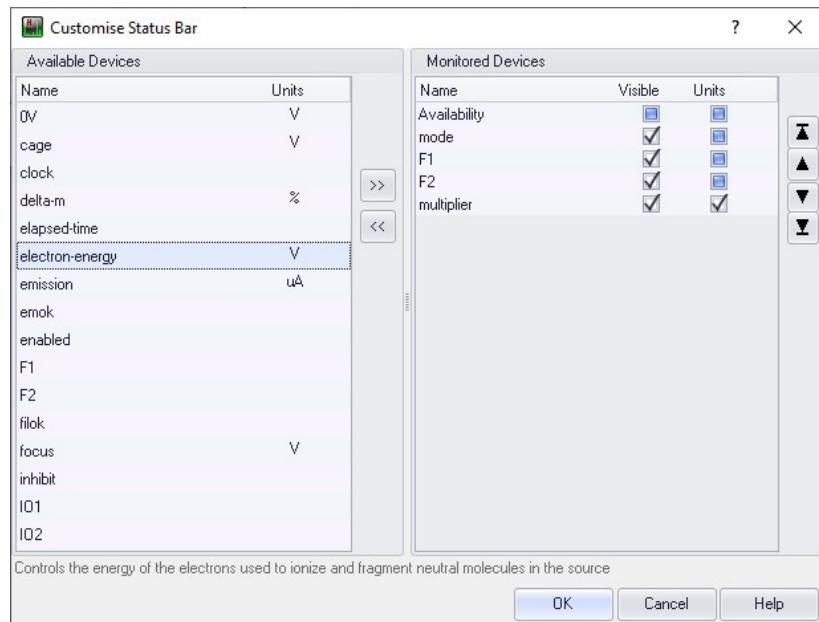
To customise the Status Bar ;

1. Select the Status bar to be customised

2. Right-click the Status Bar
- A context sensitive menu will be displayed
3. Click the Customise... menu item
- The Customise Status Bar dialog box will be displayed

Alternatively:

1. Select the Status bar to be customised
2. From the MASsoft main menu, click the Instrument->Customise Status Bar menu item
- The Customise Status Bar dialog box will be displayed



To Add a device to the status bar ;

1. Select the Status bar to be customised
2. Right-click the Status Bar
- A context sensitive menu will be displayed
3. Click the Customise... menu item
- The Customise Status Bar dialog box will be displayed
4. From the list of Available devices select the device(s) to add

- | | |
|--|---|
| 5. Click >> to add the device(s) to the monitored list | Tick/untick the Units column for a device to show/hide the device units |
| 6. Click Ok | The device(s) will be added to the Status Bar |

Alternatively, double-clicking a device in the Available Devices list will add it to the Monitored list. Drag-and-drop can also be used to move a device from one list to the other.

To Remove a device from the status bar ;

- | | |
|--|---|
| 1. Select the Status bar to be customised | |
| 2. Right-click the Status Bar | A context sensitive menu will be displayed |
| 3. Click the Customise... menu item | The Customise Status Bar dialog box will be displayed |
| 4. From the list of Monitored devices select the device(s) to remove | |
| 5. Click << to remove the device(s) from the monitored list | |
| 6. Click Ok | The device(s) will be removed from the Status Bar |

Alternatively, double-clicking a device in the Monitored Devices list will remove it from the list. Drag-and-drop can also be used to move a device from one list to the other.

Cracking Pattern

When components are ionised in the mass spectrometer ion source the process is likely to result in a number of different ions being produced. For instance nitrogen, atomic weight 14 amu, exists as a diatomic molecule N₂, molecular weight 28amu. Ionisation of nitrogen results in a “parent” N₂

ion at mass 28 plus a peak at mass 14 due to the ionisation of nitrogen atoms following the breaking of the bond (fragmentation) in the nitrogen molecule.

Also appearing in the mass spectrum are peaks due to isotopes. Nitrogen has two isotopes, 14 and 15. Ionisation of a nitrogen molecule consisting of a N14 atom and an N15 atom will result in a peak at mass 29. Fragmentation of such a molecule will result in a mass 14 ion and a mass 15 ion. A nitrogen molecule formed by two N15 atoms accounts for a small peak at mass 30.

Analysis of nitrogen results in a mass spectrum with peaks at 14, 15, 28, 29 and 30. The ratio of the 28, 29 and 30 peaks is solely determined by the ratio of the N14 and N15 isotopes that naturally occur in air and will be very stable. The 14:28 ratio (or 15:29) depends on the ionisation source.

Argon, whose main peak is at mass 40, shows another effect; it has a smaller peak at mass 20, this is due to doubly charged argon, Ar⁺⁺. It is not just the mass that matters but the mass to charge ratio. Argon also exists as an Ar36 isotope, so argon gives peaks at 18, 20, 36 and 40.

Organic, and other more complex molecules, will tend to decompose in the source and produce many fragments.

The problem is that each component in the analysis is unlikely to produce one unique peak by which it can be measured. Peaks from one component are subject to interference by contributions from fragments and minor peaks of other components.

However the minor peaks and fragments can be the solution to the problem; provided that the ratios of the peaks attributed to a component remain stable then it is possible to solve simultaneous equations to work out the contributions from each component. The ratio of minor peaks, expressed with respect to the largest or major peak, is called a “cracking pattern”. To solve the simultaneous equations accurately without “bits being left over” (residuals) the peak ratios must be accurately known for the individual mass spectrometer. This is why calibration is needed. However, before the cracking pattern can be calibrated the software needs to know which masses need measuring. There are two ways to do this:

Import data from the NIST library.

Introduce the sample into the mass spectrometer.

The NIST library contains a complete list of fragments, but the ratios may vary slightly from those produced by a particular quadrupole mass spectrometer (the NIST library is likely to have been determined using a magnetic sector mass spectrometer).

A Bar scan of gas sample introduced into the mass spectrometer can be acquired in MASsoft. Data is copied and pasted into the library where the 20 largest peaks will be included. Some of the peaks, those that are too small, carrier gas peaks or peaks from the mass spectrometer background (water and CO₂ from the filaments) may need to be deleted. The accuracy of the peak ratios is not important at this stage as this will be corrected by the subsequent accurate calibration. At this stage the identification of the peaks to measure is the aim.

See also:

[Library](#)

[Quantitative Analysis](#)

CSV File

With the view selected click **File > Export > Data As** to export the data as a .CSV file.

Bar and Profile views will then prompt the user to select which cycles they would like to export. MID scan views will export all cycles.

Export With Header	If selected include a header block containing the settings used to acquire the data.
One Iteration Per Line	If selected for Bar and Profile scans the first row contains the X values and subsequent rows contain one iteration or cycle of Y values. Each row includes the cycle number, elapsed time at start of the cycle in hh:mm:ss, elapsed time in ms followed by the Y data.
Export in X:Y Format	The data consist of one X:Y pair per line with no header, cycle number or timestamp. The format is suitable for importing to ESPionSoft.

If “One Iteration Per Line” is not selected the first row contains the column headers “cycle”, “time”, “ms”, for the first three columns and the device name and units of the output and input devices e.g. “mass amu”, “Faraday torr” for the X and Y values. For multivariant scans the X values of the parent scans precede the X value of scan with the input device.

Note: For a conventional, sequential, scan tree an “Iteration” is synonymous with a “Cycle”. For a multivariant scan the Iteration is the number of times that the scan has executed – this is product of the number of previous cycles and the number of steps in each of its parent scans plus the total of the all the steps of the parent scan so far this cycle.

Note: For historical reasons the first row of the CSV header contains a value identified as “scans”. This value actually contains the number of rows of data. For MID and, if “One Iteration Per Line” is selected, for Bar and Profile scans this is equal to the number of Cycles (or Iterations). If “One Iteration Per Line” is not selected then for Bar and Profile scans it is equal to the number of lines of data (i.e. the total number of data points).

Bar Scan – No header

Example .CSV

```
"Cycle","Time","ms","mass amu","Faraday mbar"  
0000000001,00:00:05,0000005757, 1.00, 8.02728e-07  
0000000001,00:00:05,0000005757, 2.00, 2.91351e-07  
0000000001,00:00:05,0000005757, 3.00, 4.56874e-10
```

Each line of data consists of 1 data point.

Bar Scan – One Iteration Per Line, with Header

Example .CSV

```
0000000003,scans,0000001432,DataLength  
"header",0000000026,"lines"  
"Date",02/04/2019,"Time",15:05:42  
"ID","HAL RC RGA 201 #16000","Version",4
```

```

"Scans",1
"Scan ID","Mode","Input","Scanned","Start","Stop","Increment","Dwell","Settle","RS","ReISEM"
"Scan 1","RGA","Faraday","mass",1.00,100.00,1.00,100.00%,100.00%,1.000000,1.000000,
"Tags",4
"SavedAs","C:\Users\Documents\Hiden Analytical\MASsoft10\wrl6000\instrument\bar_hd_with_tag.exp"
"SavedBy","doughton"
"SavedOn","24/04/2019"
"SavedTime","13:08:19"
"Environment",
"Global","RGA"
"Fl",1,"( 1 = on, 0 = off )"
"Fr",0,"( 1 = on, 0 = off )"
"cage",3.0,"V"
"curtail-clipping",0,"( 1 = on, 0 = off )"
"delta-m",0,"%"
"electron-energy",70.0,"V"
"emission",1000.000,"uA"
"focus",-90,"V"
"mass",5.50,"amu"
"mode-change-delay",1000,"ms"
"multiplier",0,"V"
"resolution",0,"%"
"Data",100
"Cycle","Time","ms", 1.00, 2.00, 3.00, ... 99.00, 100.00
0000000001,00:00:05.0000005757, 8.02728e-07, 2.91351e-07, 4.56874e-10, ... 3.49374e-10, 2.41874e-10
0000000002,00:00:38.000038192, 7.23715e-07, 2.32979e-07, 3.49374e-10, ... 3.49374e-10, 3.49374e-10
0000000003,00:01:10.0000070627, 6.63650e-07, 2.04303e-07, 2.68749e-10, ... 3.76249e-10, 3.76249e-10

```

Bar Scan – X:Y Format

Example .CSV

```

1.00, 8.02728e-07
2.00, 2.91351e-07
3.00, 4.56874e-10
4.00, 2.68749e-11
5.00, 1.34374e-10
...
98.00, 5.64374e-10
99.00, 3.49374e-10
100.00, 2.41874e-10

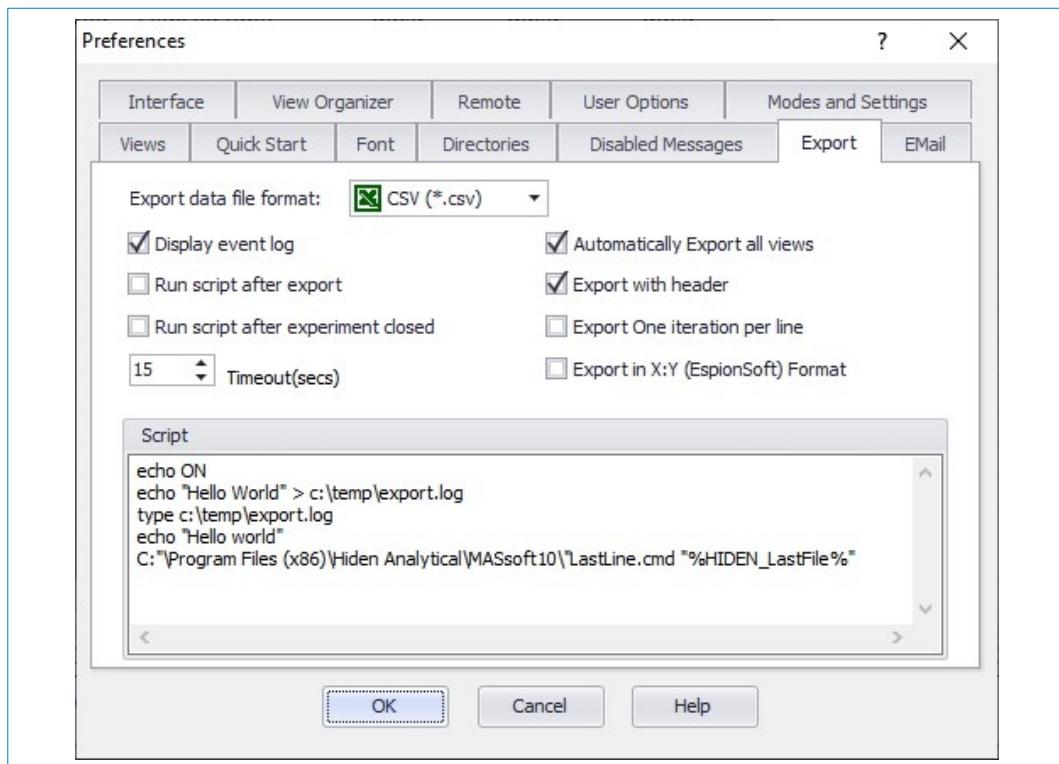
```

Each line of data consists of 1 data point. Only the X & Y values are exported. The file header and the data header line are omitted.

MID Scan

For MID Scans the Cycle Selection dialog is not shown, from MASsoft 10.31 all cycles are exported. This may be subject to change in later versions.

The header is included if the “Export With Header” option is selected in Preferences:



MID Scan - Example .CSV

```
0000000053, scans, 0000000064, DataLength
"header", 0000000023, "lines"
"Date", 02/04/2019, "Time", 15:12:08
"ID", "HAL R0 RGA 201 #16000", "Version", 4
"Scans", 3
"Scan ID", "Mode", "Input", "Scanned", "Start", "Stop", "Increment", "Dwell", "Settle", "RS", "ReISEM"
"Scan 1", "RGA", "Faraday", "mass", 18.00, 18.00, 0.01, 100.000%, 100.000%, 1.000000, 1.000000,
"Scan 2", "RGA", "Faraday", "mass", 28.00, 28.00, 0.01, 100.000%, 100.000%, 1.000000, 1.000000,
"Scan 3", "RGA", "Faraday", "mass", 32.00, 32.00, 0.01, 100.000%, 100.000%, 1.000000, 1.000000,
"Environment",
"Global", "RGA"
"Fl", 1, "( l = on, 0 = off )"
"Fl", 0, "( l = on, 0 = off )"
"cage", 3.0, "V"
"curtail-clipping", 0, "( l = on, 0 = off )"
"delta-m", 0, "%"
"electron-energy", 70.0, "V"
"emission", 1000.000, "uA"
"focus", -90, "V"
"mass", 5.50, "amu"
"mode-change-delay", 1000, "ms"
"multiplier", 0, "V"
"resolution", 0, "s"
"Data", 3
"Time", "ms", "Water", "Nitrogen", "Oxygen",
00:00:00,      531, 2.80789e-06, 7.52498e-07, 1.71999e-07,
00:00:00,      703, 2.79902e-06, 7.42426e-07, 1.68645e-07,
00:00:00,      894, 2.77349e-06, 6.88428e-07, 1.64689e-07,
00:00:05,      5500, 2.62770e-06, 6.89073e-07, 1.67484e-07,
00:00:10,     10105, 2.62634e-06, 6.86171e-07, 1.67377e-07,
00:00:14,     14711, 2.59409e-06, 6.80043e-07, 1.66087e-07,
00:00:19,     19317, 2.55849e-06, 6.73056e-07, 1.64044e-07,
00:00:23,     23923, 2.51415e-06, 6.66498e-07, 1.61034e-07,
```

Each line of data consists of one complete cycle (or iteration) of the all the Trend values from a Graphical Trend View or all the columns from a Tabular view.

Multivariant Scan – One Iteration Per Line, with Header

Example .CSV

```

0000000310,scans,0000002857,DataLength
"header",0000000020,"lines"
"Date",26/10/2017,"Time",12:12:13
"ID","HAL RC RGA 201 #16000","Version",4
"Scans",2
"Scan ID","Mode","Input","Scanned","Start","Stop","Increment","Dwell","Settle","RS","ReISEM"
"Scan 1","RGA","(Scan 2)","Electron-energy",40.0,70.0,1.0,100.000%,100.000%,1.000000,1.000000,
"Scan 2","RGA","Faraday","mass",19.00,21.00,0.01,100.000%,100.000%,1.000000,1.000000,
"Environment",
"Global","RGA"
"Fl",0,"( 1 = on, 0 = off )"
"Fr",1,"( 1 = on, 0 = off )"
"cage",3.0,"V"
"delta-m",0,"%"
"electron-energy",70.0,"V"
"emission",100.0,"uA"
"focus",-90,"V"
"mass",23.00,"amu"
"mode-change-delay",1000,"ms"
"resolution",0,"%"
"Data",201
"Cycle","Time","ms","electron-energy V", 19.00, 19.01, 19.02, ... 20.98, 20.99, 21.00
0000000001,00:00:01,0000001014, 40.0, 0.00000e+00, 1.10499e-08, 0.00000e+00, ... 0.00000e+00, 1.10499e-08, 0.00000e+00
0000000001,00:00:06,0000006555, 41.0, -5.52499e-09, 2.10999e-08, 0.00000e+00, ... 1.10499e-09, 1.10499e-09, 0.00000e+00
0000000001,00:00:12,0000012089, 42.0, -4.08849e-09, 2.32049e-09, -4.08849e-09, ... 8.83999e-10, -1.76799e-09, -4.97249e-09
0000000001,00:00:17,0000017633, 43.0, 0.00000e+00, 1.10499e-11, -3.86749e-11, ... 1.04974e-10, 8.28740e-11, 4.41999e-11
...
0000000001,00:06:22,0000382914, 67.0, 2.20999e-09, -2.20999e-09, -4.08849e-09, ... -5.52499e-10, 4.41999e-10, 3.31499e-10
0000000001,00:06:28,0000388457, 68.0, 2.98349e-09, 4.08849e-09, 6.85099e-09, ... 7.29299e-09, 1.32599e-08, 1.06079e-08
0000000001,00:06:33,0000393992, 69.0, -1.21549e-09, -2.09949e-09, 0.00000e+00, ... 3.53599e-09, 8.39790e-09, 1.43649e-09
0000000001,00:06:39,0000399547, 70.0, -2.32049e-09, 3.31499e-09, -6.62999e-09, ... -5.52499e-10, -3.09399e-09, -4.30949e-09
0000000002,00:06:45,0000405087, 40.0, 1.87849e-09, 4.86199e-09, 1.54699e-09, ... 7.73499e-10, -1.32599e-09, 5.19349e-09
0000000002,00:06:50,0000410621, 41.0, -5.52499e-12, -6.07740e-11, -5.52499e-11, ... -5.52499e-11, 1.65749e-11, -1.10499e-11
0000000002,00:07:03,0000423761, 42.0, 9.39240e-12, -2.51387e-11, 3.86749e-11, ... -2.26524e-11, 3.34262e-11, 6.27080e-11
0000000002,00:07:24,0000444470, 43.0, -4.59679e-12, 2.78459e-12, 1.37240e-11, ... -1.20886e-11, -1.99120e-11, -1.98899e-12
...
0000000002,00:13:55,0000835649, 67.0, 5.85649e-09, 3.86749e-09, 3.86749e-09, ... 2.32049e-09, 8.83999e-10, 2.76249e-09
0000000002,00:14:01,0000841711, 68.0, 3.53599e-09, 3.32049e-09, 1.76799e-09, ... -4.64099e-09, -3.97799e-09, 3.64649e-09
0000000002,00:14:07,0000847246, 69.0, 1.76799e-09, 3.86749e-09, 2.76249e-09, ... 4.86199e-09, 2.76249e-09, 3.97799e-09
0000000002,00:14:12,0000852791, 70.0, -2.09949e-09, 2.09949e-09, 7.40349e-09, ... 6.29849e-09, 4.19899e-09, 7.29299e-09
0000000003,00:14:18,0000858335, 40.0, -2.09949e-09, 2.54149e-09, 9.94490e-10, ... 7.51390e-09, 6.74049e-09, 6.51949e-09
0000000003,00:14:23,0000863872, 41.0, -3.86749e-11, -2.20999e-11, 2.20999e-11, ... 1.65749e-11, 7.18240e-11, 7.18240e-11
0000000003,00:14:37,0000877032, 42.0, 3.48074e-11, -2.73487e-11, -3.81224e-11, ... 4.41999e-11, 2.79012e-11, 6.62999e-12
0000000003,00:14:57,0000897725, 43.0, 2.00004e-11, 2.59232e-11, 2.83100e-11, ... -5.98909e-12, 3.62218e-11, 3.57356e-11
...
0000000003,00:21:29,0001289046, 67.0, 3.03874e-10, 2.65199e-10, 2.48624e-10, ... 5.52499e-12, -1.65749e-11, 5.52499e-12
0000000003,00:21:39,0001299201, 68.0, -2.20999e-10, 2.76249e-09, 1.28179e-08, ... 1.10499e-09, 5.96699e-09, 7.29299e-09
0000000003,00:21:45,0001305262, 69.0, -2.87299e-09, 2.98349e-09, 7.73499e-10, ... -5.30399e-09, -1.43649e-09, -2.20999e-09
0000000003,00:21:50,0001310776, 70.0, 7.51390e-09, 9.06090e-09, 1.11604e-08, ... 6.07749e-09, 3.64649e-09, 7.73490e-09

```

In a multivariant scan the fourth column contains the value of the topmost multivariant scan (in this case Scan 1 – electron-energy 40.0-70.0). Additional columns are added for each level of multivariant scan.

If “One Iteration per Line” is not selected then multivariant scans output in a Z:X:Y format suitable for reading by Origin™.

Layout of MASsoft CSV file

The Header - BAR scan

```

0000000003,scans,0000001432,DataLength
"header",0000000026,"lines"
"Date",02/04/2019,"Time",15:05:42
"ID","HAL RC RGA 201 #16000","Version",4
"Scans",1
"Scan ID","Mode","Input","Scanned","Start","Stop","Increment","Dwell","Settle","RS","ReISEM"
"Scan 1","RGA","Faraday","mass",1.00,100.00,1.00,100.000%,100.000%,1.000000,1.000000,
"Tags",4
"SavedAs","C:\Users\Documents\Hiden Analytical\MASsoft10\wr16000\instrument\bar_hd_with_tag.exp"
"SavedBy","doughton"
"SavedOn","24/04/2019"
"SavedTime","13:08:19"
"Environment",
"Global","RGA"
"Fl",1,"( 1 = on, 0 = off )"
"Fr",0,"( 1 = on, 0 = off )"
"cage",3.0,"V"
"curtail-clipping",0,"( 1 = on, 0 = off )"
"delta-m",0,"%"
"electron-energy",70.0,"V"
"emission",1000.000,"uA"
"focus",-90,"V"
"mass",5.50,"amu"
"mode-change-delay",1000,"ms"
"multiplier",0,"V"
"resolution",0,"%"
"Data",100

```

Start of Data - BAR Scan

```

"Cycle","Time","ms", 1.00, 2.00, 3.00, ... 99.00, 100.00
0000000001,00:00:05,0000005757, 8.02728e-07, 2.91351e-07, 4.56874e-10, ... 3.49374e-10, 2.41874e-10
0000000002,00:00:38,0000038192, 7.23715e-07, 2.32979e-07, 3.49374e-10, ... 3.49374e-10, 3.49374e-10
0000000003,00:01:10,0000070627, 6.63650e-07, 2.04303e-07, 2.68749e-10, ... 3.76249e-10, 3.76249e-10

```

Format of MASsoft CSV file

Line 1:

```
003,scans, 8470,DataLength
```

Is the number of lines of data, 8470 should be the length of a line of data. Each line of data contains the same number of characters (all the data lines are the same length).

Line 2:

```
"header", 24,"lines"
```

Indicates the number of lines in the header.

Line 3:

```
"Date",03/04/01,"Time",15:28:46
```

Is date and time of start of scan, according to the PC's clock.

Line 4:

```
"ID","HAL V RC RGA 301 #10970","Version",4
```

The text following "ID" identifies the MSIU, that following "Version" is the CSV file format version.

Line 5:

```
"Scans",4
```

Indicates the number of scans in the scan tree

Line 6:

```
"Scan ID","Mode","Input","Scanned","Start","Stop","Increment","Dwell","Settle","RS"
","RelSEM"
```

These are the column headings for the data table that follows in the subsequent 4 lines, Scan 1-4.

```
"Scan 1","RGA","Faraday","mass",28.00,28.00,0.01,100.000%,100.000%,1.000000,1.000000,
```

The following lines, one for each scan as indicated in line 5, describe the scan structure.

As this section can have a varying number of lines, depending on the number of scans in the scan tree, the following sections are not at fixed line numbers.

The Scan Section:

```
"Scan 1","RGA","Faraday","mass",28.00,28.00,0.01,100.000%,100.000%,1.000000,1.000000,
```

This contains the values in the Scan Editor and Input Selection dialogues of "Scan 1" in the scan tree. These are more easily understood when aligned with the headings in line 6:

```
"Scan ID",      "Scan 1",
"Mode",        "RGA ",
"Input",       "Faraday",
"Scanned",     "mass",
"Start",       28,
"Stop",        28,
"Increment",   0.01,
"Dwell",       100,
"Settle",      100,
"RS",          1,
"RelSEM",     1,
```

In a typical scan the "Input" will be SEM or Faraday and the "Scanned" device will be mass. When Start = Stop then the scan is a MID scan.

The Tags Section

The Tags line is optional. It is omitted if there are no tags. The value following “Tags” (4) is the number of Tags – the next 4 lines are the tags themselves. Each line consists of

<Tag>,<Value>

```
"Tags",4  
"SavedAs", "C:\User\Documents\HidenAnalytical\MASsoft10\wr16000\instrument\bartag.exp"  
"SavedBy", "doughton"  
"SavedOn", "24/04/2019"  
"SavedTime", "13:08:19"
```

The Environment Section

"Environment", This marks the beginning of the section of the header containing File Settings variables.

First the values for RGA mode are listed: “Global”, “RGA”

This will be followed by the values for other modes, if supported.

If a scan has different scan settings to the file settings then its values will be listed:

```
"Scan",1
```

This marks the beginning of the sub-section of the header containing scan settings variables for Scan 1.

If Scans 2 onward do not have local Scan Settings then these sub-sections are omitted, since they will use the File Settings, which have already been presented.

Each line consists of <variable-name>, <value>, <units> . The number of lines will vary by instrument type.

The Data Section

```
"Data",3
```

This marks the start of the data section. The value 3 indicates that 3 values are being exported.

```
"Cycle", "Time", "ms", "Nitrogen", "Oxygen", "Water",
```

These are the column headings for the data table that follows.

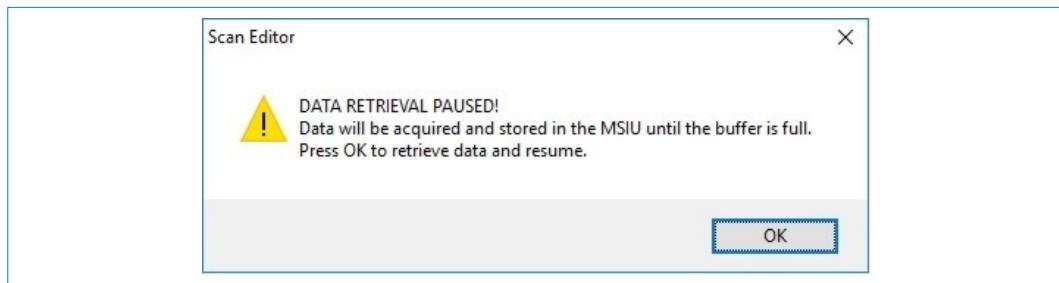
```
00:00:00,247, 170.383,1.15837e-05,3.05532e-06,5.74599e-08,
```

Data table. These values are more easily understood when aligned with the headings in the previous line.

"Cycle",	-	0000000001	-	The Cycle (or Iteration)
"Time",	-	00:00:00	-	Elapsed time in hours:mins:secs
"ms",	-	247,	-	Elapsed time in milliseconds
"Nitrogen",	-	1.15837e-05	-	Partial pressure of Nitrogen
"Oxygen",	-	3.05532e-06	-	Partial pressure of Oxygen
"Water",	-	5.74599e-08,	-	Partial pressure of Water

The elapsed time is given in ms as well as hh:mm:ss because Excel cannot read hh:mm:ss format if seconds are formatted to 3 decimal places.

Data retrieval paused



This message box may be displayed if an MID scan is optimised to scan at high speed.

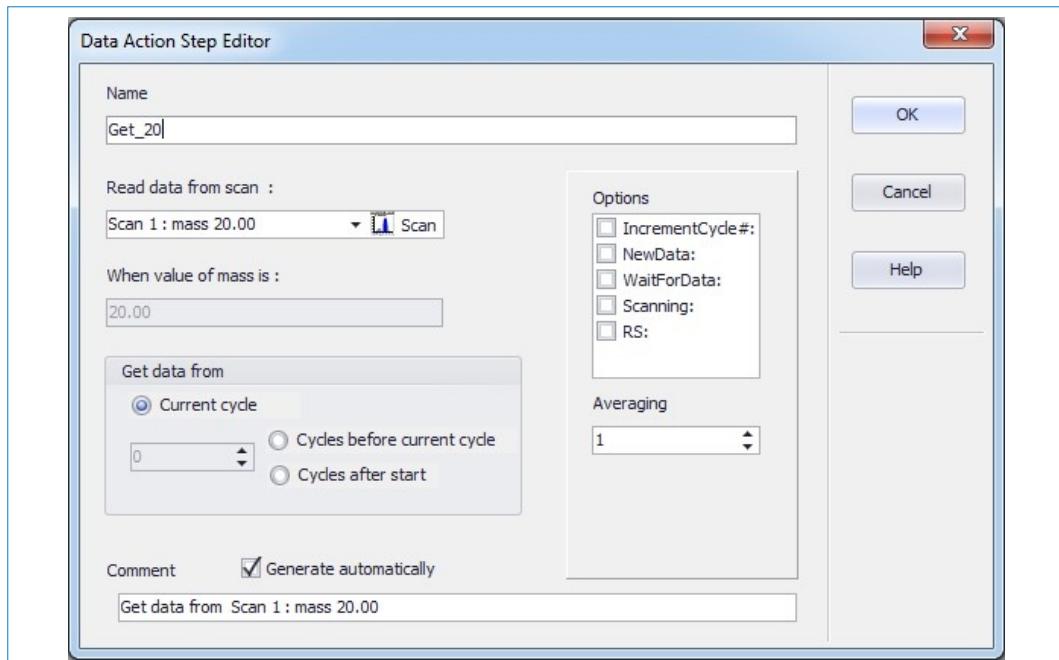
Also see: [MID speed optimisation](#)

Data Action Step Editor

The **Data Action**  , allows data to be read from a scan or another action.

The **Data Action Step Editor** is displayed when editing a **Data Action**.

An example is shown below where the value of the mass 20 peak is being read from a MID scan.



Fields **Data Action Step Editor** are:

Name	The name assigned to the Data Action.
Scan	Read data from scan: The source from where the value is being taken from. A pull down allows you to choose between Scan and Action step .
Action step	The scan which is the source for the data.
When value of mass is:	If the data is being read from a Bar / Profile scan, then this is the value of the mass at which point data is taken.
Get data from	This specifies the cycle number at which to get the data from the scan.
Current cycle	Takes data from the current cycle
Cycles before current cycle and Cycles after start	Selecting either of these options activates the field into which you enter a number of cycles before the current cycle, or after the start of the scan to at which point to take data. For Cycles before current cycle 0 specifies the current, most recent. 1 specifies the previous cycle and so on.
Options	Tick any options you wish to use from the list available
IncrementCycle#	This option is used when the Cycles before current cycle option is selected. When enabled, if Cycles before current cycle is initially 1, after cycle 1 has been read it increments to 2. This can be used to ensure every cycle is processed.
NewData	The Data Action will only process each data point once. If the action sequence loops at a faster rate than the scan, which it probably will, the Data Action will wait until new data is available, pausing the Action Sequence.
WaitForData	Causes the Action Sequence to wait if the required mass has not yet been measured, instead of producing a “No data” error.
Scanning	Checks that the scan has actually started.
RS:	Use an Evaluate Action to divide by the Relative Sensitivity.
Averaging	Calculates the mean over the specified number of values from previous cycles. If the specified number of cycles are not available then all the available cycles are averaged.

Comment	The comment associated with the Data Action. If Generate automatically is selected, the comment is generated by the selections made within the dialog.
----------------	--

See also:

[Automation page](#)

Data Overlay

When displaying a 2D Graphical View of a profile plot an overlay of a previous cycle or iteration of data can be added to the current profile plot data. The overlay appears as a semi-transparent grey watermark image. This can be of the previous cycle or iteration of data when scanning, or of a selected cycle or iteration of data when either viewing historical data or scanning.

The overlay allows you to see how a peak position moves or how the peak height changes over time, or the effect of changing another device value.

The overlay is added (and removed) via the **Overlay Data** submenu of the Bar/Profile plot menu. Options are **Previous Cycle / Iteration**, **Fix Cycle / Iteration** and **Clear Overlay**. If the scan is of a multi-variant type the options are labelled as **Previous Iteration** and **Fix Iteration**, otherwise they are labelled **Previous Cycle** and **Fix Cycle**

Previous Cycle / Iteration

The **Previous Cycle / Iteration** option is only available when scanning. When this option is selected, on the next cycle or iteration after the one that this option was selected, the plot will overlay a ghost image of the previous cycle or iteration of data behind the Graph Cursor. Note that the data ahead of the Graph Cursor by default displays the previous cycle or iteration of data, hence only data before the Graph Cursor will show the watermark image maintaining an image of the previous iterations data.

Fix Cycle / Iteration

When the **Fix Cycle / Iteration** option is selected then the current displayed cycle or iteration of the data is used as the overlay. In historical mode this iteration will be shown as a watermark image when you change iteration using the slider bars, or shown as overlay as new data is collected when scanning.

Selecting the **Fix Cycle / Iteration** again when an iteration has already been fixed will replace the overlay image with that of the current iteration at the next iteration.

Automatic scaling of the plot takes into account the height of the actual data and overlaid data.

Clear Overlay

Removes the data overlay from the plot.

See also:

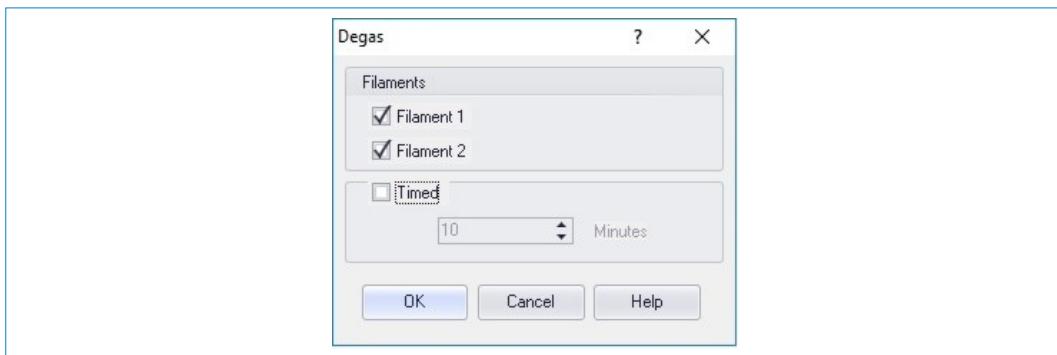
[Bar/Profile plot menu options](#)

[Bar/Profile plot view](#)

Degas

Degassing the ion source involves increasing the emission current and the electron energy. The flood of more energetic electrons and the heating effect can help to remove surface contaminants from the ion source and reduce the background spectrum. To achieve the increase in emission current the filament current is increased. This can reduce the life of the filament so care is needed and protection of the probe from a total pressure gauge is vital.

Open the **Degas** dialog by selecting **Degas** from the **Maintain** sub-menu on the **Instrument** menu.



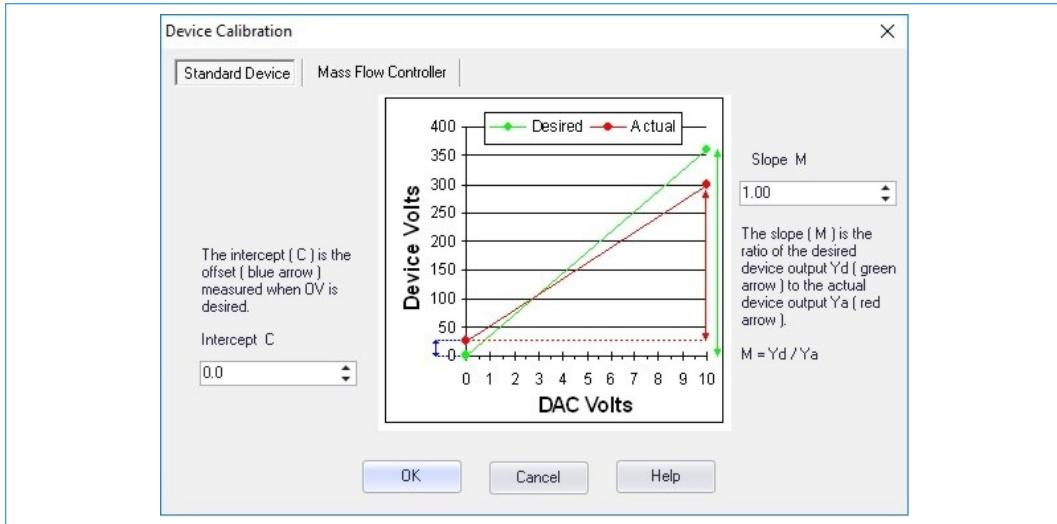
Select either Filament 1 or Filament 2 for degassing. Both filaments can be selected and be degassed together.

Check the Timed option and then set the degas period in minutes.

Scanning cannot be performed whilst degassing.

Device calibration

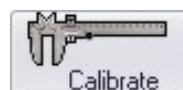
All the mass spectrometer variables are controlled by a digital-to-analogue converter (DAC), which the mass spectrometer's control unit microcomputer loads with suitable values. The physical variable is related to the DAC value by a slope and intercept, which may be altered to calibrate the variable. This dialog allows these values to be adjusted where necessary.



The diagram in the **Device Calibration** dialog is for illustration only.

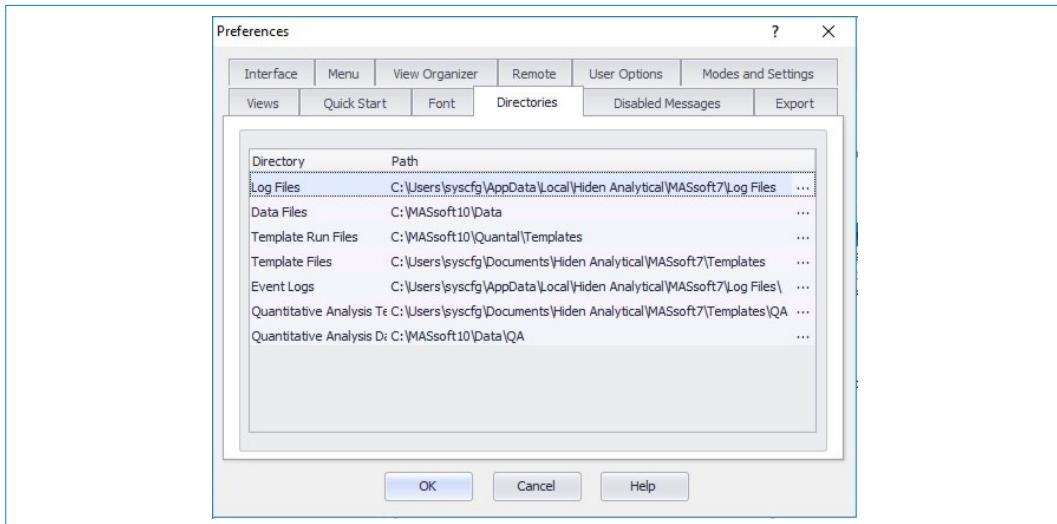
The **Device Calibration** dialog is opened by selecting **Edit Instrument Environment...** on

the **Instrument** menu, selecting an item then clicking the **Calibrate** button and selecting the **Standard Device** tab.



Also see: [Mass flow controller](#)

Directories

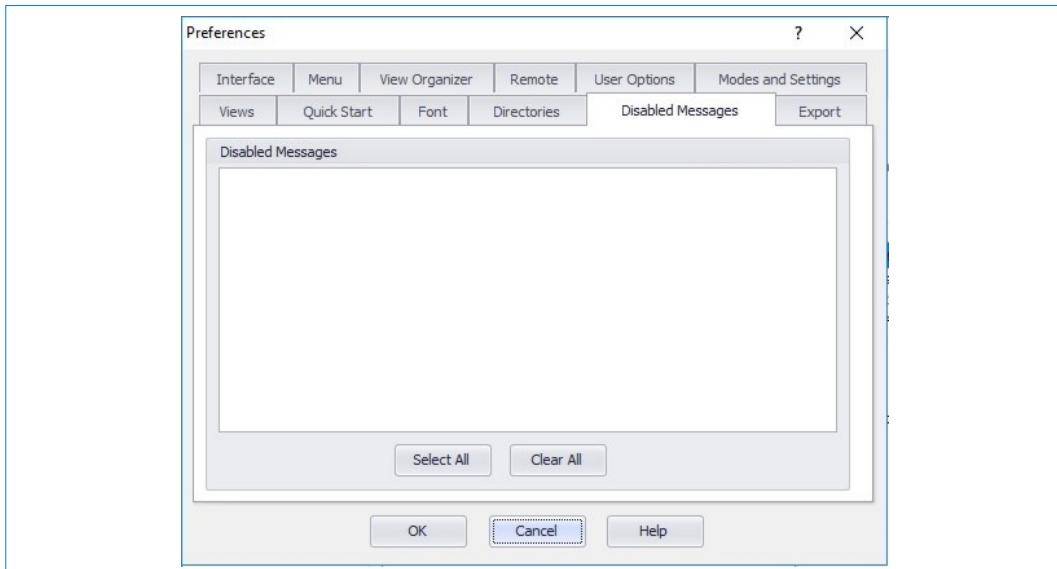


To view the Directories preferences select **Preferences..** on the **Edit** menu then select the **Directories** tab.

The **Directories** tab allows the location of log files, data files and template files to be specified.

Click on the button to the right of the Path to change the location.

Disabled messages

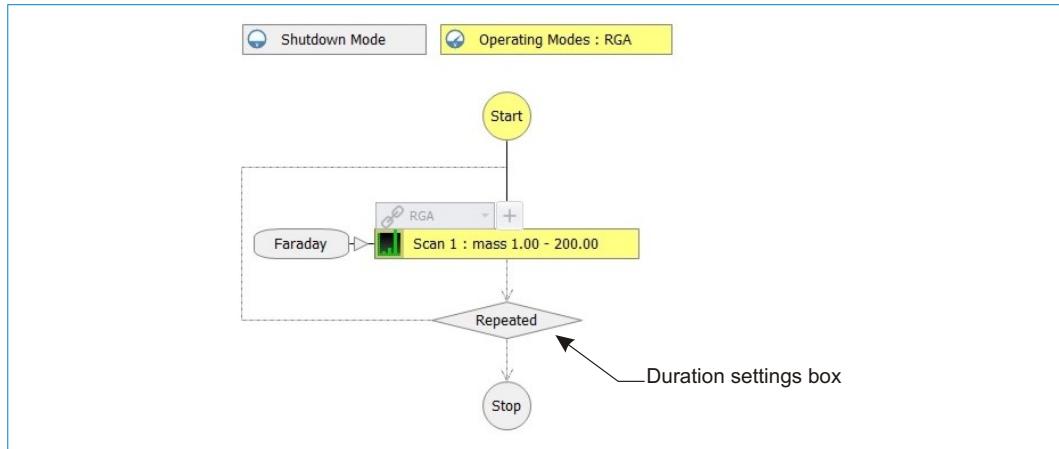


To view the Disable Messages preferences select **Preferences..** on the **Edit** menu then select the **Disabled Messages** tab.

The **Disabled Messages** tab allows the user to choose whether certain messages are displayed.

Some error message boxes have a "**Don't show this message again**" option. If this is selected the message box is added to the list displayed in this tab.

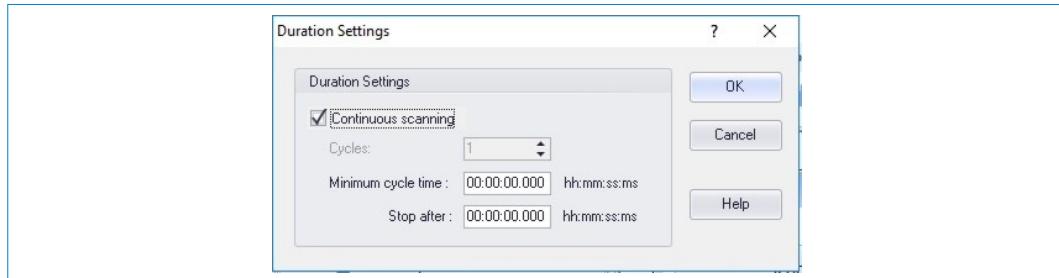
Duration settings box



The Duration settings box holds the settings which define for how long the experiment will run. These values may be adjusted by double-clicking on the Duration settings box, which opens the Duration Settings dialog.

See also: [Duration settings dialog](#)

Duration settings dialog



Continuous scanning

When this box is checked, the scan tree is executed continuously until stopped by the user.

Cycles

The number of cycles for which the scan tree is to be executed is entered in this box; the box is grayed out if the Continuous scanning box is selected.

Minimum cycle time	The time between execution of scan tree cycles can be entered in hours:min:sec. Multiple cycles repeat as fast as possible if this value is set to zero (default), but, if a value is entered which is longer than the time required to complete one cycle of the scan tree, scanning pauses until the set time has expired before a new cycle is started.
Stop after	The scan tree is executed for the time defined in this box.

Dwell and settle times

The three tables below show the settle and dwell times used with control units fitted with the HAL 7 micro board.

In the tables the double line indicates the change from the low gain amplifier to the high gain amplifier.

The switching times between the Faraday and Electron Multiplier detectors are reduced for the HAL 7 micro board.

Low gain SEM to high gain Faraday 9.4s

High gain SEM to high gain Faraday 6.4s

These times were 16.4s and 13.4s for previous versions of micro board.

Mode	MID & BAR		Profile		
	Range (Torr)	Settle (ms)	Dwell (ms)	Settle (ms)	Step (ms)
10^{-5}	5	25	5	4	10
10^{-6}	5	16	5	4	10
10^{-7}	150	10	150	40	10
10^{-8}	250	160	250	80	40
10^{-9}	300	640	300	40	160
10^{-10}	400	2750	400	10	640

Faraday detector settle and dwell times

Mode	MID & BAR		Profile		
Range (Torr)	Settle (ms)	Dwell (ms)	Settle (ms)	Step (ms)	Dwell (ms)
10^{-7}	5	10	5	4	10
10^{-8}	5	25	5	4	10
10^{-9}	5	16	5	4	10
10^{-10}	150	160	150	10	40
10^{-11}	250	1600	250	10	400
10^{-12}	300	1600	300	10	400
10^{-13}	400	2750	400	10	800

SCEM detector settle and dwell times

Mode	MID & BAR		Profile		
Range (Torr)	Settle (ms)	Dwell (ms)	Settle (ms)	Step (ms)	Dwell (ms)
10^{-7}	5	25	5	4	10
10^{-8}	5	16	5	4	10
10^{-9}	150	16	150	40	10
10^{-10}	250	160	250	10	40
10^{-11}	300	1600	300	10	400
10^{-12}	400	2750	400	10	800

Channel plate detector settle and dwell times

Dwell time

Dwell time is the time the instrument spends acquiring a single measurement.

The longer the dwell time the more stable the measurement as it is less likely to be affected by noise. But high dwell times lead to slower data acquisition speeds. Reducing the dwell time will increase scan speed at the expense of accuracy.

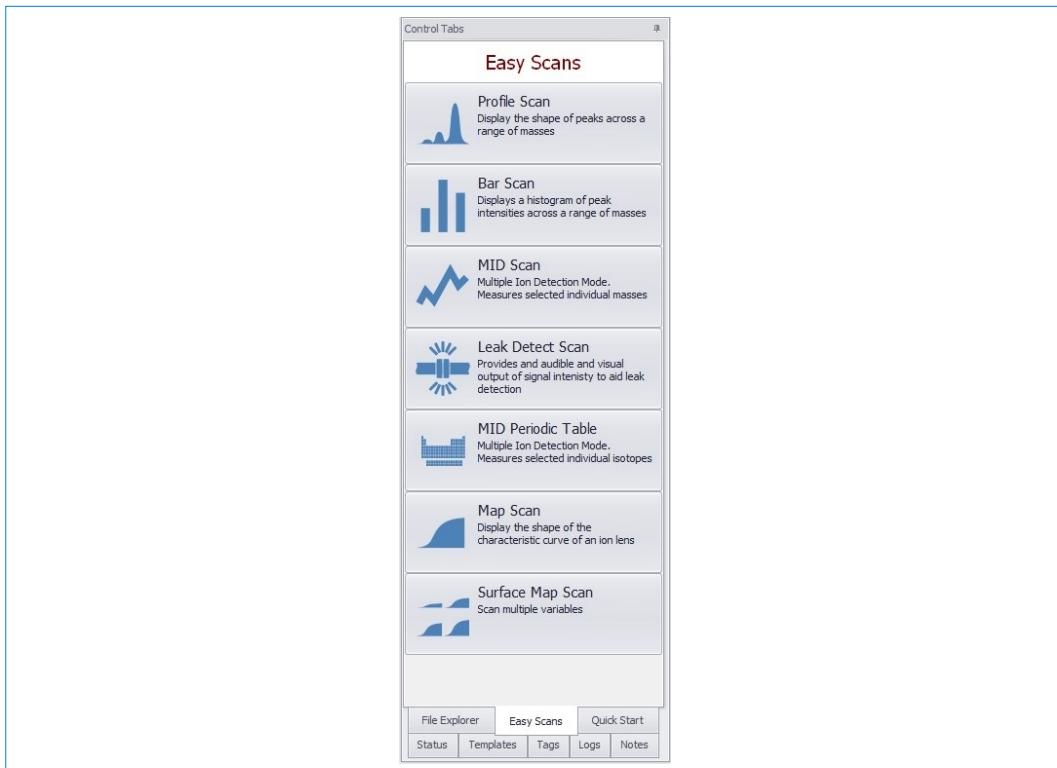
See also: [Dwell and settle times](#)

Easy scans

The Easy Scan buttons are displayed in the Control Tabs frame when the **Easy Scans** tab is selected.

Easy Scans provide a quick and easy way to setup scans. To create a specific scan type, click on the required button and the corresponding scan creation dialog will be displayed. Use the dialog to customise the scan, click the **OK** button, MASsoft will create the appropriate scan tree in a new scan tree window as well as any additional view windows. Each scan creation dialog remembers the settings that were last used.

The buttons which are displayed depend on what instrument is connected. If MASsoft does not have any instruments interrogated then all options will be disabled.



If an interrogated instrument is connected the following Easy Scans are always displayed.

Profile Scan, Bar Scan, MID Scan and Leak Detect Scan.

The **MID Periodic Table, Map Scan** and **Surface Map Scan** are not available for all instrument types.

See also:

[Bar Mode dialog](#)

[Profile Mode dialog](#)

[MID Mode dialog](#)

[Leak Detect Mode dialog](#)

[MID Periodic Table](#)

[Map Scan](#)

[Surface Map Scan](#)

There are many common items used in the various scan creation dialogs.

See also: [Common dialog items](#)

Edit File Settings dialog - Operating Mode

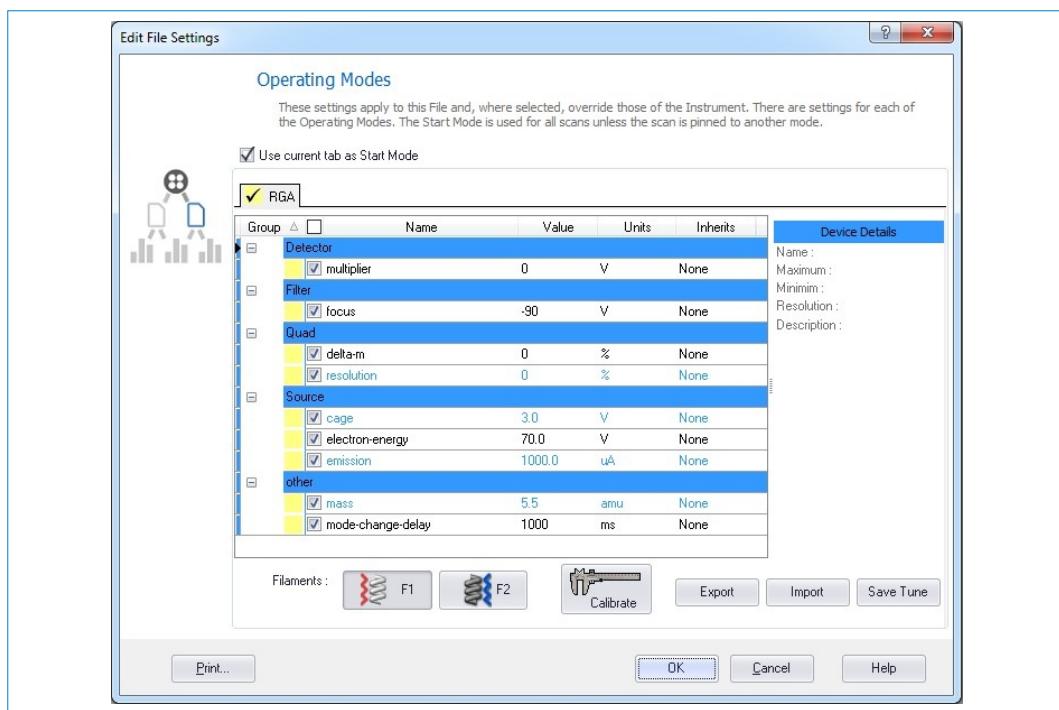
In previous versions of MASsoft the File Settings were called the Global Environment.

The file settings encompass the variable values of all the acquisition modes. The file settings for each operating mode contain the current device values for that mode. These device values are used whenever that operating mode is selected for a scan, unless overridden by the scan settings associated with that particular scan.

The device values for each type of acquisition mode can be edited in the Edit File Settings Operating Modes dialog.

In the MASsoft settings hierarchy the File Settings are overridden by Scan Settings but override Instrument Settings.

To open the File Settings Operating Modes dialog double-click on the **Operating Modes** box in the scan tree.



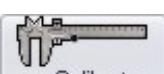
The dialog will contain a tab for each available operating mode. In the figure above there is just the **RGA mode** tab which is typical for an RC-RGA instrument.

Each mode has a different set of device settings, therefore the values displayed in the device table will change when a different tab is selected.

When the **Use current tab as Start Mode** box is ticked, the mode of the currently selected tab is used as the start mode. The **Start Mode** is used by default for all scans which have not had a specific mode assigned to them (the scan will have the icon displayed before the mode name in the Scan Canvas).

Column headings

Group	Values may be grouped by function. Each group contains devices with a related function. This column cannot be edited.
	Also see: Modes and settings
Checkbox	<p>The check box column determines whether the device values should be taken from those entered in this dialog or inherited from the Instrument environment settings.</p> <p>The check box in the header of this column allows all the device values in the table to be checked on (all values here override the Instrument values), or checked off (all values to are inherited from the Instrument values).</p> <p>Selected values are NOT over-written when a scan's File Settings are copied to the Instrument at the end of a scan.</p> <p>Also see Copy current settings to Instrument Settings at end of scan in Modes and settings.</p> <p>A tick does NOT mean that the value will be always be used as the value may be overridden by the value in the Scan Settings.</p>
Name	The name of the device. This is cannot be edited.
Value	Shows the current value of the selected variable. The value may be edited.
Units	The units of the value. This is cannot be edited.
Inherits	The Inherits column will set as None , when a device is checked on (✓) using the value entered in this dialog. It will be set as Instrument showing the value has been inherited from the Instrument environment settings when check box is off.
Additional Information	
Additional information about the currently selected device is shown in the right hand panel.	
Minimum	The minimum allowable value for the currently-selected device; this cannot be edited.
Maximum	The maximum allowable value for the currently-selected device; this cannot be edited.
Resolution	The minimum allowable increment value for the currently-selected device; this cannot be edited.
Description	A brief description of the currently-selected device.

Export	The Export button exports the device values of the currently displayed mode tab to a mode file (default extension “.mde”). A default name is created for the file, which can be edited. The state of the check box column (whether the value overrides the instrument setting) is saved in the mode file. This option is only visible when using the Advanced user interface preference.
Import	Import allows the values saved within a mode file to be imported. These values can be imported into chosen modes of this dialog. When this button is pressed first a previously exported mode file (.mde) must be opened. All the devices found in this file must match all the devices (and units) displayed in the device table. You will be warned if you attempt to open a file containing conflicting devices. On successfully opening the file you will be presented with the Import Mode dialog. The state of the check box column (whether the value overrides the instrument setting) is restored from the mode file. If a value is edited in the Import Mode dialog the override check box will be enabled. This option is only visible when using the Advanced user interface preference.
Save Tune	Saves a Tune file (which contains device values for all the modes). This may be done after carrying out the export and import procedure to create a tuned environment for all the modes. This option is only visible when using the Advanced user interface preference.
Print...	Prints the device values in the device table via a Print Preview screen.
F1 Button	Selects Filament 1 in the RGA mode. 
F2 Button	Selects Filament 2 in the RGA mode. 
Calibration Button	Displays the Device Calibration dialog. Allows the actual output of the device to be adjusted for better correspondence with the device value.  Also see: Device calibration

Cancel Button

Cancel

The Cancel button is disabled when the instrument is scanning. When not scanning Cancel returns the values in place when the **Edit File Settings Dialog - Operating Modes** was opened.

See also:

[Import Mode dialog](#)

Edit File Settings dialog - Shutdown Mode

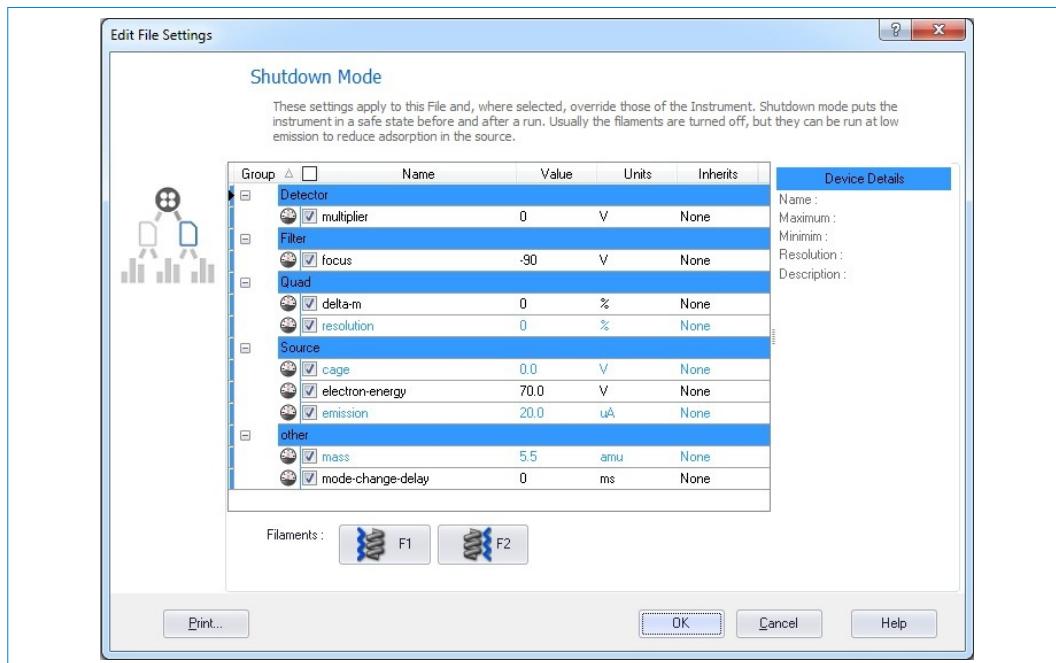
CAUTION

Ensure that the filaments are not inadvertently turned on in the Shutdown mode. In the Shutdown Mode dialog the Filament buttons reflect the state the filaments would have if the instrument was in the Shutdown state, not the current state of the filaments. If a filament is selected in the Shutdown Mode dialog, when the instrument next switches to the Shutdown state (at the end of a scan), the filament will be on.

The Shutdown environment contains a set of device values that are appropriate for the instrument when it is not in use. For example, when not in use for short periods, it makes sense to keep the instrument powered-up but to switch off the filaments; this saves energy and prolongs the equipment life.

The device values for the Shutdown Settings are edited in the **Shutdown Mode** dialog.

The Shutdown Settings are stored in the Experiment file.



The scan tree Shutdown settings box holds the settings for the Shutdown mode. These values may be adjusted by double-clicking the **Shutdown** settings box, which opens the Shutdown Mode Edit File Settings dialog.

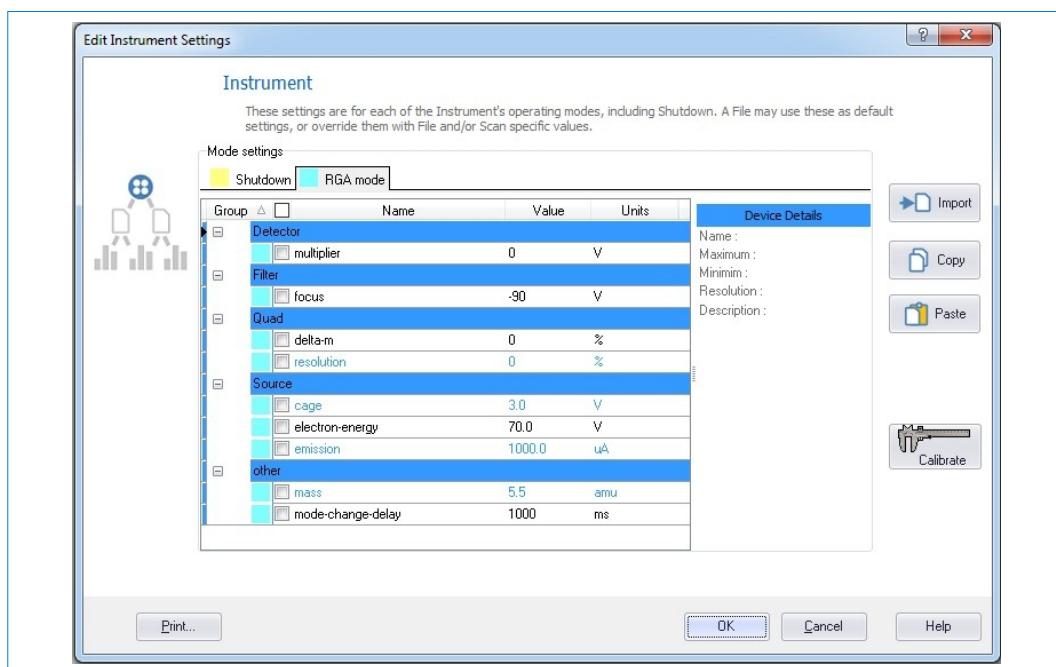
Group	Values may be grouped by function. Each group contains devices with a related function. This column cannot be edited.
Checkbox	<p>The check box column determines whether the device values should be taken from those entered in this dialog or inherited from the Instrument environment settings.</p> <p>The check box in the header of this column allows all the device values in the table to be checked on (all values here override the Instrument values), or checked off (all values to are inherited from the Instrument values).</p>
Name	The name of the device. Name cannot be edited.
Value	<p>Shows the current value of the selected variable. If the Use column is ticked (✓) the Shutdown Environment value will be displayed. If the Use column is not ticked the Instrument Environment value will be displayed. The Value may be edited.</p> <p>As soon as a value is edited the Use column is ticked.</p>
Units	The units of the value. Units cannot be edited.
Inherits	The Inherits column will set as None , when a device is checked on (✓) using the value entered in this dialog. It will be set as Instrument showing the value has been inherited from the instrument environment settings when check box is off.
Additional information about the currently selected device is shown in the right hand panel.	
Minimum	The minimum allowable value for the currently-selected device; this cannot be edited.
Maximum	The maximum allowable value for the currently-selected device; this cannot be edited.
Resolution	The minimum allowable increment value for the currently-selected device; this cannot be edited.
Description	A brief description of the currently-selected device.
Filament buttons	The filament buttons show the state of the filaments <u>in the environment</u> and allow them to be turned on or off by clicking the appropriate button. A filament is shown red when switched on and blue when switched off.
Print...	Prints the device values in the device table via a Print Preview screen.

Cancel button

The Cancel button is disabled when the instrument is scanning. When not scanning Cancel returns the values in place when the **Edit File Settings - Shutdown** was opened.

Edit Instrument Settings dialog

The Edit Instrument Settings dialog is displayed as a result of selecting **Edit Instrument Environment...** on the **Instrument** menu.



The Edit Instrument Settings dialog will contain a **Shutdown** tab and one tab for each available operating mode. In the figure above there is just the **RGA mode** tab which is typical for an RC-RGA instrument.

Column headings

Group

Values may be grouped by function. Each group contains devices with a related function. This column cannot be edited.

Also see: [Modes and settings](#)

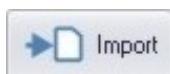
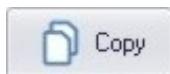
Checkbox	If the checkbox for the device is ticked (✓) this indicates that the value should be taken from the Instrument Settings in new files. When ticked the equivalent field in the File Settings dialog is not ticked by default on File New Ticked values are NOT over-written when a scan's File Settings are copied to the Instrument at the end of a scan. Also see Copy current settings to Instrument Settings at end of scan in Modes and settings . A tick does NOT mean that the value will be always be used, as the value can be overridden by a tick in the File Settings .
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Name	The name of the device. This is cannot be edited.
Value	Shows the current value of the selected variable. The value may be edited.
Units	The units of the value. This is cannot be edited.

Additional Information

Additional information about the currently selected device is shown in the right hand panel.

Minimum	The minimum allowable value for the currently-selected device; this cannot be edited.
Maximum	The maximum allowable value for the currently-selected device; this cannot be edited.
Resolution	The minimum allowable increment value for the currently-selected device; this cannot be edited.
Description	A brief description of the currently-selected device.

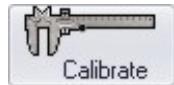
Import Button	 Import	Imports settings from a .tun file. This button is disabled when the instrument is scanning.
Copy Button	 Copy	Copy values so they may be put into other settings using the Paste button.

Paste Button

Pastes values into the Instrument settings that have been copied from other settings. This button is disabled when the instrument is scanning.

Clicking the Paste button opens a dialog in which clicking the **OK** button will Paste values that have **Use** selected, clicking the **All** button will Paste all values.

All should only be used when pasting from another Instrument settings because the significance of the **Use** option is different in the Instrument settings.

Calibration Button

Displays the **Device Calibration** dialog. Allows the actual output of the device to be adjusted for better correspondence with the device value.

Also see: [Device calibration](#)

Print...

Prints the device values in the device table via a **Print Preview** screen.

Cancel Button

The Cancel button is disabled when the instrument is scanning. When not scanning Cancel returns the values in place when the **Instrument Environment Editor** was opened.

Edit menu

Below are the menu items found on the Edit menu.

Edit...

Selecting the **Edit...** menu item will open a dialog defined by the currently selected element in the scan tree.

Insert Co-variant

Adds a co-variant scan to the currently-selected scan. This command is grayed out if no scan tree window is active.

The **Co-variant scan** command may be used to create “co-variant” scans in which several variables can change in step with each other. Where the optimum value of a control voltage changes with the mass (or other variable) being scanned, co-variant scanning can be used to change the tuning as the mass changes, or where an external voltage must be varied synchronously with the scanned mass, it can be controlled by a co-variant scan.

To attach a co-variant scan, first select the **Scan** in the scan tree, by clicking on it, and then clicking **Co-variant** on the **Edit** menu.

Insert	Adds a multi-variant scan to the currently-selected scan.
Multi-variant	This command is grayed out if no scan tree window is active. The Multi-variant scan command is used to create “multi-variant” scans in which a scan generator is linked to one or more subordinates. Here, the master scan control voltage is altered stepwise and, at each step, the complete subordinate scan set is performed. This can be used to optimise a variable, look at peak shape and size over a range of variable values, or it can be used for multi-dimensional mapping. To append a subordinate scan, first select the master scan in the scan tree, by clicking on it, and then click Multi-variant scan on the Edit menu.
Insert Sequence	Creates the next scan in sequence. This command is grayed out if no scan tree window is active. The Insert new Sequence command creates the next scan in the scan tree. Scans in the sequence may be of any type, so, for example, a histogram scan may be followed by MID-type single-mass scans which may be followed by a peak profile scan of a particular mass. Sequences of co-variant or multi-variant scans may be created, or a multi-variant scan may execute a scan sequence. To append a new scan, first select the previous scan in the scan tree, by clicking on it, and then click Insert new Sequence on the Edit menu.
Scan setting	Select Attach to attach Scan settings to the selected scan. The Scan settings will override the File setting for the selected scan. Select Detach to remove the Scan settings from the selected scan. Once the Scan settings have been attached to the scan they can be changed by selecting Edit . Scan setting can be copied and pasted between scans. See also: Scan settings
Cut	May be used when editing Scans, Environments, Events and Trips.
Copy	May be used when editing Scans, Environments, Events and Trips. Copies data to the clipboard for use in DDE client-compatible applications through paste-linking. The data copied is defined by the File , Export , DDE command prior to using Copy . Copy is grayed out if no view is selected. Copy may be used when editing Events and Trips.

Paste	May be used when editing Scans, Environments, Events and Trips.
Delete	Deletes a scan, trip or an environment. This command is grayed out if no scan tree window is active.
Select All	Selects all the scans in the scan tree. Scans will be highlighted when selected.
Library...	A library is a database of cracking patterns for reference compounds. A default RGA library is supplied as part of MASsoft. Selecting Library... opened the Library dialog. See also: Library
Calibration bottles...	Opens the Calibration bottle editor dialog box; this provides an interface for maintaining the library of calibration and check gas bottles that are required for calibration of the optional Quantitative Analysis module. See also: Calibrate Bottle Editor
Preferences...	The overall configuration of MASsoft can be controlled from the Preferences dialog opened by clicking Edit on the Preferences menu. See also: Preferences
Recent Toolbars	Returns the Toolbars to their default state.

This topic is not fully described in this version of the manual. Please contact Hiden Analytical for a manual update.

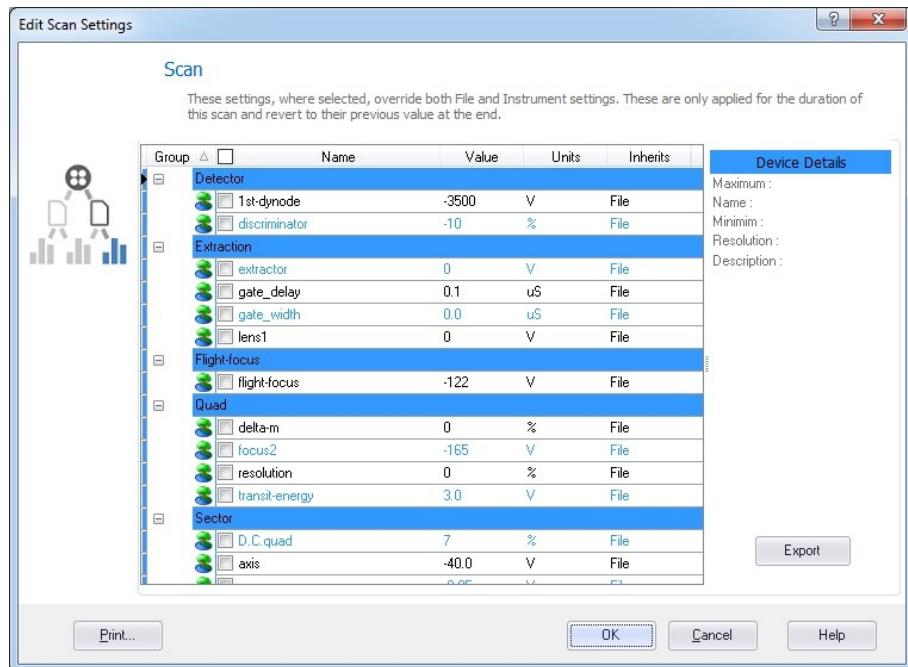
Edit Scan Settings dialog

In previous versions of MASsoft the Scan Settings were referred to as the Local Environment.

Scan settings can be created for any individual scan. The scan settings override the file settings for that scan's selected acquisition mode.

In the MASsoft settings hierarchy the Scan Settings override both the File Settings and the Instrument Settings.

The scan settings can be edited in the Edit Scan Settings Scan dialog.



Column headings

Group	Values may be grouped by function. Each group contains devices with a related function. This column cannot be edited.
Checkbox	The check box column determines whether the device values should be taken from those entered in this dialog or inherited. They may be inherited from either the File or Instrument environment settings.
	The check box in the header of this column allows all the device values in the table to be checked on (all values here override inherited values), or checked off (all values to are inherited from the File or Instrument values).
Name	The name of the device. This is cannot be edited.
Value	Shows the current value of the selected variable. The value may be edited.
Units	The units of the value. This is cannot be edited
Inherits	The Inherits column will set as None , when a device is checked on (✓) using the value entered in this dialog. It will be set as File showing the value has been inherited from the File environment settings when check box is off, and is checked on in the Operating Modes. Otherwise if checked off in the Operating Modes then the value inherits from the Instrument .

Additional Information

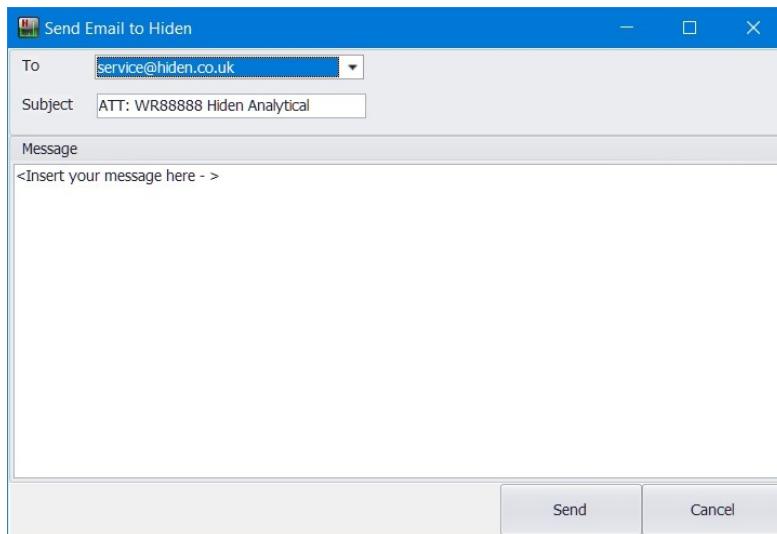
Additional information about the currently selected device is shown in the right hand panel.

Minimum	The minimum allowable value for the currently-selected device; this cannot be edited.
Maximum	The maximum allowable value for the currently-selected device; this cannot be edited.
Resolution	The minimum allowable increment value for the currently-selected device; this cannot be edited.
Description	A brief description of the currently-selected device.
Export	The Export button exports the device values to a mode file (default extension “.mde”). A default name is created for the file, which can be edited. This option is only visible when using the Advanced user interface preference.
Print...	Prints the device values in the device table via a Print Preview screen.
Cancel Button	The Cancel button is disabled when the instrument is scanning. When not scanning Cancel returns the values in place when the Edit Scan Settings dialog was opened

Emailing Files

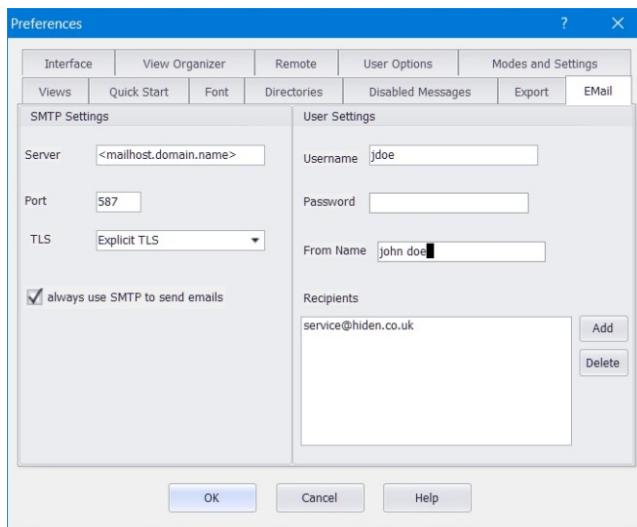
This is performed by selecting the **Send File(s) to email client** from the **File** menu.

This will cause a file select dialog box to open and once you have selected the file(s) the following form is then displayed:



To	This control is populated from the email addresses specified in the Recipients control in the Email tab located in the preferences.
Subject	This is automatically generated and will consist of the WR of the MSIU and your company name (if specified). This can be edited but we recommend that, if emailing files to Hiden Analytical, that you leave this information as it is.
Message	Allows you to construct a message for the recipient
Cancel	Abandon the attempt to send emails
Send	Will either cause your default email client to open with a new email message ready to be sent (with the above information filled in) OR attempt to send the email via the SMTP settings specified (in the Mail tab in preferences dialog)

Email Preferences



To view the EMail preferences select **Preferences...** on the **Edit** menu then select the **EMail** tab.

These settings are required to allow MASsoft to connect to an email server and send the email.

Column headings

SMTP Settings

Server	Outgoing mail server (for example, “smtp.example.com”).
Port	Port upon which the Server is listening on. (example port 587).
TLS	Security setting for the connection with the server (for example, “STARTTLS” or “SSL/TLS” and whether or not to use secure authentication)
always use SMTP to send emails	This checkbox instructs MASsoft to not use the default email program to send emails. MASsoft will always attempt to use this first and when this fails will attempt to use SMTP to transmit the files. However certain email clients do not always work (Outlook) and so setting this option allows MASsoft to skip the attempt and always use SMTP.

User Settings

Username	This is the name of the email account (for example, if your email address is johnDoe@gmail.com, then your user name is “johnDoe”).
-----------------	--

Password	This is the password of the email account. If this is left blank MASsoft will prompt you for a password when you first attempt to email files. (note for security reasons this will NOT be stored on the PC and will need to be re-entered every time MASsoft is started).
From Name	The name that will appear in the ‘From’ field
Recipients	Contact Email addresses from which you can select to email files to. Note, service@hiden.co.uk is automatically added and cannot be deleted.

If you require further guidance about the settings that apply to you then please contact your email administrator.

See also:

[Emailing](#)

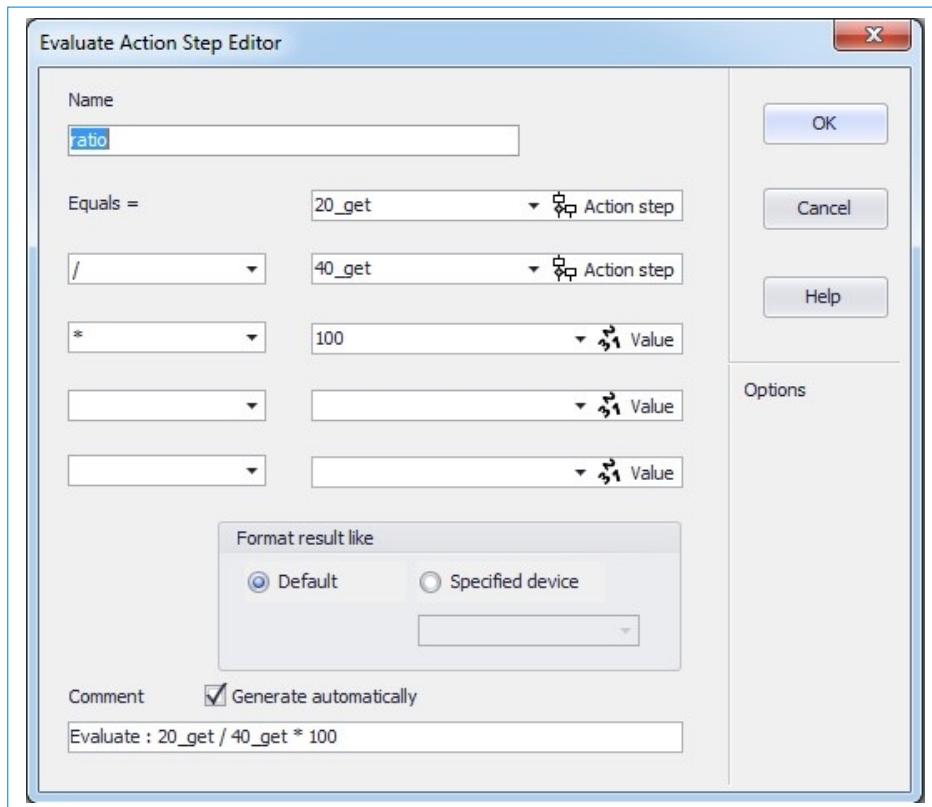
Evaluate Action Editor



The **Evaluate Action** , can be used to perform calculations.

The **Evaluate Action Step Editor** is displayed when editing an **Evaluate Action**.

The Evaluate Action calculates from top to bottom as displayed in the editor with no operator precedence. An example is shown below where the value returned from the 20_get **Data Action** is divided by the value returned from the 40_get **Data Action** and multiplied by value 100.



Fields **Evaluate Action Step Editor** are:

Name	The name assigned to the Evaluate Action.
Equals=	Up to 5 fields are available into which are entered the source values which are to be used in the evaluation. A pull down allows you to choose between Device , Action step and Value .
Device	The value returned for the given device is used.
Action step	The value is that returned from an action is used.
Value	The source is a constant value.
	Up to 4 operator fields are available. These apply the operator to the resulting value from the steps above the operator to the linked source value to the right of the operator. In addition to the basic arithmetic operations +, - * and /, are Log and InvLog , Power and Root , Min and Max .
	The value returned by the Evaluate Action is that resulting from the top to bottom evaluation of the entered fields. Fields left empty are ignored.

Format results like	Defines how the result will be formatted. Either the Default format or if a Specified device is selected then the number format used by the specified device will be applied to the result of the Evaluate Action.
Comment	The comment associated with the Evaluate Action. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation Page](#)

Events

This topic is not described in this version of the manuals. Please contact Hiden Analytical for a manual update.

Event Logs

Selecting the **Events Log** option of the **Instrument** menu generates an **Event Log** for the currently selected instrument.

When messages are received during acquisition, **Event Log** windows are created, on a per mass spectrometer basis, if not already open. Each new message from a given mass spectrometer is displayed below the last. The window automatically scrolls to ensure that the most recent message is visible. Messages can be generated using **Print Text Action** of Action Sequences. Other messages may be automatically generated to inform of other events associated with the instrument.

If the Control Tabs frame is visible, then the log will be displayed docked within the **Logs** tab. Otherwise the events log is opened in a floating window an example shown below

An example is shown below.



A log can be closed by clicking on the X button of the associated log.

MASsoft will only display events in the Event log and then only up to a maximum of 500 events. However, both the Archive and Event logs are text files and can be viewed via any text editor. The log file has the extension .log and the archive file .old. They are stored in the MASsoft program folder and are named after the IU's WR number (without the preceding WR).

When the Event log window is created the Event log will be interrogated before the most recent events are displayed. If the Event log exceeds 64kb it will be reduced in size by about 25%, with the oldest events being archived. The Archive log will then be interrogated and if it exceeds 1Mb it will be reduced in size by about 10%, with the oldest events being discarded. This ensures neither log grows indefinitely and the most recent events are retained.

Right clicking when the cursor is in the **Event log** window opens the **Event log** window menu.

The following options can be selected from this menu:

Show Time and Date When selected, this option displays, at the end of the message, the time and date at which the message arrived.

Clear Log	The Clear Log option will archive the events, resulting in an empty Event log.
Edit Font...	This opens a dialog box which allows the text font on the Event log window to be changed.
Edit New Entry Colour	This opens a dialog box which allows the text colour of new messages to be defined.
Copy	Copy the selected text.
Select All	Select all the text.

See also:

[Logs Tab](#)

[Print Text Action Step Editor](#)

Exporting

Data may be exported in various formats for use in other applications.

Windows screen copy

A bitmap copy of all or part of the MASsoft screen can be made using the normal Windows copy options. To copy an active MASsoft application window, press the *Alt, Print Screen* key combination. To copy the whole screen, where MASsoft is not maximised, press the *Print Screen* key. With either method, the resultant bitmap may be copied into other Windows applications by pasting from the clipboard.

Exporting

Data may be exported for use in other graphics packages and spreadsheets by clicking **Export** on the **File** menu which provides four export options:

- **Data as** enables the current data to be exported in one of three formats for use by other packages.
- **DDE** provides the ability to transfer, in real time, data to other Dynamic Data Exchange (DDE) client-compatible applications by defining the relevant data and then using **Edit, Copy** to copy the data to the clipboard.
- **NIST** [NIST Export](#)
- **Plot As**

Export Data As

When **File, Export, Data As...** is selected, the Export View Data To dialog is opened. This dialog is a standard Windows save type dialog where a file name is entered, a file location can be selected and the file type selected. The file types supported are:

Ascii Files (*.csv)

ANDI-MAS Files (*.cdf)

JCAMP-DV Files (*.jdx)

ASCII files comprise values separated by the default Windows separator character for the view currently selected. For a normal sequence or co-variant scan, the whole of the scan is exported, but when a multi-variant scan is selected, the whole of the major (i.e. highest level) scan is output, which may include several subordinate scans, resulting in a large output file. The **.csv** extension name allows the resultant file to be read into other applications as ASCII comma-separated values, after which the data can be manipulated as required.

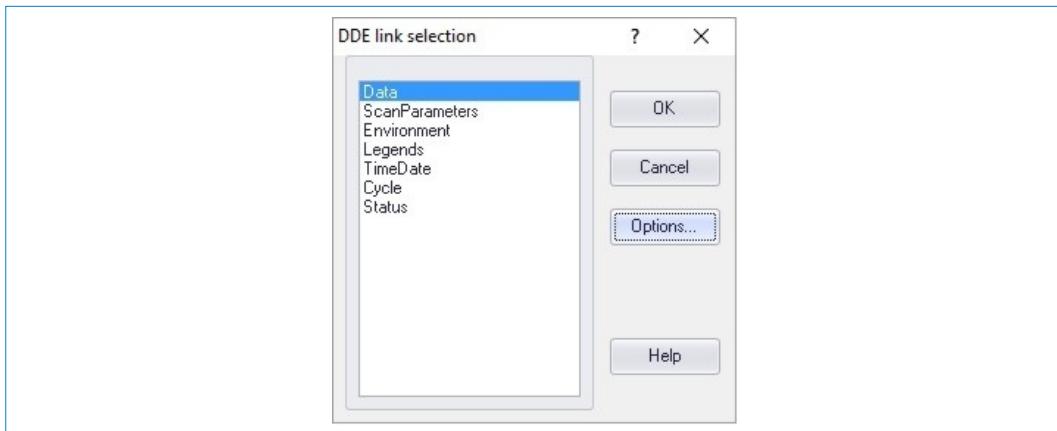
Refer to the Windows Control Panel documentation for details of the Separator character and International settings.

CAUTION

Changing the Separator character may cause MASsoft and other Windows applications to function incorrectly.

Export DDE

Selecting **Export, DDE** on the **File** menu opens the **DDE link selection** dialog.

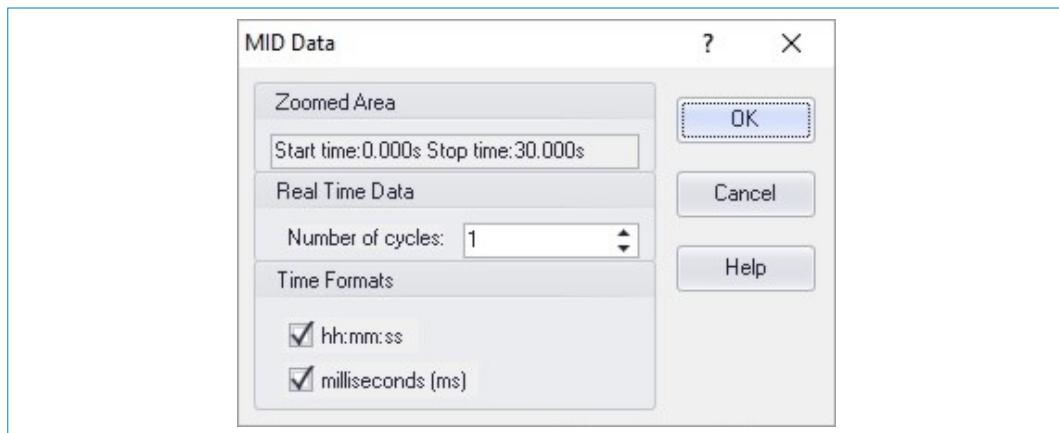


The type of information to be linked is selected by clicking on it, then clicking the **OK** button. To transfer information, select the view containing the scan to be copied or linked, click **Copy** on the **Edit** menu to transfer the information to the clipboard. The client application can then import the data using the **Edit, Paste** command, or link to it, using the **Edit, Paste Special** command.

When a view is copied to the clipboard, using the **Edit, Copy** command, two sets of data are transferred. One set is text data, which allows DDE values to be transferred, the other is the view as a Windows metafile picture. If the **Edit, Paste** command is used when pasting the data into another application, the client application will take the most suitable data set for its normal operation. For example, a word processor will take the text, whereas a drawing application will take the picture.

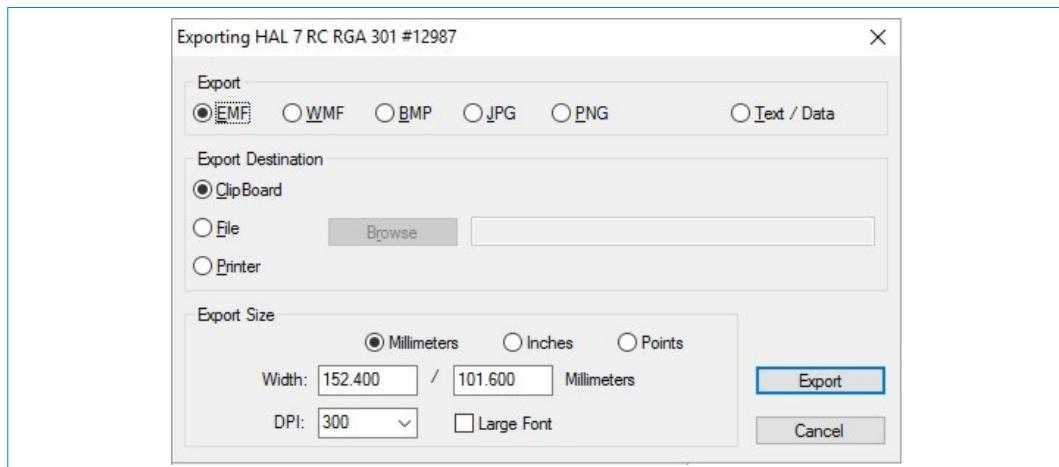
To force the client application to take the other data set (for example, a picture into a word processor) the **Edit, Paste Special** command must be used; this allows the input object to be selected. If the **Paste:** option in the **Paste Special** dialog box is selected, the data is copied into the client application and the transfer ends. If the **Paste Link:** option in the **Paste Special** dialog box is selected, a link is set up between the client and the MASsoft server. If the data in the MASsoft view now changes (e.g. during acquisition) the new data will automatically be transferred to the client. This “hot link” can be used with a spreadsheet, for example, to extend MASsoft’s data-processing capabilities.

The **Options...** button is only available if the selected information is **Data** and the view is a Multiple Ion Detection (MID)-type. Selecting this button opens the **MID Data** dialog box, which allows the **Number of cycles** and **Time Formats** to be selected.



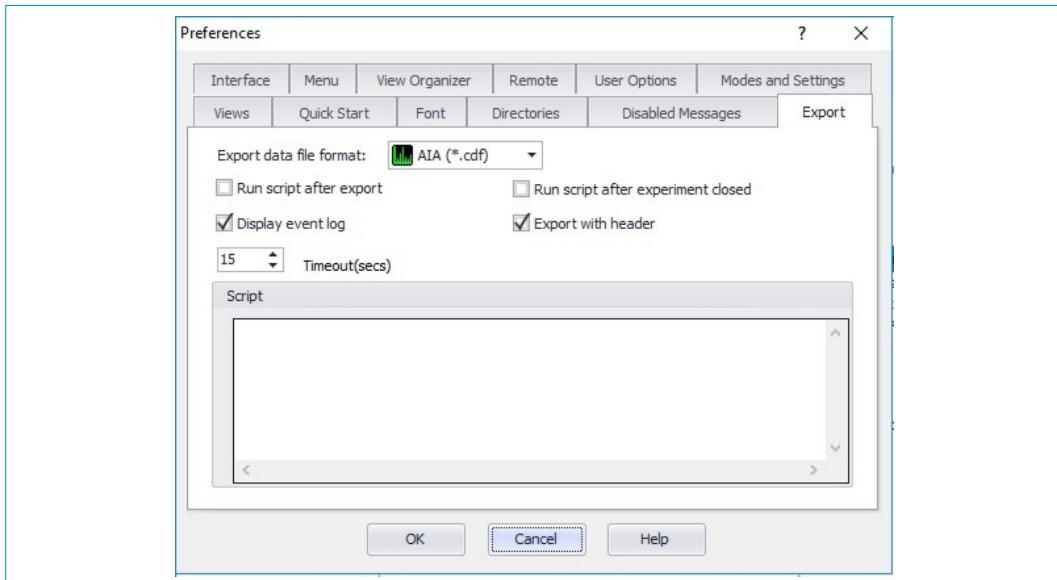
Export plot

The current view may be exported in a number of file formats. Select **Export, Plot As ...** on the **File** menu to open the **Exporting** dialog.



File type, export destination and plot size may be selected before clicking the **Export** button.

Export preferences



To view the Export preferences select **Preferences..** on the **Edit** menu then select the **Export** tab.

The **Export** tab allows a MASsoft experiment to be exported in a format that can be imported into another application. To enable exporting the **Export after scanning** option must be selected in the **Completion Options** dialog.

See also: [Completion options dialog](#)

The **Export** tab allows the user to select the required export format and to perform a series of DOS commands after the exporting has been completed.

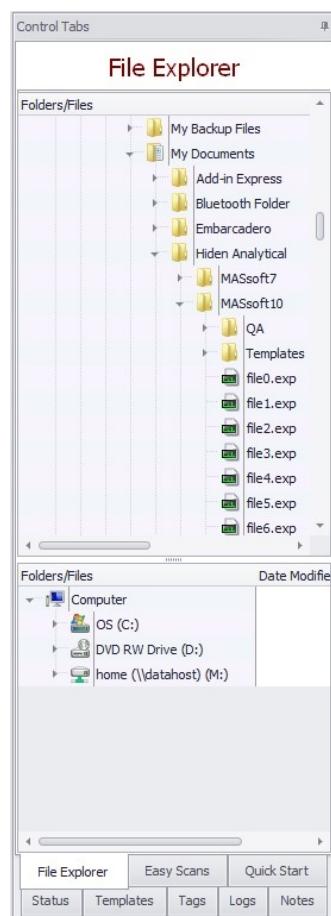
Export data file format	This control lists all the available formats.
Run script after export	Select this control to run the script after the experiment has been converted to the select format.
Run script after experiment closed	Select this control to run the script after the experiment has been closed.
Display event log	Brings the event log to the front.
Export with header	When selected a header providing information about the scan settings and environment values used to acquire the data precedes the CSV data. Omitting the header can make the data easier to import into some programmes.
Timeout (secs)	The script timeout value.

Script

This control lists a series of DOS commands to be run after the exporting has been completed.

File explorer

The **File Explorer** tab of the Control Tabs frame provides a convenient way of managing Windows folders and MASsoft experiment files. It provides a function similar to Windows Explorer, allowing a number of actions to be performed on MASsoft files and folders. However, only folders and MASsoft files are listed.



The File Explorer contains two views of the PC's file structure separated by an adjustable splitter bar that can be positioned to suit. Clicking in the centre of the splitter bar will expand the topmost view to accommodate the entire File Explorer panel, clicking it again will restore it to its previous size. To reposition the splitter bar press and hold the left mouse button, drag the splitter bar to the new position, and then release the mouse button.

File Explorer treats all five MASsoft files as a single .exp file entity. When performing actions such as copy/paste/rename or delete the actions taken on the five hidden files are made invisible to the user. If such operations were to be attempted using Windows Explorer

care must be taken to ensure that none of the files are omitted from the procedure. File explorer will also copy .log and .csv files if they exist.

Right-clicking on an item in the File Explorer will display a context-sensitive popup menu containing actions to be taken that are appropriate for that selection.

Items that may appear in the popup menu include:

Expand	Expands a folder showing any folders or MASsoft file it contains.
Collapse	Closes a folder hiding any folders or MASsoft file it contains. A folder may be expanded or collapsed by double-clicking on it. A folder may be expanded or collapsed using the left and right arrow keys.
New Folder	Create a new folder.
Open	If a MASsoft file is selected, that file is opened. If a folder is selected a file browser displays the contents of the folder. A file can be opened by double-clicking on it. A file can be opened by selecting it then pressing the ENTER key. A file can also be opened by dragging it onto the view tab.
Copy	Copy the folder or MASsoft file.
Paste	Paste a copy of the folder or MASsoft file. This will create another copy of the file or folder copied earlier. Another method to copy files is to press and hold the mouse button, and then drag the selected item to the target folder before releasing the left mouse button. To select consecutive experiment files in the same folder, click the first file, press and hold the SHIFT key, and then click the last item. To select non-consecutive experiment files in the same folder, press and hold CTRL , and then click each item. Only multiple experiment files can be selected, not folders.
Rename	Rename the folder or MASsoft file. A file or folder can also be renamed by clicking on it when it is already selected. The names of system folders such as Documents and Settings, Windows or System32 cannot be changed. They are required for Windows to run properly.
Send file(s) to e-mail client	The selected file can be e-mailed to the current e-mail client with an inserted message.

Delete	Delete the folder or MASsoft file. A file can be deleted by pressing DELETE whilst it is selected. Deleted files and folders are moved to the recycle bin.
Properties	Displays the properties of the selected file or folder. The properties page displayed for a MASsoft experiment file is that of the xxx.exp file and does not include the other 4 files (.ann, .dat, .env, .scn) that make up an experiment.

See also:

[Easy Scans](#)

File menu

The File menu items are described below.

New	Creates a new experiment file containing a basic scan tree based on the values last used by the current instrument. This command is grayed out if no instrument is selected.
Open	Opens and displays an existing experiment file. A standard Windows open dialog is displayed from where a file can be selected. MASsoft experiment files have the file extension .exp. Existing experiment files contain scan tree information that may be used to acquire new data, which may be saved in a new experiment file. When a file is opened, the first scan in the file is displayed. This command is grayed out if no instrument is selected.
Close All	Closes all the currently open data files and all their associated views. A message box is displayed if the file has not been saved.
Save	Saves the current scan tree information, either in its original file, or in a new one if the information has not been saved previously. The experiment's previously acquired data will be lost. This command is grayed out if no instrument is selected.
Save As...	Saves the current scan tree information in another file of the same format. A standard Windows Save As dialog will be opened. This command is grayed out if no mass spectrometer window is active.

Save As Template...	Creates a template from the current experiment file. Everything associate with the file is saved except data.
	See also: Save as template
Save Options	This command is used, prior to starting acquisition, to specify which data are to be saved; it opens the Save Options dialog. This command is grayed out if no scan tree window is active.
Send File(s) to Email client	This will e-mail a data set from the users PC to Hiden Service When selected an Open dialog is displayed where the user selects an experiment file. Associated experiment files are zipped, a blank e-mail in the user's client e-mail application is created and addressed to service@hiden.co.uk with the subject as the instrument WR. This feature is designed to make it easier to obtain support from Hiden.
Close	Closes the currently open data file and all its associated views. A message box is displayed if the file has not been saved.
Import	<p>NIST Opens the NIST Import dialog to allow a scan from a NIST library to be imported. Only scans with the scanned device set to mass can be imported from a NIST library.</p> <p>See also: NIST import</p>
Analysis	<p>Environment Values Imports a saved tune file (extension .tun) to a scan. This command is grayed out if no scan tree window is active.</p> <p>See also: Tune files</p>
Export	Export is only visible o the File menu when a view is selected.
Data as	Allows data to be exported in one of three file formats: ASCII Files *.csv ANDI-MS Files (*.cdf) JCAMP-DX Files (*.jdx).

DDE	Provides the ability to transfer, in real time, data to other Dynamic Data Exchange (DDE) client-compatible applications by defining the relevant data and then using the Edit, Copy command to copy the data to the clipboard.
NIST	Allows data to be exported is a NIST database. See also: NIST export
Plot As	Allows the data view to be exported as a graphics file such as jpeg or Windows metafile.
Run Recipe	<i>This Topic is not described in this version of the manual. Please contact Hiden Analytical to see if an updated version of the manual is available.</i>
Convert	<p>Converts files created by a different instrument to allow them to run on the current instrument.</p> <p>Conversion will ignore any settings that are not present on the current instrument and use default values from the Instrument Settings for any missing variables. The scan's input and output devices are also checked. Conversion makes any data associated with the file invalid. If the converted file is saved to the same file as the original, over-writing it, then the data will be lost. To avoid this use the File, Save as command.</p> <p>If Automatically convert from earlier version of firmware (Edit, Preferences, Modes and Settings tab) is selected files without data created using an earlier version of the instrument's firmware are automatically converted when the file is opened. Files with data are automatically converted if the file is run.</p> <p>If Allow files from a different instrument to run without conversion (Edit, Preferences, Modes and Settings tab) is selected MASsoft will run files without requiring them to be converted. Variables in the file's environments that are not present on the current instrument will produce an "Unknown logical device" error, missing variables will have an undefined value. Incompatible input and output devices will cause errors and MASsoft may not be able to display the data. This behaviour is the same as previous versions of MASsoft. Use of this option is NOT recommended.</p> <p>See also: Modes and settings</p>

Unlock	Unlocks file with data to allow editing. When a file that contains data is opened it will be locked to prevent inadvertent editing. Editing files invalidates the data. When a file is locked the OK button in the scan and environment editing dialog boxes is replaced with a locked symbol; no values can be changed. The Cancel button is used to exit the dialog. Unlocking the file allows the user to edit the file. Unlocking makes any data associated with the file invalid. If the unlocked file is saved to the same file as the original, over-writing it, then the data will be lost. To avoid this use the File, Save as command.
Print Page Setup...	Selects the printer to be used via the standard Windows Printer Setup dialog. This command is grayed out unless a view is selected.
Print Preferences	Allows the user to choose whether to print the displayed graph and/or its associated environment data. The default user and company names may be changed, for printing with the data. This command is never grayed out.
Print	Prints the currently selected view. The command is grayed out unless a view is selected.
Print Preview	Reviews data in print layout format before it is selected for printing. This command is grayed out unless a graphical view is selected.
Recently used files	A list, up to a maximum of five, of most recently used files. Clicking on a file in the Recently Used Files will open it.
Exit	Closes the MASsoft application. This command should be used only after acquisition has been stopped, or an error dialog will be opened.

File settings

In previous versions of MASsoft the File Settings were called the Global Environment. The file settings encompass the variable values of all the acquisition modes. The file settings for each operating mode contain the current device values for that mode. These device values are used whenever that operating mode is selected for a scan, unless overridden by the scan settings associated with that particular scan.

The device values for each type of acquisition mode can be edited in the Edit File Settings Operating Modes dialog.

In the MASsoft settings hierarchy the File Settings are overridden by Scan Settings but override Instrument Settings.

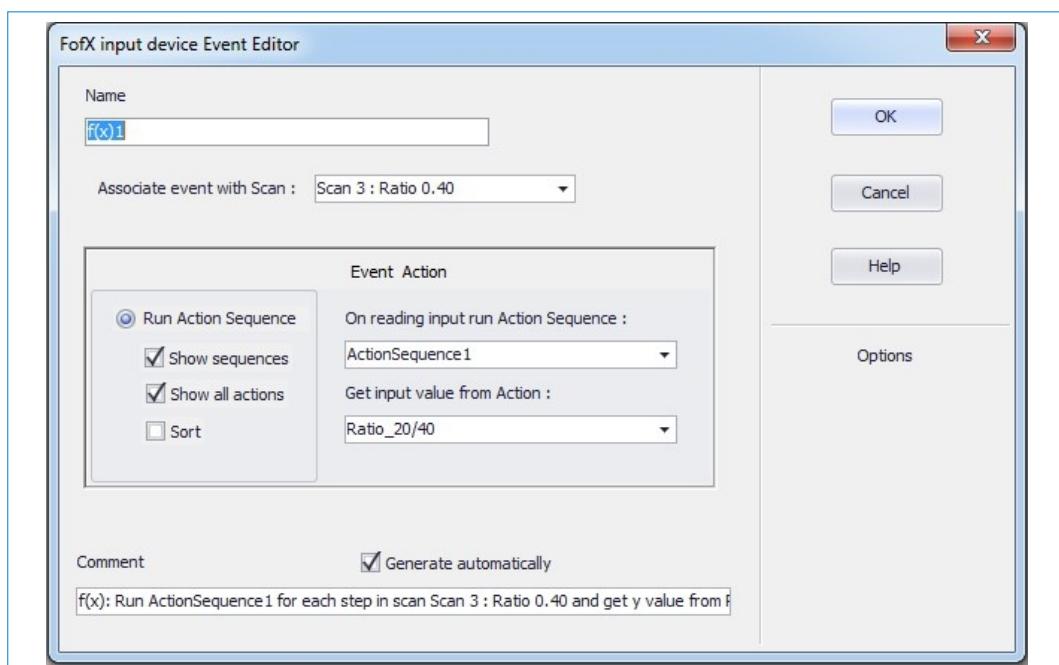
FofX Input Device Event Editor

The **f(x) Input Device** associate a f(x) input with an action sequence to calculate and return the result. The action sequence is run once for each step in the associated scan. The value read from the step is returned as the result, as if it were a reading from a normal input device. The specified scan must have f(x) as its input device.

To do this additional scans need to be added to your scan tree in to which the newly calculated data can be linked, allowing the resulting data to be viewed.

The **FofX input device Event Editor** dialog is opened when a **New f(x) Input event** is selected from the **Automation** popup menu, or when an **f(x) Input event** is edited.

An example which calculates a ratio value, and inputs that value to a scan is shown below.

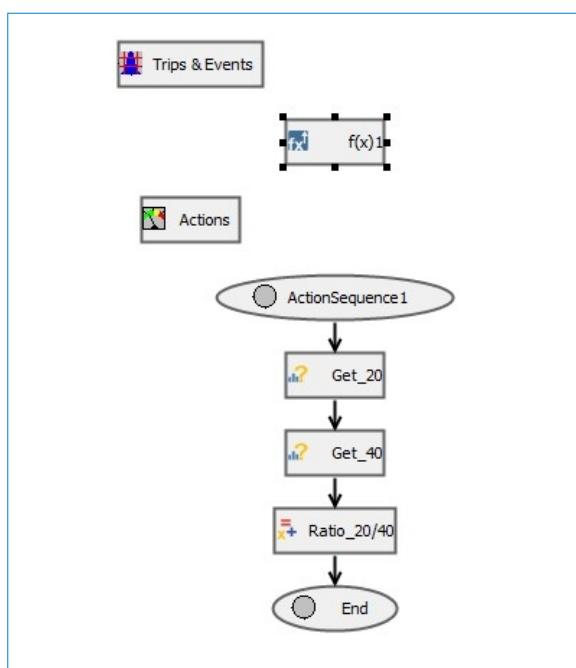


Fields **FofX input device Event Editor** are:

Name The name assigned to the f(x) input.

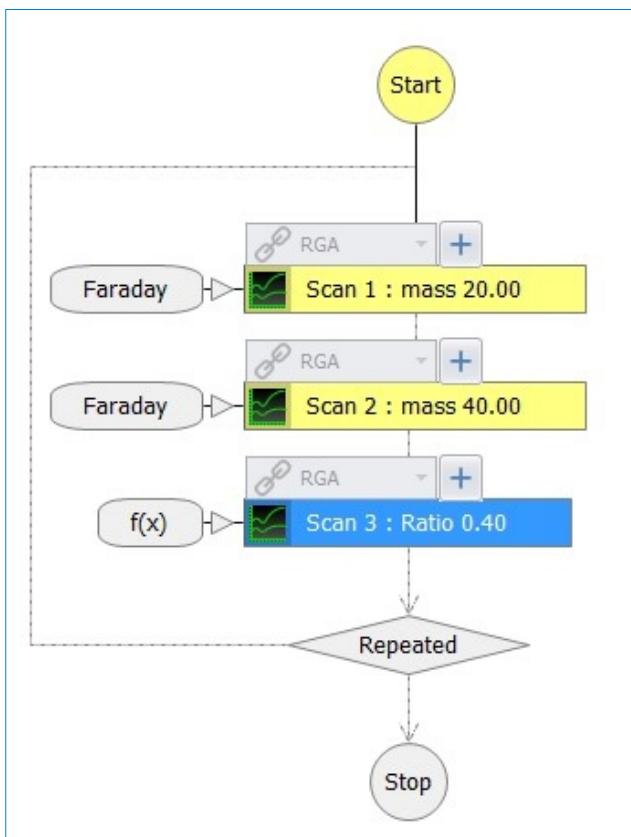
Associate event with Scan	The scan which the event is associated with, that you want to input your calculated value from your event sequence.
	Event Action : Run Action Sequence
	Choose a previously created action sequence from the pulldown box boxes. The type of actions listed can be filtered using the Show sequences , Show all actions and Sort options.
On reading input run Action Sequence:	This is the point in the action sequence from where you want the calculations to be performed. For example setting this as ActionSequence1 runs the first action sequence from the beginning. May be omitted if the result has already been calculated by an earlier call to a f(x) input.
Get input value from Action:	The action step which you wish to get a value from, after running through earlier steps in the action sequence. For example you may get a value calculated from an Evaluate Action step. This value will be input into the scan associated with this action, and displayed as data for the scan.
Comment	The comment associated with the f(x) input event. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

An example of a simple ratio Action Sequence using the f(x) input event to generate data is given below.



Two Data Actions collect the values of MID scans at peak mass 20 and mass 40. The Evaluate Action calculates a ratio of the two scan values. The f(x) input event runs

ActionSequence1 and associates the output from Ratio_20/40 with Scan 3. Where a scan must be added associated scan structure.



If now we plot the data returned from Scan3 it would be the ratio value.

See also:

[Automation page](#)

FofX Ouput Device Event Editor



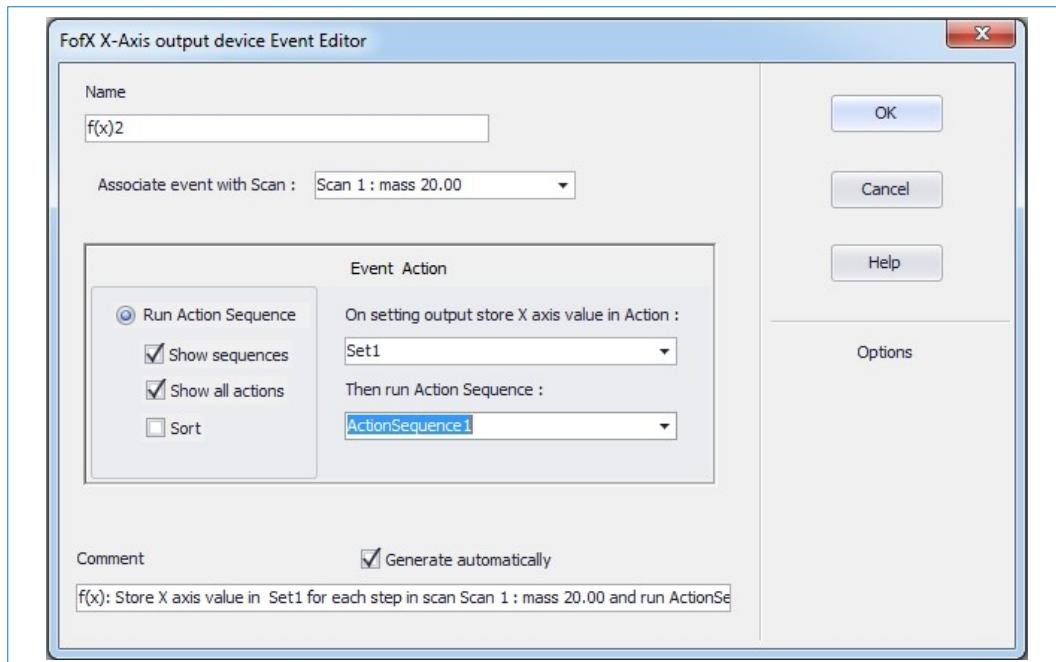
The **f(x) Output Device**, is used associate an f(x) output (i.e the scan's scanned device) with an event sequence; this sequence can then take the x axis ordinal and use it to calculate a value to output.

For each step in the scan specified by associated scan the X axis value is stored in the step specified action and an action sequence is run. The specified scan must have f(x) as its output device.

The **FofX X-Axis output device Event Editor** dialog is opened when a **New f(x) Output event** is selected from the **Automation** popup menu, or when an **f(x) Output event** is edited.

An example shown below where a value output from an associated scan is stored in a Set Action, then an action sequence started using the value. The sequence runs to completion and returned to the scan.

Care must be taken that the step referred to in **On setting output store X axis value in Action** does not have its value over-written by running the sequence before the value has been retrieved.



Fields **FofX X-Axis output device Event Editor** are:

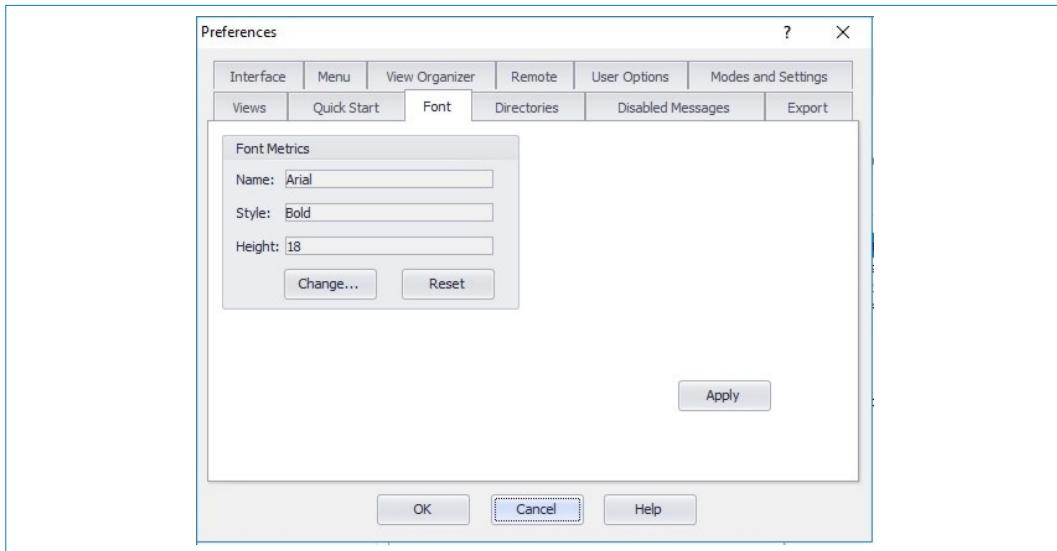
Name The name assigned to the f(x) output.

Associate event with Scan	<p>Specifies the scan for which the f(x) output is to be calculated.</p> <p>Event Action : Run Action Sequence</p> <p>Choose a previously created action sequence from the pulldown box boxes. The type of actions listed can be filtered using the Show sequences, Show all actions and Sort options.</p>
On setting output store X axis value in Action:	<p>Specifies the sequence step to store the X axis value for each step of the scan in.</p> <p>Then run Action Sequence:</p> <p>Specifies the sequence step to run.</p>
Comment	<p>The comment associated with the f(x) output event.</p> <p>If Generate automatically is selected, the comment is generated by the selections made within the dialog.</p>

See also:

[Automation page](#)

Font preferences



To view the Font preferences select **Preferences..** on the **Edit** menu then select the **Font** tab. The settings in **Font Metrics** determines the settings of the font used in the Scan Views.

Graphical/Tabular view editor

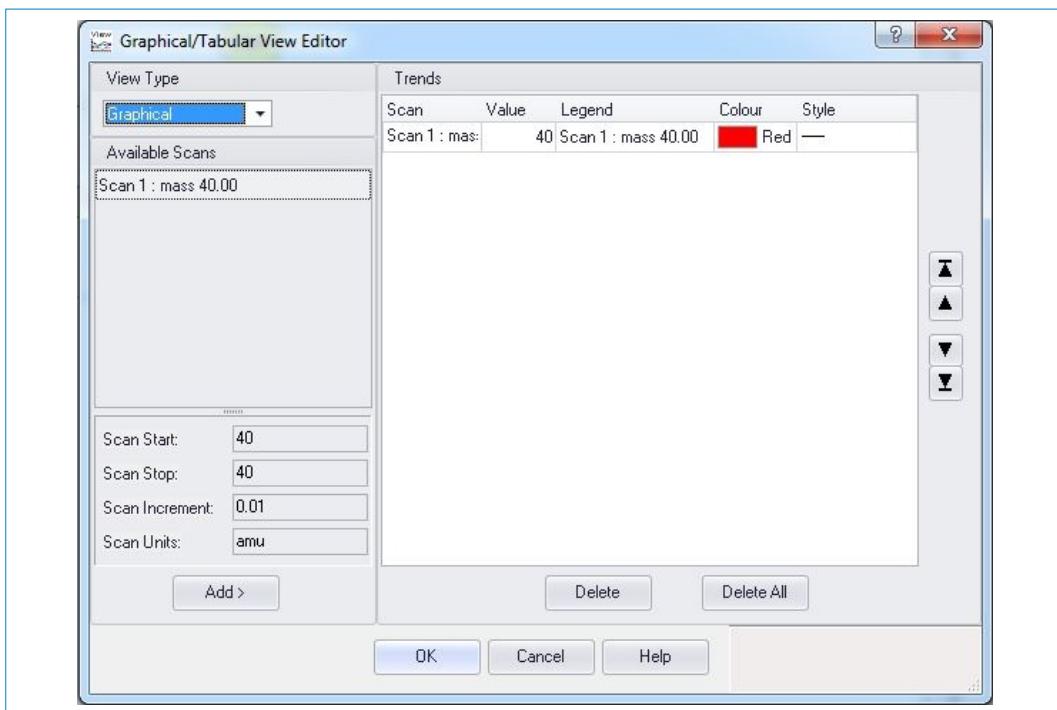
Note

Previously the Graphical/Tabular View Editor dialog was called the Trend View Setup dialog.

The **Graphical/Tabular View Editor** is used to create a new or edit an existing MID Tabular View or Graphical Trend View.

The dialog is displayed by selecting **New Trend View...** from the **Views** menu when highlighting a scan within the Scan Tree. It can also be accessed by selecting **Edit Trend View...** when a MID Tabular View or Graphical MID Trend View is the active view. The **Trend View Setup...** option from a Graphical Profile plot also opens the dialog.

An example is shown here where a new trend view is being created from an MID scan.



View Type

The **View Type** determines if the view created will be **Tabular** or **Graphical** or **One of Each**. When editing a MID Tabular View only the Tabular view is enabled.

Available Scans

To add new trends to the view being edited or created, select one of the scans from the list of **Available Scans**. This list can include MID scans or Bar/Profile scans. Details of the scan are displayed below the **Available Scans** list. Click the **Add** button to add the scan to the **Trends** box.

Trends box

If editing a MID Tabular View or Graphical Trend View the current trends of the selected view are displayed in the **Trends** box. When creating a new trend view from a MID scan within the Scan Tree then the current scan is added. Otherwise if you are creating a new trend from a Bar/Profile scan or from a Bar / Profile Plot View then the **Trends** box is empty. For a non-MID scan the Value of the trend should be edited in the entry added to the table.

The **Delete** and **Delete All** buttons below the **Trends** box are used to delete entries in the Trends box table. The arrow buttons to the right allow you to change the order of the trends, which will affect the sequence they are displayed within the MID Tabular View.

Click the **OK** button to create or edit the view.

Also see:

[Views menu](#)

[Scan tree](#)

Graphical view tool bar

When either a Bar / Profile View or MID Graphical View becomes the active window, the Toolbar displays a series of buttons which allow operations to be performed on the plot.

For the Bar/Profile view the left-hand axis is the only axis, so operations are always performed on this axis.

For the MID Graphical view it can have both a left and right hand axis, and most of the operations apply to currently selected axis. An axis is selected by clicking on any of the number annotations which mark the values of on that axis. The selected axis is drawn in red.

Increase Magnification



Zooms in on the selected axis by 25%.

Decrease Magnification



Zooms out on the selected axis by 25%.

Set Axes Limits to Full Scale



Sets the X-axis to its full range, then auto scales all the Y-axes. This returns the view back to its default starting state, as when the view is first created.

Auto Scale Y Axis

Auto scales the selected Y axis. The Y-axis upper limit is adjusted, so that the maximum peak size within the visible X range is close to the Y axis maximum, and fills the plotting area. The visible X range is changed by zooming or via the X Axis Properties.

For Bar/Profile plots this option alternates between scaling the Y axis, to the Y values of the current cycle of data or with the Y values of the previous cycle of data.

If the **Autoscale Lower** option of the Y Axis Properties is checked on this also scales the Y axis minimum to the lowest Y value in the visible X range.

Vertical /Horizontal Zoom Style

Set the zoom type to Vertical / Horizontal, surrounding this button with a box.

Horizontal Zoom Style

Set the zoom type to Horizontal, surrounding this icon with a box.

Vertical Zoom Style

Set the zoom type to Vertical, surrounding this icon with a box.

See also:[Bar/Profile plot view](#)[MID Graphical view](#)[Tool bars](#)[X Axis properties dialog](#)[Y Axis properties dialog](#)[Zooming](#)

Grid options

The **Grid Options** is a sub menu of both the **Bar/Profile Graphical** and **MID Graphical Views** menu. These options control the appearance of grid lines which can be optionally superimposed over the plot data. The chosen option is marked with a tick.

Show X-Y Grid Lines

Displays a grid on both the X and Y axes.

Show X Grid Lines

Displays a grid only on the X axis.

Show Y Grid Lines

Displays a grid only on the Y axis.

No Grid Lines

Displays no grid lines

Bold	When Bold is checked on the grid lines are shown in black, otherwise they are shown in a more subtle grey colour.
Thick Grid Line	The grid lines are thick.
Thin Grid Line	The grid lines are thin.
Dotted Grid Line	The grid lines are dotted.

Help menu

This topic is not described in this version of the manuals. Please contact Hiden Analytical for a manual update.

Highest Peak Value

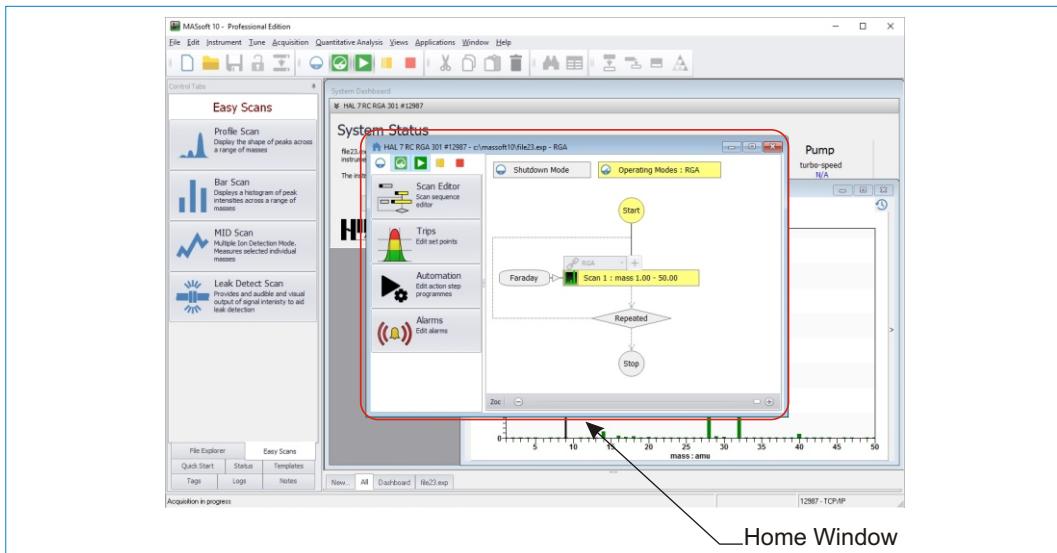
Pressing the SHIFT button and moving the mouse while the cursor is over a Bar / Profile plot or MID graphical view will display a vertical line and below the plot the X coordinate value and highest peak value of the data displayed at that point in the plot.

For the MID graphical view where the trend for more than one peak can be displayed on the same plot axis, the value of the highest peak on the currently selected axis is returned.

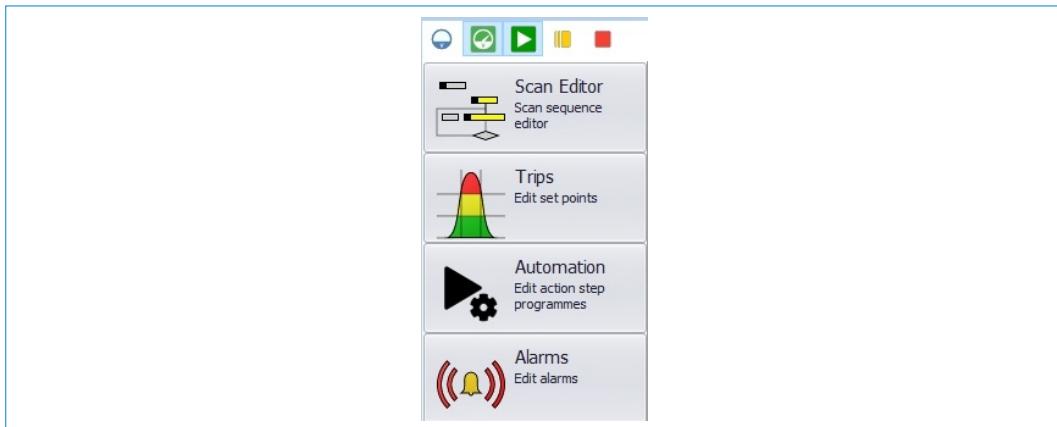
If you use this feature with the Bar / Profile plot while scanning then peak values displayed after the graph cursor (current X position of the scan) are zero. This is because although the plot may display data from the previous cycle the value returned is for the current cycle.

Home window

The Home Window is a multi-page window which facilitates the configuration of the MASsoft experiment file.



Pages are selected from the toolbar on the left side of the window.



Buttons for the Scan Editor, Trips, Automation and Alarms pages are always visible. Additional Raster and Mimic Diagram buttons may also be displayed if they are configured for the instrument for which the experiment has been created.

See also:

[Scan editor](#)

[Trips](#)

[Automation](#)

[Alarms](#)

[Rastering](#)

The Home window can have a number of associated windows, called Views. These views include Bar and Profile Plots, together with Graphical MID Views and MID Tabular Views. The views including the experiments Home window are organised onto a View Tab.

See also:

[Views](#)

[View tab](#)

Views can be easily created from the Scan Tree by using the Home window Views menu.

See also:

[Scan tree](#)

[Home window views menu](#)

Home window views menu

The Views menu options associated with the experiments Home window depend on which page of the Home window is selected.

When the Scan Editor page is selected by clicking on the **Scan Editor** button, the Scan Tree is displayed. The Views menu options are disabled or enabled depending on which box is selected within the Scan Tree.

New Trend View... Opens the **Graphical/Tabular View Editor** dialog which allows the creation of a new **MID Tabular View** or **Graphical MID View**.

Graphical View This option is enabled if a Bar, Profile or MID scan is selected within the Scan Tree. This displays either a **Bar/ Profile Plot View** or **Graphical MID View**.

MID Tabular View This option is only enabled when a MID scan is selected within the Scan Tree. This displays a **MID Tabular View**.

These views can also be displayed from the Tool Bar using the following buttons:

Bar Plot ,  , Profile Plot  , MID Graphical View  and MID Table  .
View

See also:

[Home window](#)

[MID graphical view](#)

[MID tabular view](#)

[Scan Editor](#)

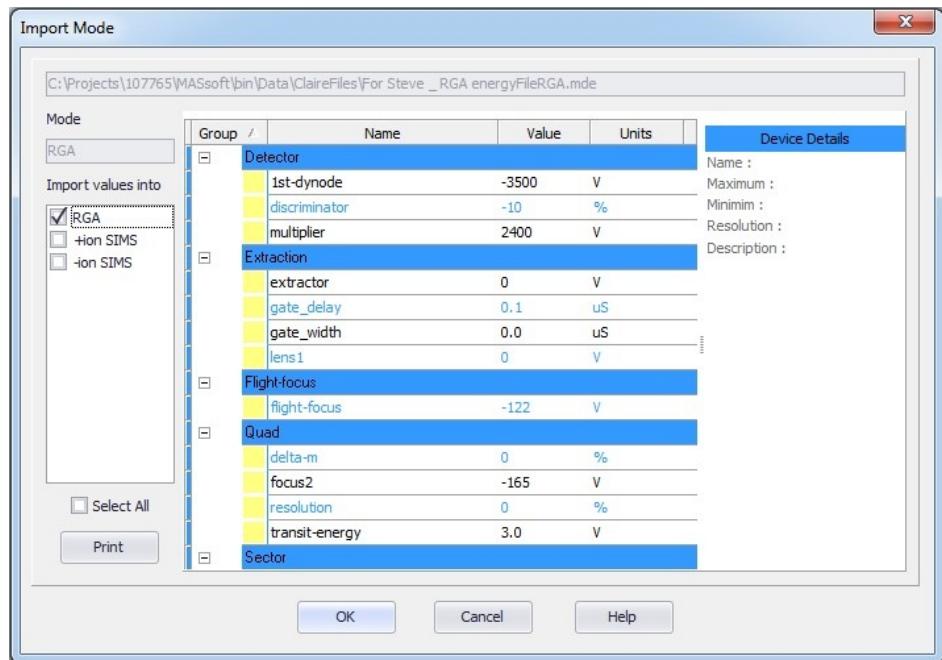
[Scan tree](#)

[Tool bars](#)

[Views menu](#)

Import Mode dialog

The **Import Mode** dialog is displayed when the **Import** button of the **Operating Modes** dialog is pressed, and a valid file to import has been selected.



The mode file name is displayed in the top text field which cannot be edited.

The mode which is saved in the file is displayed in the **Mode** box which cannot be edited.

A table of the device values in the mode file is displayed.

Column headings

Group Values may be grouped by function. Each group contains devices with a related function. This column cannot be edited.

Name The name of the device. This is cannot be edited.

Value Shows the current value of the selected variable. The value may be edited.

Units The units of the value. This is cannot be edited

The state of the check box column (whether the value overrides the instrument setting) is saved in the mode file, but is not displayed on this table.

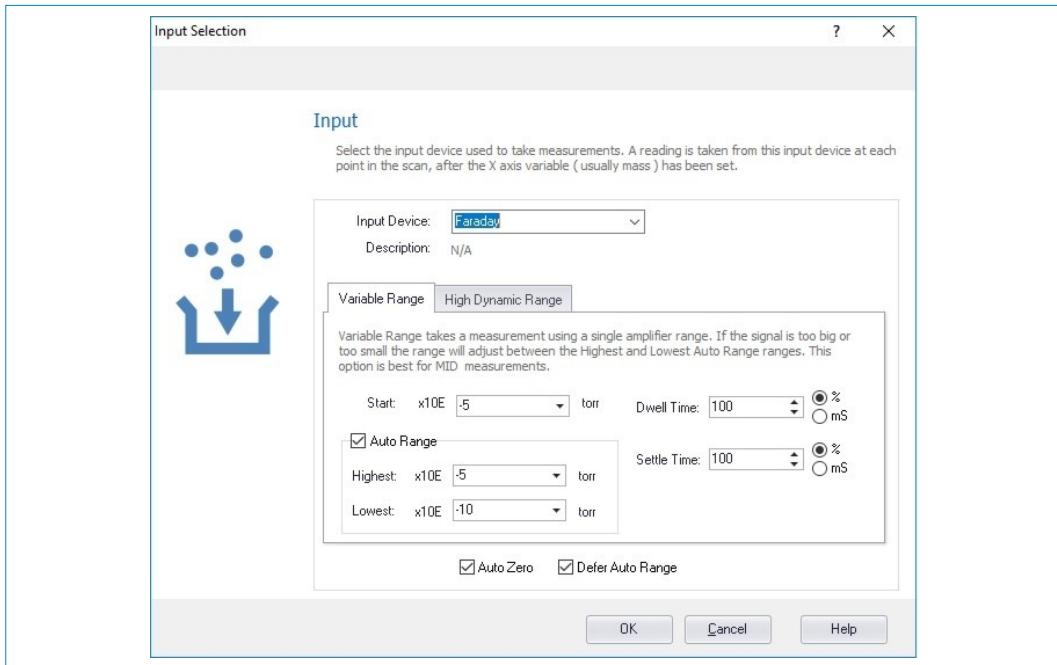
Import values into

The device values can be imported into the chosen modes of the Operating Modes dialog by ticking on those modes you wish to import the values into. By default only the mode of the file is checked on.

Pressing **OK** will import the values into the selected modes of the dialog.

If a value is edited in the **Import Mode** dialog the override check box will be enabled for that device in the **Edit File Settings – Operating Modes** dialog. Otherwise the state of the check box column is maintained as that when the export file was created.

Input selection dialog



Double-clicking the Input device box opens the **Input Selection** dialog box. If the mass spectrometer supports more than one input device, this dialog allows selection of the input device used by a scan.

The dialog supports range-switched input devices and allows the user to specify upper and lower auto-range limits to prevent auto-ranging to slower, high-gain ranges when very small peaks are not of interest, or to low-gain ranges which would suppress very small peaks.

The high dynamic range option allows data to be collected over a larger dynamic range by combining data from scans on two or three ranges as if they were a single scan. This allows measurements to cover a range of two, four, six or even eight decades.

The data values in the **Acquisition Range** and **High Dynamic range** tabs are independent, modifying the **Start** value in one tab will not modify the value in the other tab. The value from the selected tab will be used when the dialog box is closed.

InputDevice

The **Inputs Device** box contains a list of the input devices available on the instrument. The input device may be selected by clicking on the required name or by typing the name in the box. The devices available on pulse-counting and analogue analysers are shown below.

Input device	Pulse-counting analyser	Analogue analyser	Units
SEM	Yes	Option	c/s (Pulse-counting) Torr (Analogue)
Raw counts	Yes	-	counts
Faraday	Option	Yes	Torr
Total	-	Yes	Torr
auxiliary1	Yes	Yes	volts *
auxiliary2	Yes	Yes	volts *
f(x)	Yes	Yes	-
f(<unit>)	Yes	Yes	unit
none	Yes	Yes	
vacuum	Option	Option	Torr
Muxn	Option	Option	-

* default but may be user defined

Faraday	Faraday cup detector. This detector is standard on analogue instruments and optional on pulse counting instruments.
SEM	Secondary electron multiplier; the gain of the SEM is controlled by the multiplier voltage setting in the scan's environment and the 1st dynode voltage (if fitted). This detector is standard on pulse-counting instruments and optional on analogue instruments.
Total Pressure	The total pressure input device configures the analyser to pass ions of all masses, thus giving an approximation of the total pressure in the system. The ions are collected by the Faraday detector. The mass selected is irrelevant when this input device is used. This detector is only available on analogue instruments.
Raw counts	This is an alternative to the SEM on pulse-counting instruments; it reports the intensity as counts instead of counts/second.

auxiliary1	These are analogue inputs which can be read as a scan's input; each input has user-selectable -10 V and -1 V ranges.
auxiliary2	The ranges are to the power 10, i.e., range 0 represents a x1 gain (10×10^0 full scale, -10 V) and range -1 represents a x10 gain (10×10^{-1} full scale, -1 V).
	These detectors are standard on all instruments.
	The names and ranges of auxiliary1 and auxiliary2 may be configured by the user.
	See also: Analogue inputs
f(x)	This input device allows an input value to be calculated as a function of data previously acquired, or of another data value. Please contact Hiden Analytical Limited if further information is required.
	This is standard on all instruments.
f(<unit>)	The f(v) , f(Torr) , f(%) , f(mbar) , f(ppm) , f(c/s) and f(Pa) devices are identical to the f(x) device except for the units used by the device.
none	No input device is selected.
vacuum	Reports the total pressure as read by the Hide Vacuum Control Unit or Edwards Turbo Interface Controller.
Muxn	These input devices are used when an Analogue Input Module is used in conjunction with the control unit to expand the number of analogue inputs.
	These detectors are an option on all instruments.

Variable Range tab

The unit will depend on the selected input.

Start x10E	This combination box contains the range used at the start of a scan. The value entered is a power of ten; i.e. if -7 is entered, the range set is 10^{-7} Torr. For instruments with a pulse counting detector Start specifies the maximum number of counts counted. It should normally be left set to 7 (10^7 counts). If it is set to a lower value the instrument will measure how long it takes to acquire the specified count and calculate the c/s from the time. The time will not exceed the dwell time.
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Auto Range

When selected, this allows the analyser to automatically change the range and follow changes in the input signal.

The manner in which automatic ranging is applied can be controlled by the user, using the **RestartAutoRange** and **No DeferAutoRange** options.

See also: [Advanced scan options](#)

Highest x10E

This combination box contains the highest range to which the input device may autorange; the entered value is a power of ten. **Highest x10E** is not applicable to pulse-counting instruments.

The **Highest x10E** value should be set to the expected maximum intensity, i.e. the pressure in the vacuum system as indicated by the vacuum gauge.

Lowest x10E

This combination box contains the lowest range to which the input device may autorange; the entered value is a power of ten. **Lowest x10E** is not applicable to pulse-counting instruments.

Dwell Time

Defines the time used to acquire a single point in the scan. A value may be typed directly into the text box.

If the radio button marked **mS** is selected, the value in the text box will be specified as milliseconds. Note that if the instrument changes range the set dwell time will be used on the new range and this may affect the signal to noise ratio.

If the **%** radio button is selected, the value will be interpreted as a percentage of the default dwell time for that range. The default dwell time for a given system and range is contained within look-up tables in the control unit; it is selected to give a good signal-to-noise ratio for the selected range.

Settle Time

Defines the time to allow the electronics to settle before the scan is started. A value may be typed directly into the text box.

If the radio button marked **mS** is selected, the value in the text box will be specified as milliseconds.

If the **%** radio button is selected, the value will be interpreted as a percentage of the default settle time for that range. The default settle time for a given system and range is contained within look-up tables in the control unit; it is selected to allow adequate settling on the selected range.

When the scan has started, a "point time" is applied between each measurement; this time cannot be defined by the user. There are also other delays which contribute to the overall scan time.

See also: [Dwell and settle times](#)

Auto Zero

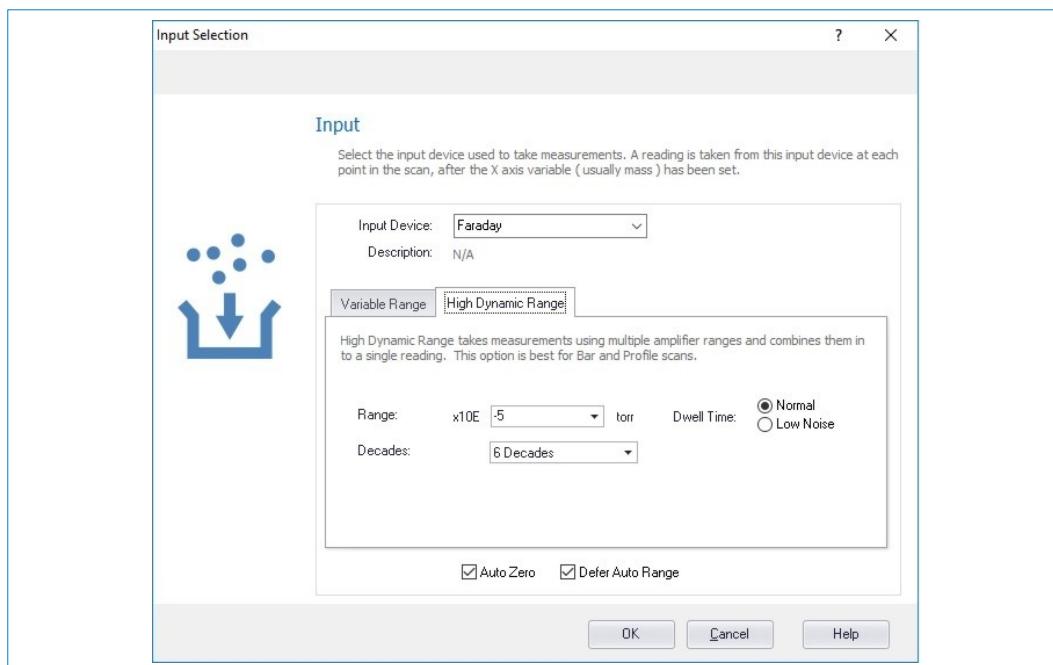
When selected, this forces the analyser to perform an automatic zeroing function at the start of each scan. This corrects any errors due to amplifier offsets and leakage currents.

Defer Auto Range When selected, the scan is completed before any data are displayed. If out of range values are detected, the scan will be restarted with different range settings.

When not selected data are displayed immediately. If out of range values are detected the range is changed before the next cycle.

For the SEM input on pulse-counting instruments, the **Auto Zero** and **Auto range** (and hence **Highest x10E** and **Lowest x10E**) entries are not applicable; **Acquisition range**, **Start** sets the maximum expected count rate which affects the **Settle time** and **Dwell time** when they use the percentage mode.

High Dynamic Range tab



The units displayed in the **High Dynamic range** depend on the input selected.

Start x10E The range maximum at the start of the scan. The value entered is a power of ten. If **-7** is entered, the range is set to 10^{-7} .

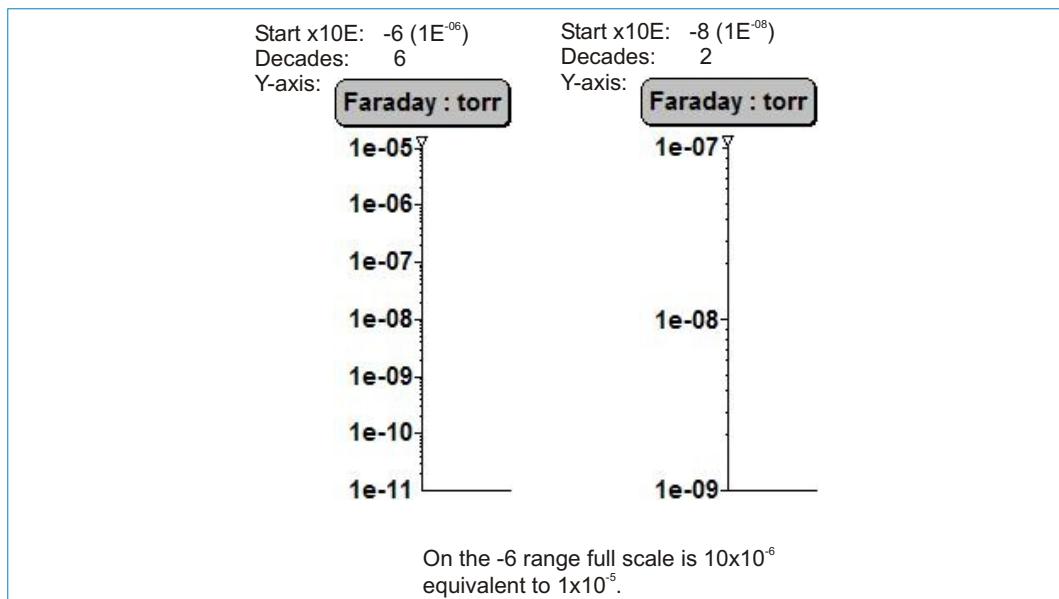
Decades The number of decades to be displayed. The possible options are 2, 4, 6 and 8. However, not all the options may be available, they are dependent on the input device and start value.

Dwell Time The time used to acquire a single point in the scan as a percentage of the default dwell time for the range. **Normal** is 100%, while **Low Noise** is 400%.

When the **Input Selection** dialog is opened from a graphical view only the **Start x10E**, **Decades**, and **Dwell Time** controls can then be modified. Closing the dialog by clicking the **OK** button will result in the modifications being sent immediately to the control unit.

The user will not be able to change the input device.

The Y-axis range will be changed to match the new settings. The Y-axis will be changed to a log axis with a maximum value set to the **Start x10E** value and the number of displayed decades matching the **Decades** value.



The Y-axis minimum value will never be set to less than the input device resolution. If the **Start x10E** value was set to -7 and the **Decades** was set to 6 the Y-axis minimum would still be **1e-11**, (Faraday detection limit), and not **1e-13**.

Decades

The high dynamic range option allows data to be collected over a larger dynamic range by combining data from scans on two or three ranges as if they were a single scan. This allows measurements to cover a range of 2, 4, 6 or even 8 decades.

Decade	Meaning
2	Will perform one scan covering two decades.
4	Will perform two scans with each covering two decades.
6	Will perform two scans with each covering three decades.
8	Will perform three scans, covering eight decades.

Instrument menu

Menu items on the Instrument menu are described below.

Edit Instrument Environment...	Select Instruments, Edit Instrument Environment... to open the Edit Instrument Settings dialog where device values for all the operating modes and the shutdown mode may be edited. See also: Instrument settings
Show Status Bar	When selected the control unit Status Bar is displayed. See also: Status bar
Customise Status Bar...	Opens the Customise Monitored Devices dialog where the user can select which devices are monitored and added to the Status Bar. See also: Monitored devices
Events Log	Displays messages generated by the Print text and Print number event sequence objects.
View Error Log	Error messages appear, when generated, at the bottom of the MASsoft window. The last twenty messages are stored as the error log (on a per mass spectrometer basis); this can be accessed by this command which enables the error log for the current session to be displayed. This command is grayed out if no error log has been generated.
Maintain	The Maintain sub-menu provides access to the following functions; Degas, Auto Tune, Auto Mass Align and Clear Mass Table. See also: Degas Auto Tune Auto Mass Align Clear mass table
Configure Auxiliary Inputs...	Configure the auxiliary analogue inputs by opening the Auxiliary Input Editor dialog. See also: Analogue inputs
Add New Instrument...	This option is used to define the communication settings for a new instrument by opening the Connections Settings dialog. See also: Connection settings
Import Instrument...	<i>This feature is not described in this version of the manual. Please contact Hiden Analytical for a manual update.</i>
Export Instrument...	<i>This feature is not described in this version of the manual. Please contact Hiden Analytical for a manual update.</i>

Connection Settings...	The Connections Settings dialog will be opened and the settings for the currently connected instrument can be examined and changed. See also: Connection settings
Connection State	Connected, Disconnected, Removed.
Reinterrogate	<i>This feature is not described in this version of the manual. Please contact Hiden Analytical for a manual update.</i>
Explore	Allows the presence of recently switched-on mass spectrometers to be confirmed. Any mass spectrometer found by this command is added to the Instruments list. If a new mass spectrometer is detected, it is interrogated and its configuration read back. The status of a mass spectrometer is shown on the title bar of the mass spectrometer's window. Where an existing mass spectrometer is detected, the relevant mass calibration table will be downloaded from the PC.
Instruments list	<i>This feature is not described in this version of the manual. Please contact Hiden Analytical for a manual update.</i>

This topic is not complete in this version of the manual. Please contact Hiden Analytical for a manual update.

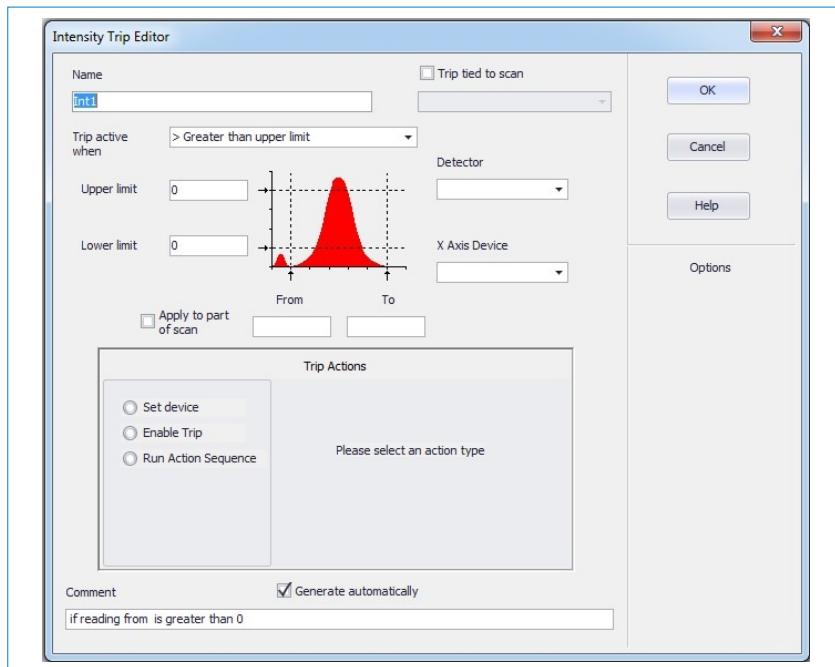
Intensity Trip Editor



The **Intensity Trip** , performs a comparison of acquired data against set limit values, and perform output actions as a result of these comparisons. Data may be acquired from one particular scan, or it may be derived from any scan acquiring the correct data.

Intensity trips can be used to enable other trips, start an event sequence or provide a signal to external equipment when an acquired signal is in a certain state.

The **Intensity Trip Editor** dialog is opened when a **New Intensity Trip** event is selected from the **Automation** popup menu, or when an **Intensity Trip** is edited.



Fields in the **Intensity Trip Editor** are:

Name

The name assigned to the Intensity Trip.

Trip tied to scan

When this is checked, the associated combination box contains a list of the current scans in the tree, and the trip may be tied to one of these. If this option is not checked, the trip applies to any scan which acquires data over the defined X-axis region and with the defined X-axis device.

Trip active when

This control gives a list of the comparison functions available; these are associated with the values entered into the **Upper limit** and **Lower limit** text fields.

Detector

Selects the detector (input device). If the trip is tied to a scan, this control is grayed out (not active) and the detector selected in the tied scan is displayed, but if the trip is global, i.e. not tied to a scan, an input device MUST be selected.

Upper limit

Selects the upper limit for the trip, in the units of the input device in the **Detector** field.

Lower limit

Selects the lower limit for the trip, in the units of the input device in the **Detector** field.

X Axis Device	This combination box contains a list of available output devices. One must be selected if the trip is global. If the trip is tied to a scan, this control is grayed out (not active) and the scanned device selected in the tied scan is displayed.
Apply trip to part of scan	When checked, the From and To text fields are enabled to allow the output device range to be set. If this is not set, the trip operates over the full range of the output
From	Sets the lower boundary of the output device range.
To	Sets the upper boundary of the output device range. To monitor a single point, set the From and To fields to the same value, e.g. to trip on mass 40 set From and To both equal to 40.
Trip Actions	This frame contains controls which allow the trip's output action to be programmed. Choosing one of the Set device , Enable Trip or Run Action Sequence options configures the frame contents and the controls to suit the output action selected.
Set device	When this option is selected, the values in the Value set when: Trip Active and Value set when: Trip Inactive fields are set for the output device selected in the pulldown box when the trip switches between active and inactive modes.
Enable Trip	The pulldown box contains a list of the trips and actions which can be enabled. When the trip goes active, the selected trip or action is enabled, and vice-versa.
Run Action Sequence	When this option is selected you can set an Action Sequence to run when: Trip Active and Trip Inactive . Choose a previously created action sequence from the pulldown box. The type of actions listed can be filtered using the Show sequences , Show all actions and Sort options.
Comment	The comment associated with the Intensity Trip. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation page](#)

Instrument settings

The instrument settings contains the default variable values of all the acquisition modes and the shutdown mode for an instrument. These device values are copied to a file's Global environment when a file is created. The instrument settings may hold values for variables that need to be shared by all files, e.g. the current multiplier voltage. The device values for each mode can be edited using the **Edit Instrument Settings** dialog, described below. There is one set of instrument settings per mass spectrometer. The instrument settings are independent of any experiment file currently in use.

The instrument settings contain the default variable values of all the acquisition modes and the shutdown mode for an instrument. These are used in place of File settings or Shutdown settings when its **Use** check box is not checked.

The Instrument settings are copied to a file's Global settings when a file is created.

The instrument settings may hold values for variables that need to be shared in common by all files, e.g. the current multiplier voltage.

There is one instrument environment per mass spectrometer. The Instrument settings are not part of the Experiment File. They do not change when a different file is opened.

When MASsoft is started, the Instrument settings in use the last time it was closed are reinstated. This means that the Instrument settings for each mass spectrometer are persistent, and will only change if edited or overwritten by opening and running an existing experiment file when the **Copy current settings to Instrument Settings at end of scan** option is selected in the **Edit, Preferences, Modes and Settings** tab.

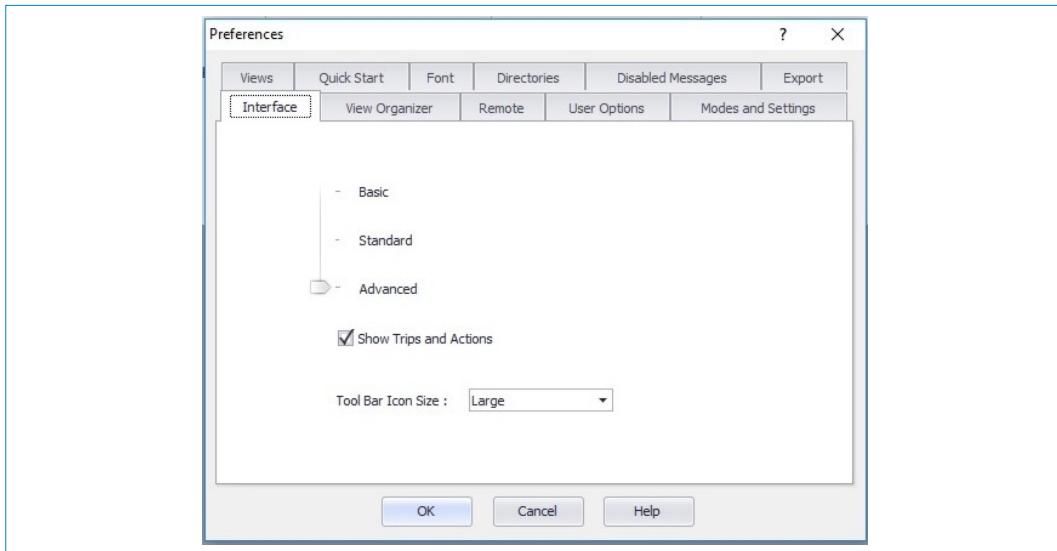
See also: [Modes and settings](#)

When a new MASsoft installation is started for the first time, the Instrument settings for each acquisition mode are default values interrogated from the control unit. It is recommended that the user save these values by creating a file, DEFAULT.EXP; this file can then be used to reload the original, default file settings if required.

If the instrument is being interrogated after a firmware upgrade then the control unit will have been reset to safe default values. The multiplier and first-dynode voltages (if fitted) will be set to 0V. Both filaments will be off. The original values may be re-instated by running a recent file created prior to the upgrade.

See also: [Edit Instrument Setting dialog](#)

Interface preferences



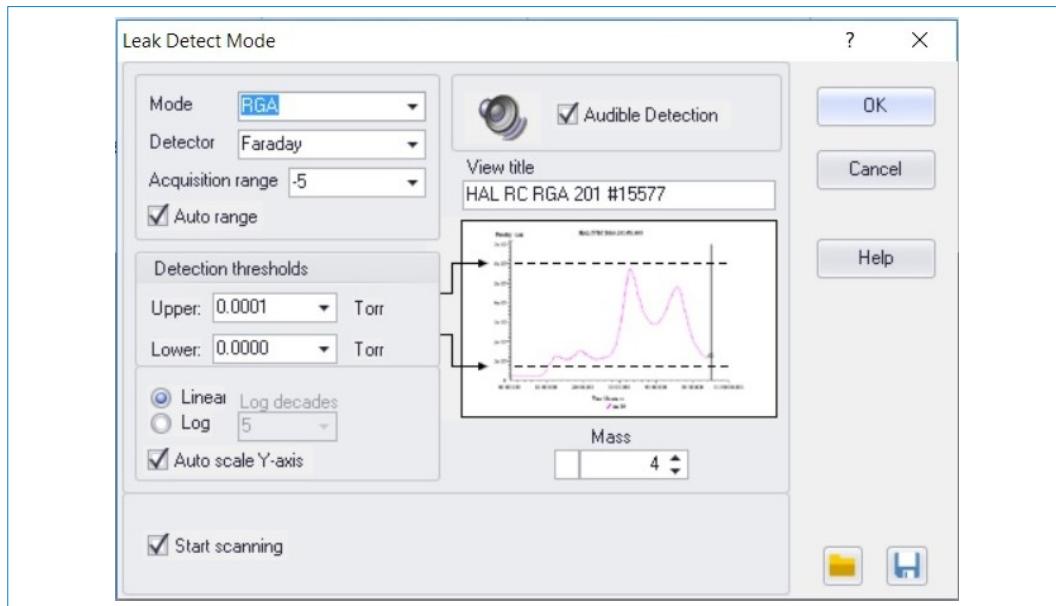
To view the Interface preferences select **Preferences..** on the **Edit** menu then select the **Interface** tab.

- | | |
|------------------------------|--|
| Basic | Provides the bare minimum of MASsoft features. MASsoft files may be opened and run but not edited or created. |
| Standard | Basic scan creation options are allowed, trips and events are enabled. Tune, system and library options are permitted. |
| Advanced | More scan creation options are available, background subtraction is enabled. |
| Show Trips and Events | Trips and events are available in Standard, Advanced and Full but may be hidden if Show Trips and Events is disabled. |
| Tool Bar Icon Size | A choice from three sizes for the Tool Bar Icon Size may be made. |

Leak Detect Mode dialog

Clicking the Leak Detect Scan button in the Easy Scans opens the **Leak Detection Mode**

dialog which sets the variables to build a scan tree for easy leak detection; it creates a display for the monitored mass on the automatically-attached view.



Some of the dialog box items in the **Leak Detection Mode** dialog are common to other scan mode dialogs.

See also:

[Common dialog items](#)

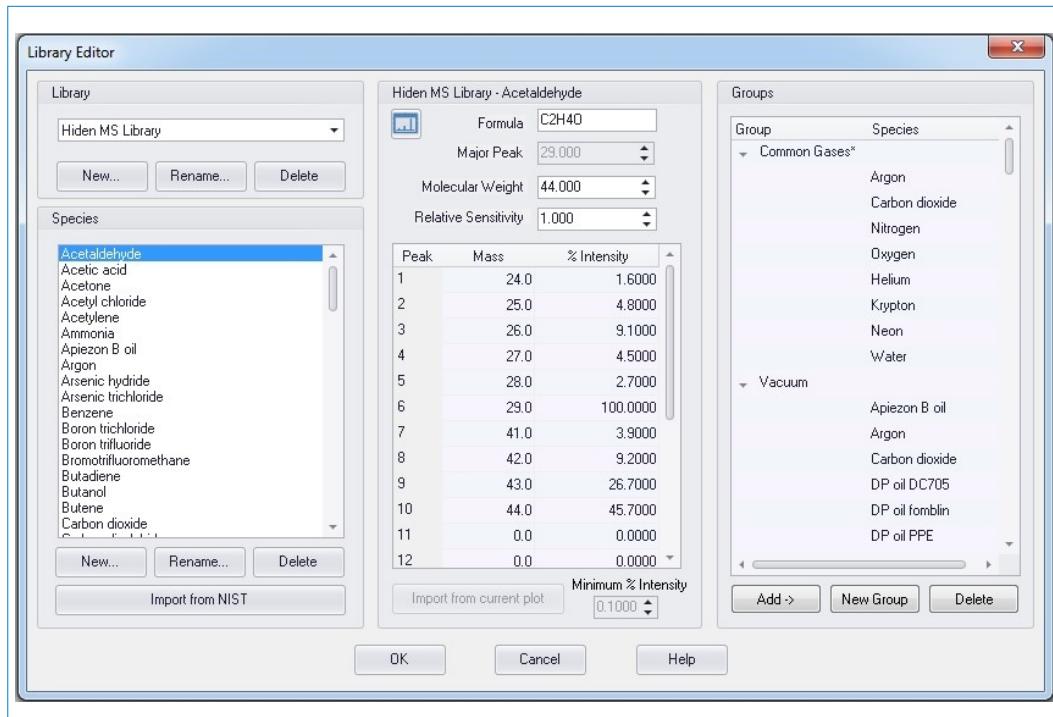
- | | |
|------------------------------------|---|
| Detection thresholds Upper: | Selects the upper leak detection rate. |
| Detection thresholds Lower: | Selects the lower leak detection rate. |
| Audible Detection | If selected, the PC gives an audible indication of leak rate. If the PC is capable of generating a variable frequency, the tone rises with increasing leak rate. Where the PC cannot generate a variable frequency, the audio output is a series of single frequency pulses, the rate of which increases with the leak rate. The audio capability of the PC is determined by the hardware fitted and the drivers loaded. Check the PC and the Windows sound drivers to determine the system's capabilities. |
| Mass | The mass of the gas used for leak checking. Usually, this will be mass 4 for helium. Mass 40 for argon is often used when leak checking cryo-pumped vacuum systems. |

Library

A component library is a database of information on the cracking pattern and relative sensitivity of reference species acquired under standard conditions. Libraries of spectra acquired in various acquisition modes (such as RGA, positive ion SIMS and negative ion SIMS modes, etc.) and for various purposes (e.g. Gas Analysis, Plasma etching, etc.) may be created. There is no limit to the number of libraries which can be created. A default library (called Hiden MS Library) is supplied with MASsoft. Other libraries (such as SIMS) may be supplied with particular instruments. The values in the default Hiden MS library are either taken from literature, or obtained from a typical Hiden RGA MSIU at 70 eV.

Component libraries are used in **Peak Identification**, **Quantitative Analysis** and to create **Easy Scans**.

The **Library Editor** dialog is accessed from the **Library...** option of the **Edit** menu. An example is shown below for the **Hiden MS Library**.



Library panel

The Library dropdown list box allows you to select an existing library. The default Hiden MS Library is supplied with MASsoft. Below the library pulldown list are buttons for:

New	Create a new library. Enter a name for the library in the displayed dialog. A name may be up to 32 characters long but it must not contain any spaces. Library names are case insensitive; “SIMS” and “sims” are deemed to be the same.
Rename	Rename an existing library using the displayed dialog. If the library name is not unique a warning box will be displayed
Delete	Delete an existing library. A warning message is displayed if you select this option. Click the Yes button to complete the deletion.
Import from NIST	Imports a species from a NIST file (.msp), which can be exported from the NIST database. A dialog is displayed where you choose the file to open and the spectra of the species to import from within that file. The name for the new entry will default to that of the NIST species. A new entry is created in the species list and the peaks table is set to the cracking pattern data of the species in the file. You are still required to enter a Formula, Molecular Weight and Relative Sensitivity of the species.
Species Panel	<p>Below the Library panel, the Species box lists all the species which are included in the currently selected library. When a new library has been created this list is empty.</p> <p>Control buttons allow the editing of the library contents:</p>
New	Create a new library entry. Enter the name for the library entry in the displayed dialog. If the compound name is not unique, a warning box is displayed.
	Species names are case insensitive; “AIR” and “air” are deemed to be the same.
Rename	Rename an existing library entry using the displayed dialog.
Delete	Delete the selected library entry. A warning message is displayed if you select this option.
Library entry panel	<p>For each Species entered into a library the details for that entry are displayed in the middle panel. This panel contains fields for Formula, Major Peak, Molecular Weight, Relative Sensitivity and a table of the cracking pattern associated with the entry. Existing values can be viewed or edited.</p> <p>When a new entry has been added to the library the Formula, Molecular Weight, Major Peak and Relative Sensitivity fields will be blank or set to 0.</p> <p>Mass and Intensity values for up to twenty peaks may be entered, these fields are initially set to 0.</p>

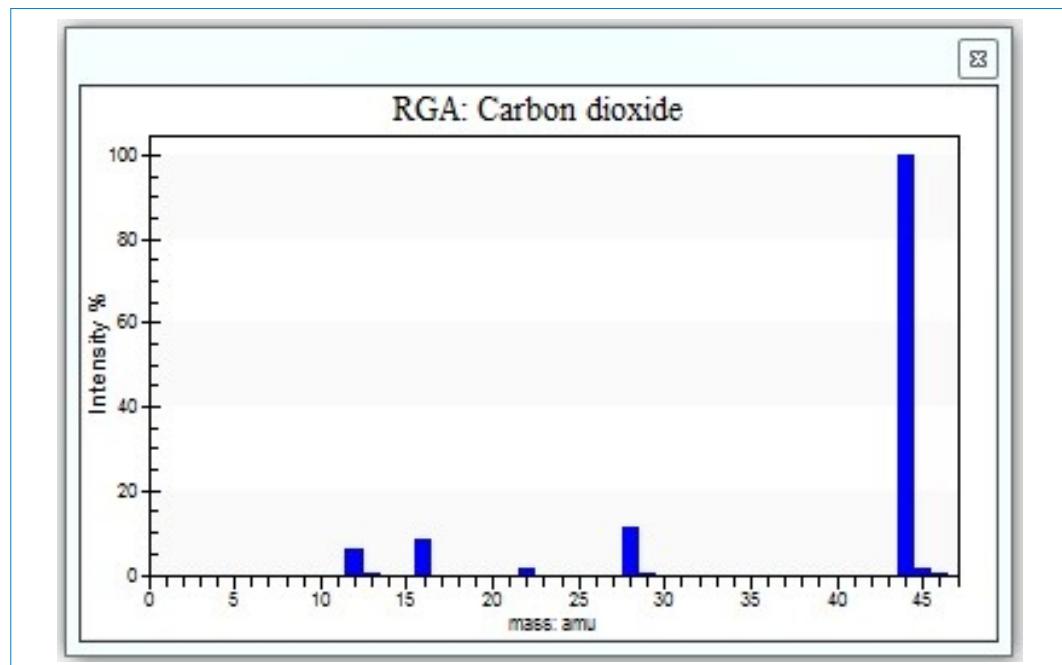
Formula	Enter the formula of the current library entry. This may be left blank.
Major Peak	Enter the mass of the largest peak in the cracking pattern of the current library entry.
Molecular Weight	Enter the molecular weight of the current library entry in atomic mass units (amu). This may be left set to 0.
Relative Sensitivity	Enter the relative sensitivity of the current library entry. If the relative sensitivity is not known enter a value of 1.
	The sensitivity of the mass spectrometer to different species varies for a number of reasons; how easily the component is ionised in the source, how efficiently the resultant ion is transmitted through the mass spectrometer quadrupole filter and, if using a Secondary Electron Multiplier (SEM), how many electrons are produced when the ion hits the detector (or the probability of producing an output pulse if using pulse-counting SEM).
Peaks Table	Each library entry contains a table of mass and intensities for up to twenty peaks. The table has columns for Peak , Mass and Intensity . Peaks should be added in ascending order starting from the first peak in the mass spectrum.
Peak	Displays the identification number of the peak. This field can not be edited.
Mass	Displays the mass of the constituent peak. To edit, click in the field and type a new value.
% Intensity	Displays the intensity of the constituent peak as a percentage of the major peak intensity, in the range 0.001 to 100. The major peak intensity should always be set to 100.00. All other peak intensities are relative to this. To edit, click in the field and type a new value.

Import from current plot

Imports the data from the currently selected bar plot view. A message is displayed asking if you wish to create a new species, clicking Yes will display a dialog asking for the name of the new species to add to the list of species in the current library, with peaks imported from the plot. Clicking No will paste the peaks from the plot into the peak table of the currently selected species. A bar plot must have focus (the title bar of the plot must be clicked on), prior to displaying the **Library Editor** dialog in order to carry out this operation. The **Minimum % Intensity** determines the cut off in peak height. Peaks with normalised intensity below this value are not added to the table. This reduces the number of small peaks and removes noise. Up to 20 peaks are added to the table in mass order. If more than 20 peaks meet the minimum height, then the highest intensity peaks are added.



Pressing the icon button in the top left corner of the **Library entry panel** pops up a plot showing the peaks which have been entered into the table for the currently selected species. This is to give a visual representation of the cracking pattern / peaks associated with that species. An example is shown below for Carbon dioxide in the Hiden MS Library.



Groups

On the right of the dialog is the **Groups** panel showing which groups have been added to the library and what species they contain. These groups are used in MASSsoft, for example with

Peak Identification, to allow a subset of a library to be considered based on known chemistry.

The Hiden MS Library has groups **Common Gases, Vacuum, Semiconductor, Reaction chemistry and catalysis, Bio-process, Medical, Solvents, Environment and Refrigerant**.

Below the groups list are three buttons:-

- | | |
|------------------|--|
| New Group | Creates a new empty group. A dialog appears into which you can enter the group name. The group name can not already exist. |
| Add-> | Adds the currently selected Species to the currently selected Group. A species can be added to multiple groups, but only once to each group. |
| Delete | Deletes either the currently selected Group, or the currently selected Species from the group. |

Right-Clicking in the groups list displays a popup menu including the above and in addition the following options

- | | |
|--|--|
| Unselect default for Peak Identification / Select default for Peak Identification | Library groups are used in the peak identification method to filter the species which are included in the optimisation based on known chemistry. When a group is selected for peak identification, its name is post-fixed with an asterisk (*). Species which are members of this group will be included by default in the peak identification. An unselected group is not by default included for peak identification, but can be manually selected if required via the Peak Identification dialog. |
| Rename Group | The group name can be edited using this option |
| Changes to libraries | Permanent changes to the library files only occur when the Library Editor dialog is exited.

Pressing the Library Editor dialog OK button will close the dialog making all changes to the libraries permanent. If any invalid entries have been made you are warned.

If you have made changes and the Cancel button is pressed then a warning message is displayed asking if you want to discard the changes. Click Yes to close the dialog discarding changes, or No to return to the dialog. If no changes have been made then Cancel will close the dialog. |

See also:

[Cracking Patterns](#)

[Relative Sensitivity](#)

[Quantitative Analysis](#)

[Peak Identification](#)

[Easy Scans](#)

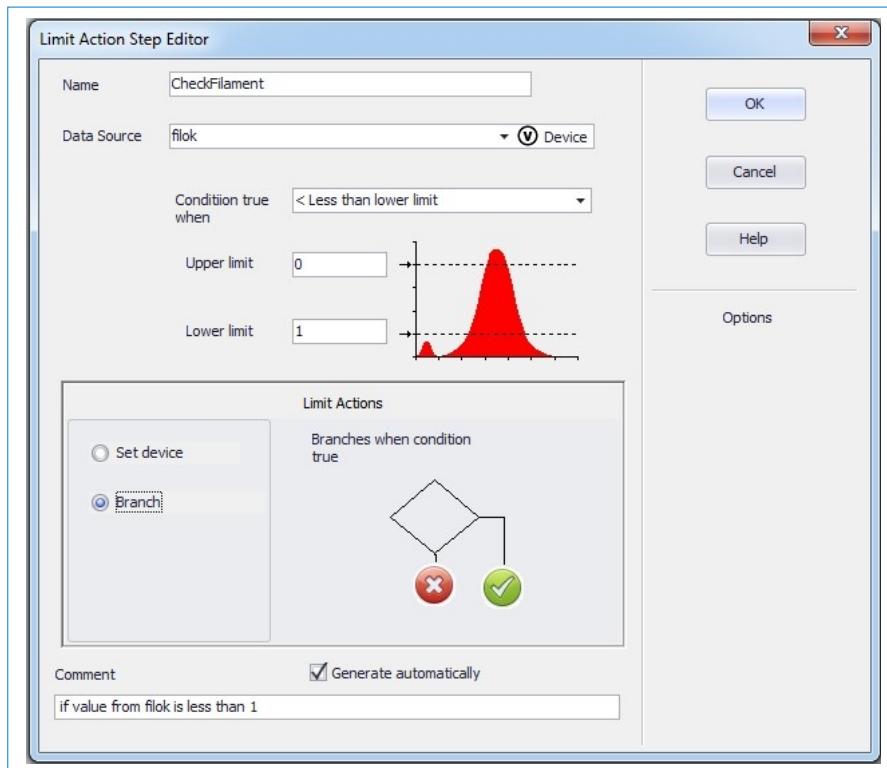
Limit Action Step Editor



The **Limit Action** , allows a value to be compared with upper and lower limits and an action taken depending on whether or not the limits were met. One of the actions a Limit Action can take is to branch to another Action object. The Limit Action is equivalent to an IF statement in high level programming languages.

The **Limit Action Step Editor** is displayed when editing a **Limit Action**.

An example is shown below where the device *filok* is read, which returns 1 if the filament is intact, 0 if it is open circuit. Action is taken when *filok* is less than the lower limit of 1.



Fields **Limit Action Step Editor** are:

Name	The name assigned to the Limit Action.
Data source	The source where the value to check is being taken from. A pull down allows you to choose between Device and Action step .
Device	The data source is a device.
Action step	The data source is a value returned from an action.
Condition true when	Specifies a list of logical condition with which to check the source value, against either the Upper limit and / or Lower limit .
>Greater than upper limit	True if the value is greater than the Upper limit .
< Less than lower limit	True if the value is less than the Lower limit .
> Greater than upper limit with hysteresis	True if the value is greater than the Upper limit and Lower limit .

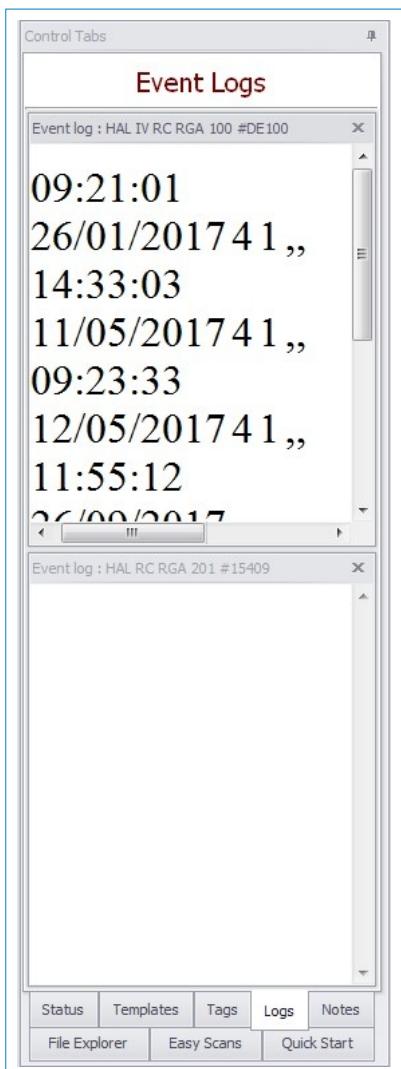
< Less than lower limit with hysteresis	True if the value is less than the Lower Limit and Upper limit .
Out of band limit	True if the value is out of the band limit from Lower limit to Upper limit .
>< In band limit	True if the value is within the band limit from Lower limit to Upper limit .
= Comparison	True if the value is equal to both the Lower limit to and the Upper limit . Enter the values for comparison in the Upper limit and / or Lower limit fields. Note that counter intuitively, the value for the Lower limit can be higher than for the Upper limit (as pictured in the example)
Limit Actions	The limit actions can be used to set a device value or to create a branch in the Action Sequence.
Set device	Choose the Device to set , and the Value set when the condition is false and when it is true.
Branch	A branch is added to the Action Sequence. One path of the branch occurs when the condition is false, and other when the condition is true.
Comment	The comment associated with the Limit Action. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation page](#)

Logs

When the **Events Log** option of the **Instrument** menu is selected, an **Event Log** is generated for the currently selected instrument. If the Control Tabs frame is visible, then the log will be displayed docked within the **Logs** tab. An example is shown below where logs for two instruments have been added to the tab, although one log is empty.



A log can be undocked from the Logs tab becoming a floating window.

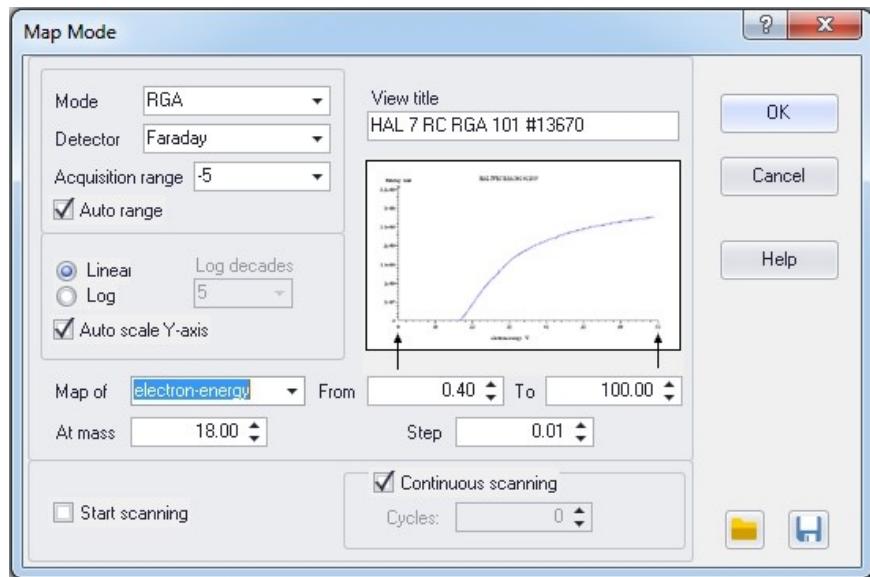
See also:

[Event Logs](#)

[Easy Scans](#)

Map Mode Scan

Clicking the **Map Scan** button of the **Easy Scans** tab in the Control Tabs frame opens the **Map Mode** dialog box for a simple linear scan with a choice of variable to be scanned and mass to be used.



Map scans are useful for selecting suitable variable operating points, for setting limits for auto-tune operations, or for appearance potential experiments where electron energy is scanned.

Map of	Sets the mapped variable. The Map of list box only contains the commonly mapped variables; other variables can be entered by typing the name into the box..
From	Sets the initial value of the variable specified in the Map of option.
To	Sets the final value of the variable specified in the Map of option.
At mass	Sets the mass at which the variable is to be mapped. The mass selected here is set into the Global box in the mass spectrometer control window.
Step	Sets the increment for the specified variable.

The other items in the **Map Mode** dialog are common to other scan mode dialogs.

See also:

[Common dialog items](#)

[Easy Scans](#)

Mass alignment

The microcomputer in the control unit maintains a mass calibration table to allow it to accurately set the masses demanded by the scans, and the automatic mass alignment option is used to update and modify this table. Up to eight masses can be used as alignment markers for which the system knows the accurate mass and the corresponding DAC value.

The easiest way to perform mass alignment is by selecting Instrument, **Maintain, Auto Mass Align...**

See also:

[Auto mass align](#)

This allows easy setting of alignment masses and selects the correct **Scan Editor Advanced** dialog box options automatically.

See also:

[Advanced scan options](#)

If used manually, a scan tree of up to eight PROFILE scans should be set up. The start and stop masses of these scans must symmetrically span the calibration peaks to be used within the vacuum environment of the analyser, as the calculated centre of the peak is assigned to the exact centre of the scan. Thus, if M is the accurate mass of the calibration compound:

$$M = \frac{\text{stop mass} - \text{start mass}}{2} + \text{start mass}$$

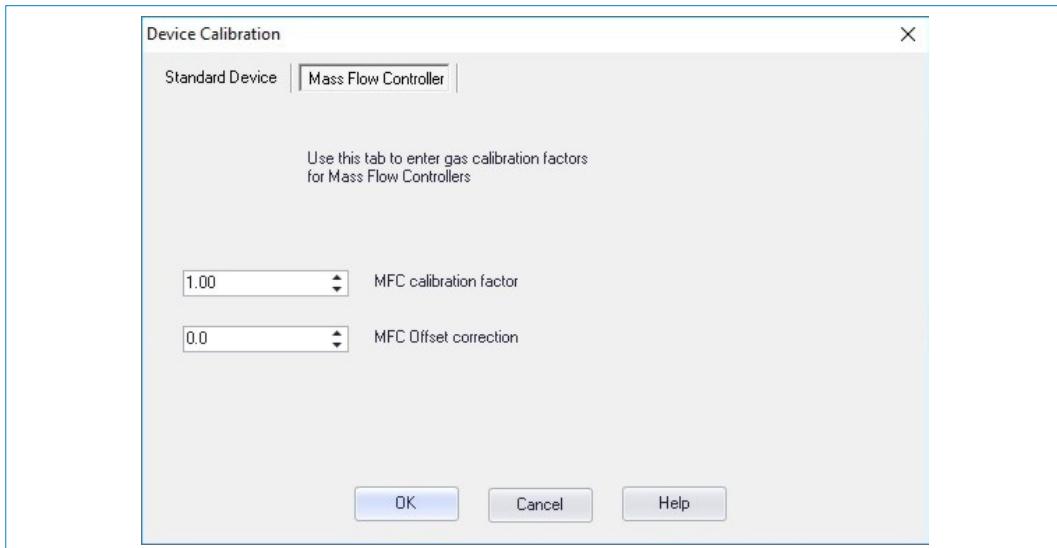
In practice, a total scan width of 1.5 amu (i.e. ± 0.75 amu) is recommended where the mass scale is not far out, so the start and stop masses can be assigned as:

$$\text{start mass} = M - 0.75 \quad \text{stop mass} = M + 0.75$$

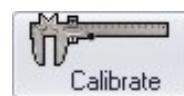
Calibration masses should, where possible, be equally distributed over the mass range of the instrument. Choosing the last (highest mass) peak too close to the next lower mass peak can give problems as small errors are magnified. In case of doubt, or if problems arise, please contact Hiden Analytical Limited.

Mass flow controller

The **Mass Flow Controller** tab allows the slope and intercept to be entered using published Mass Flow Controller (MFC) gas calibration factors when the output DAC is controlling a MFC. The **Slope** value in the **Standard Device** tab will be calculated as the reciprocal of the **MFC calibration factor**.



The dialog is opened by selecting **Edit Instrument Environment...** on the **Instrument**



menu, selecting an item then clicking the **Calibrate** button and selecting the **Mass Flow Controller** tab.

Also see: [Device calibration](#)

MASsoft files

For a single experiment, MASsoft saves data in several files in a directory on the PC's hard disk; the files all have the same name but have different extensions as follows:

xxx.EXP	Master file
xxx.SCN	Scan structure
xxx.ENV	Environmental data
xxx.DAT	Experimental data
xxx.ANN	Annotation file – this file is written when the file is closed and contains data about the views

MASsoft terms

The table below gives a definition of MASsoft terms and where appropriate the equivalent terms in previous versions of MASsoft.

MASsoft Term	Previous MASsoft versions	Description
Instrument Settings	Instrument Environment	A collection of device values (variables) for Shutdown mode and all Operating modes that belongs to the Instrument.
File Settings	Global Environment	A collection of device values (variables) for all Operating modes that belongs to the File.
Scan Settings	Local Environment	A collection of device values (variables) for one Operating mode that belongs to a specific scan in the File.
Shutdown Settings	Shutdown Environment	A collection of device values (variables) for Shutdown mode that belongs to the File.
Shutdown state	Shutdown	The state of having the values in the Shutdown Settings applied in the instrument.
Active state	Active	The state of having the values in the Operating settings of the Active mode applied in the instrument.
Protected state	disabled	In the Protected state the values of the Shutdown Settings are applied in the instrument and power supplies are disabled. The instrument boots up in the Protected state.
Tripped state	disabled	In the Tripped state the values of the Shutdown Settings are applied in the instrument and power supplies are disabled as a result of a Protection Trip having occurred.

MASsoft Term	Previous MASsoft versions	Description
Shutdown (v)	Shutdown	
Activate (v)	Active	
Start (v)	Go	
Stop (v)	Stop	
Abort (v)	Abort	
mode	mode	
Shutdown mode	Shutdown	
Active mode	The Global mode	The current Operating mode. The values of the settings in the Operating mode are applied in the instrument when the Activate or Start menu options are selected. The Active mode is the default mode of all scans unless a scan is Pinned to a specific mode.
Pinned mode	The scan's mode	When a scan is pinned to an Operating mode the scan will use that mode regardless of the mode chosen as the Active mode.
Operating modes		All modes other than shutdown:RGA , +ion SIMS –ion SIMS –ion RGA etc
Operating settings		The settings in an operating mode
Shutdown settings		The settings in shutdown mode
Settings		A collection of device values (variables).
Variable		Device value.
Parameters		Avoid this term. Parameters are named values that can be set or read from the instrument, that are not associated with a device. e.g IP-address.
Device	Device	Something that can be set (an output device), read (an input device) and usually scanned in the instrument. Often correspond to a variable voltage power supply

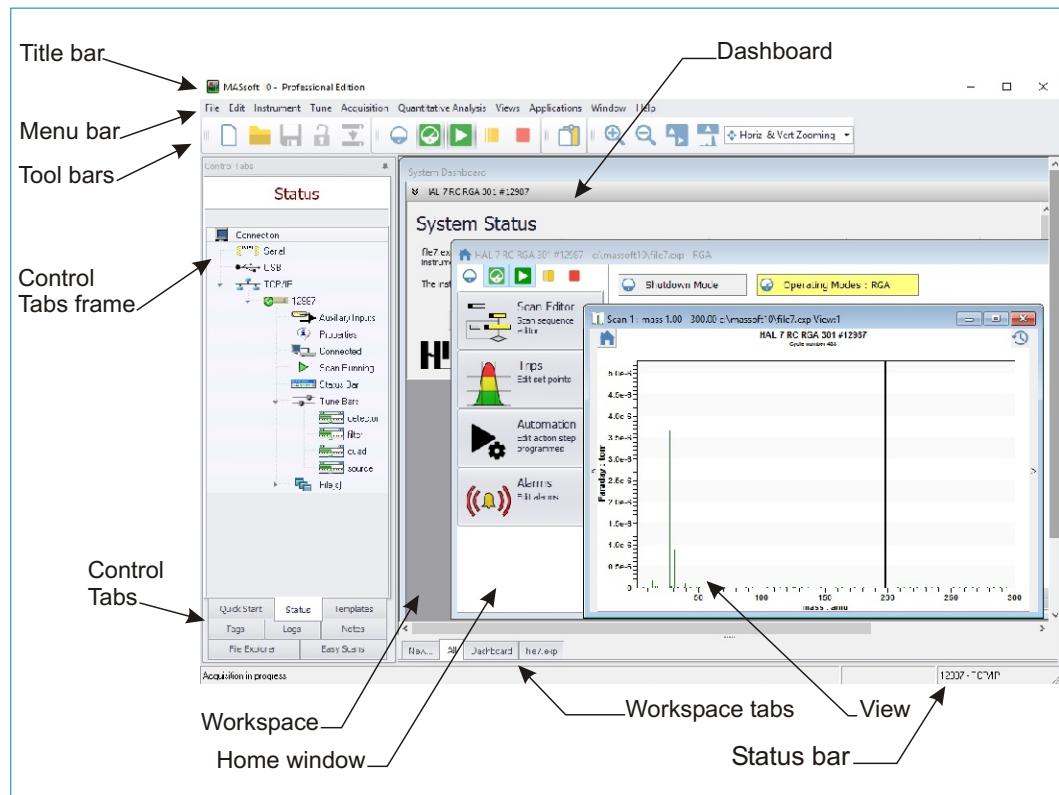
MASsoft Term	Previous MASsoft versions	Description
Action Sequence	Event Sequence	A programme consisting of individual Action steps.
Action step	Event	
Trip	Trip	Events that occur when a set-point is exceeded.
Event	Trip	Something that triggers an action, either running an Action Sequence or setting a value to a device.
Event state		An Event can either be Active (Tripped) or Inactive (Normal).
Protection Trip		Built in trips that check that it is safe to operate the instrument. External trip, Source pressure trip (“Source pressure too high”), SEM limit trip (“Signal too high for SEM”).
Instrument	Mass Spec	The generic term instrument is used in place of Mass Spec
Instrument menu	Mass Spec menu	Contains all actions relating to a specific instrument
Acquisition menu	System menu	Contains actions for setting the mode and starting and stopping scans. Maintenance has moved to the Instrument menu and is now Maintain.
Home Window	Scan Tree Window	The home window now includes multiple pages, one of which is the scan tree. The pages are selected from a toolbar down the left side of the Home Window.
View	View	A Window containing graphical or tabular data.
Scan Editor Page	Scan Tree Window	The Scan Editor page is on the Home Window.
Automation Page	Event Sequence Editor	The Tree View based Event Sequence Editor has been replaced with a flow chart Action Sequence editor. Action Sequence run in the Interface Unit.

MASsoft Term	Previous MASsoft versions	Description
Trips Page	(Formerly part of the Event Sequence Editor)	A page containing a Trip Table. Generates an action sequence that runs in the Interface Unit.
Alarms Page		A page containing an Alarm Table. Alarms allow MASsoft to take actions when limits are exceeded.
Mimics Page		A page on the Home Window containing mimic diagrams of the system.
Raster Page	(Raster dialog box accessed from the Global Environment)	Not Yet Implemented!
Easy Scans	Gallery	Same thing, different name and icons!

Control unit	The main electronics unit running the mass spectrometer. This will be either the 2U high RC Interface typically used in RGA and gas analysis systems or the 7U high Mass Spectrometer Interface Unit typically used with the science instruments. The control unit connects to the PC running Windows 10 via a serial communications interface.
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MASsoft window

A typical MASsoft window is shown in the figure below.



Title Bar

Contains the application title, MASsoft, and the normal Windows maximize, minimize, close and restore buttons.

Menu Bar

Gives access to all the MASsoft control commands. A description of each Menu bar command is given in the Reference chapter of this manual.

Some of the Menu bar commands will only be available when the mass spectrometer is running, at other times they will be grayed out.

See also: [Menu bar](#)

Tool bars

There are a series of Tool bars that are initially displayed in one line. Which Tool bars are displayed and which buttons are active depends on the state of MASsoft.

See also: [Tool bars](#)

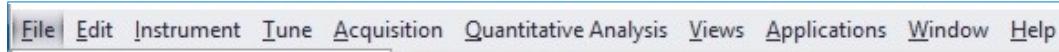
Control Tabs

In the bottom left of the MASsoft window are the eight Control Tabs.

See also: [Control tabs](#)

Control Tab frame	The Control Tab frame occupies the left of the MASsoft window and its contents change depending on which control tab is selected.
Workspace	The right hand side of the MASsoft window is occupied by the Workspace in which the Home window, Views containing MASsoft data and other MASsoft windows are displayed.
Dashboard	The Dashboard is displayed on the Workspace and displays the instrument status for all the instruments for which MASsoft is configured..
Home window	The Home window is displayed in the Workspace. It contains multiple pages one of which is the Scan Editor Page.
View	A Window on the Workspace showing data in either a graphical or tabular format.
Workspace tabs	A series a tabs which determine what is shown on the Workspace.
Status bar	The bar at the bottom of the MASsoft window displays useful status information. This bar contains no controls.

Menu bar



The Menu bar gives access to all the MASsoft control commands.

Some of the Menu bar commands will only be available when the mass spectrometer is running, at other times they will be grayed out.

Also see:

[File menu](#)
[Tune menu](#)
[Applications menu](#)
[Help menu](#)

[Edit menu](#)
[Acquisition menu](#)
[Windows menu](#)

[Instrument menu](#)
[Views menu](#)
[Quantitative Analysis Menu](#)

MID graphical view

A MID Graphical View displays data as a trend plot.

This view can be created by highlighting a MID scan within the Scan Tree and selecting the **MID Graphical View** option from the Views Menu or clicking on the MID Graphical View

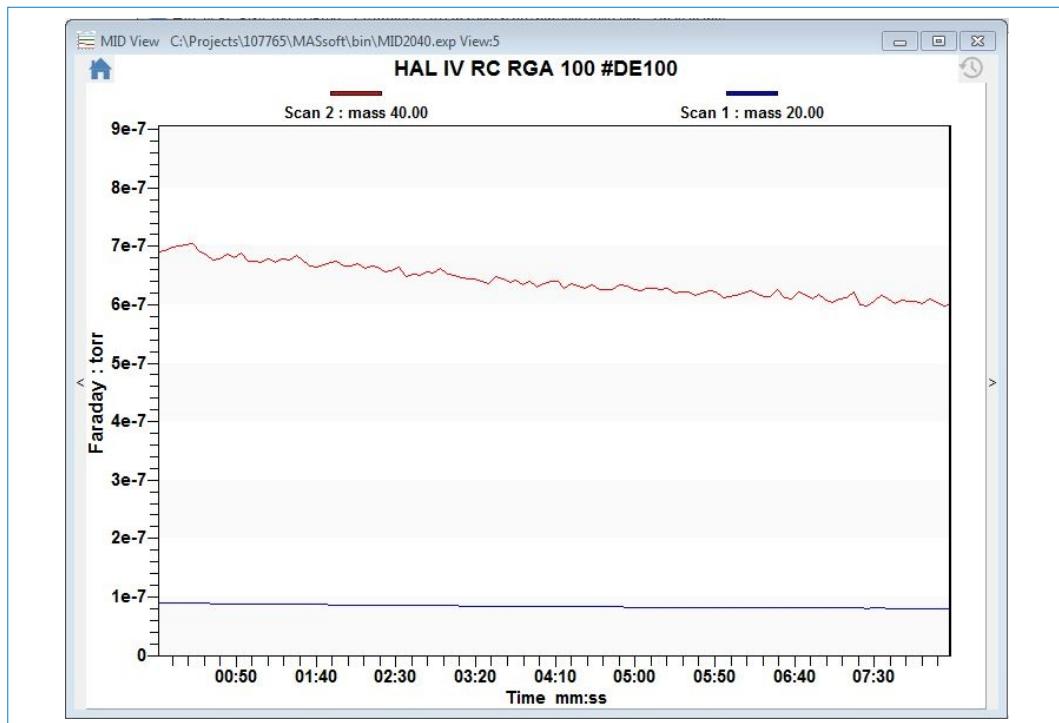


button on the toolbar. Alternatively a view can be created via the

Graphical/Tabular View Editor displayed using the **New Trend View...** option of the Views Menu.

When a MID graphical view is created or while a **MID Graphical View** is the active window, the Views Menu options change to include options applicable to the **MID Graphical View**.

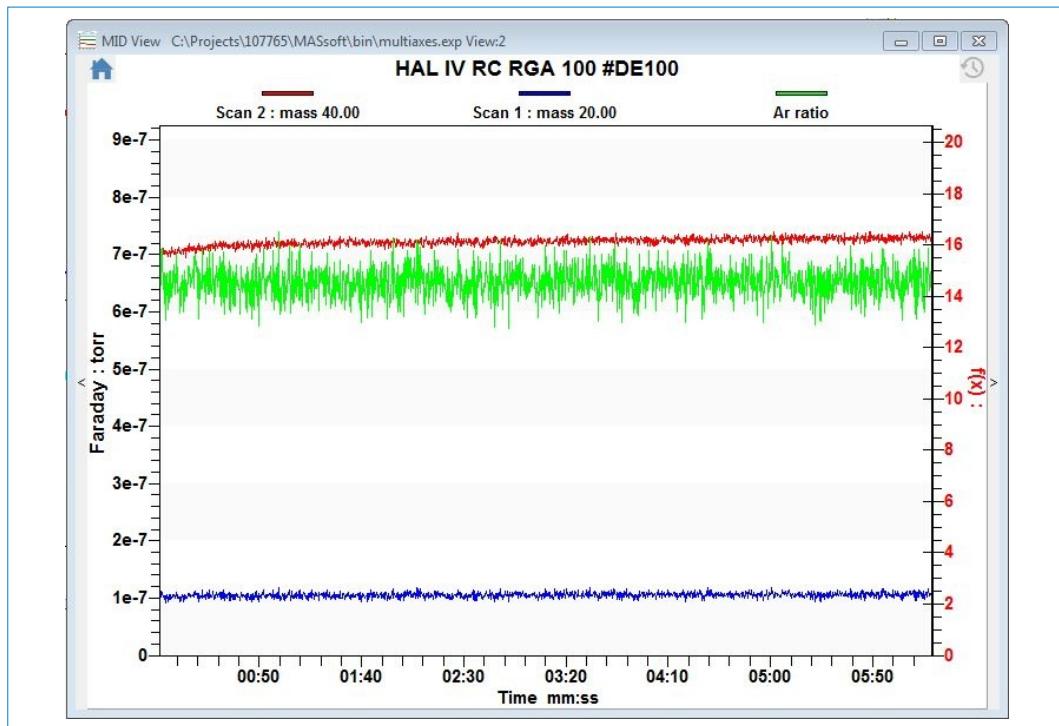
The example, below, shows trends for two mass values, 20 amu and 40 amu, plotted against elapsed time since the start of the scan.



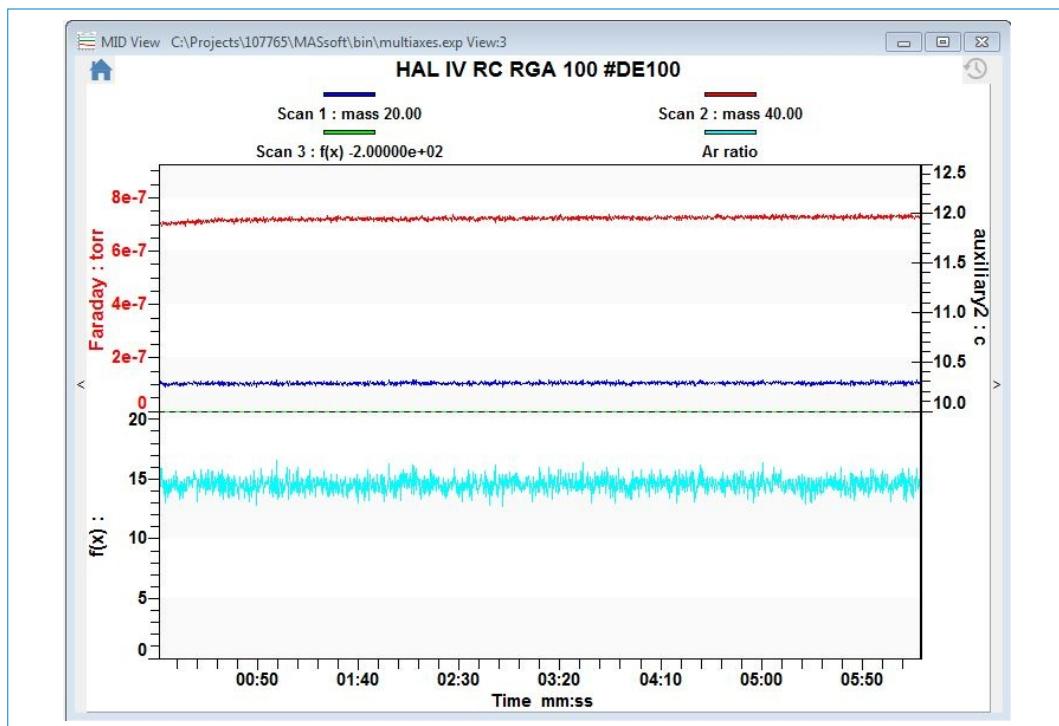
A tabular view, corresponding to the same data is shown in the MID Tabular View topic.

For the MID Graphical View the icon in the top right hand corner of the view is greyed out.

MID Graphical Views can have data displayed on a right-hand, as well as left-hand Y axis. When the plot has two or more Y axes, the axis is selected by clicking on any of the number annotations which mark the values of on that axis. The annotations on the selected axis are drawn in red. The following example shows a plot with **Ar Ratio (f(x))** added to the plot on the right-hand axis.



If a third or more axis types are required, then the axes can stack on the left, then right for multiple axis types. As shown below.



Note that it is not possible to zoom on stacked axes.

When an MID graphical view becomes the active window, the Toolbar displays a series of icons which control zooming and scaling operations to be performed on the plot.

MID Trend to MID Tabular View Statistics Tracking

Pressing the SHIFT button and moving the mouse while the cursor is over a MID graphical view will display a vertical line and below the plot the X coordinate value and highest peak value of the data displayed at that point in the plot.

If the left mouse button is clicked while pressing the SHIFT button, this displays a vertical line marking a position (X1) on the plot. Clicking a second time will mark a second (X2) line on the plot. If there is a MID Spreadsheet View associated with the same scan as the plot, the data range from X1 to X2 is then locked as the selected range in the MID Spreadsheet View. The statistics for the selected range are automatically shown including the Mean, Minimum, Maximum, Range, Standard Deviation, and Peak Integration. If there is no MID Spreadsheet View associated with the same scan as the plot, a MID Spreadsheet View spreadsheet is automatically created with the statistics displayed. If the SHIFT button is released and the mouse moved the X1 and X2 selections are cleared.

See also:

[Graphical view toolbar](#)

[MID Tabular view](#)

[Highest Peak Value](#)

[Scan tree](#)

[Views menu](#)

[Zooming](#)

MID graphical view menu options

Edit Trend View... Opens the **Tabular View Editor** allowing new data trends to be added to the current **MID Graphical View**.

Plotting Types Displays a sub-menu of Plotting Types. For a MID plot only the **Line** option is selectable. Data may be plotted on a **Linear** or **Log** (Log10) scale.

Grid Options Displays a sub-menu of Grid Options.

Title Opens a dialog to edit the title in the graph area of a view. By default, the view's title is the name of the currently connected mass spectrometer. The title is shown immediately below the view's title bar.

Configure X Axis Opens the **X Axis Properties** dialog for an MID plot.

Configure Y Axis Opens the **Y Axis Properties** dialog for an MID plot.

Graph Cursor When acquiring data, the graphics cursor can be switched on or off using this command.

- Source View** Designates the MID Graphical view as the “source” view for the **Background subtract** function. A tick mark beside **Source view** indicates whether a selected view is the source view.
- Background Subtract** Designates the MID Graphical view as the “target” view for the **Background subtract** function, then subtracts the data values in the “source” view from the data values in the selected “target” view. The result displayed in the “target” view. An operations window, describing the operation that has been performed, is displayed by default in the “target” view.
- Show Operations** If this view has been a target for **Background subtract**, then this toggles the operations panel on and off.
- Copy** This option only appears on the right-click popup menu. It copies the currently displayed range of data from the Graphical view to the Windows clipboard, allowing it to be pasted into another application such as Excel. In order to copy the plot as a graphic image use the **File Menu** and choose the **Export Plot As...** option.

See also:

[Background subtraction](#)

[Grid options](#)

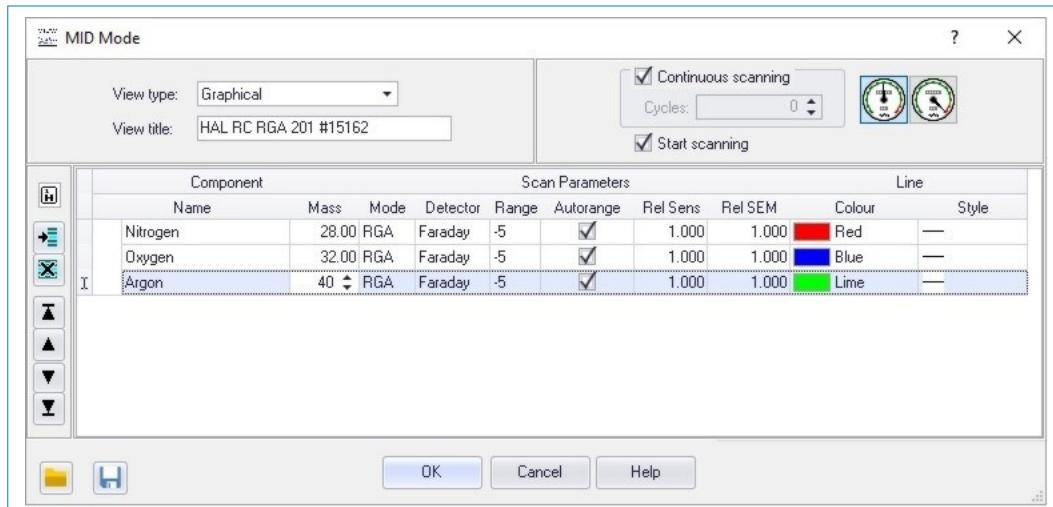
[MID graphical view](#)

[Plotting types](#)

[X Axis properties dialog](#)

[Y Axis properties dialog](#)

MID Mode dialog



Clicking the MID Scan button on the Easy Scans tab opens the **MID Mode** dialog for a multiple ion detection scan where a component (usually mass but could be total pressure or an analogue input) is plotted over time.

View type:	May be either Graphical, Tabular or one of each.
Optimise for Accuracy button	 The standard settings, 100% dwell and 100% settle, will be used.
Optimise for Speed button	 Optimises the scan structure so that data can be acquired as quickly as possible; this is achieved by setting all scans in the scan tree to use the Instrument mode currently selected in the global Environment Editor dialog. The Dwell time and Settle time are set to 3 ms and 2 ms respectively for scan structures containing a single scan; for scan structures containing multiple scans, the Dwell time is set to 10% and Settle time is set to 60%. <i>For example, when using either SEM -10 or Faraday -7 gain ranges, the settle time changes from a delay which allows the signal to fall to less than 0.05% of full scale to a delay which allows it to fall to less than 1% of full scale.</i>
	When the scan is started data retrieval will be paused.
Add component from library button	 Displays a drop-down list of components from the Library. Select the component to analyse. The major peak of the component will be added to the MID table, unless there is a conflict with another component in which case the Alternative Peak Selection dialog is displayed.
Insert component button	 Will add a new component after the currently selected component.
Delete component button	 Deletes the selected entry from the components list.
To Top button	 Moves the selected component to the top of the components list.
Move Up button	 Moves the selected component up one place in the components list.
Move Down button	 Moves the selected component up one place in the components list.

To Bottom button



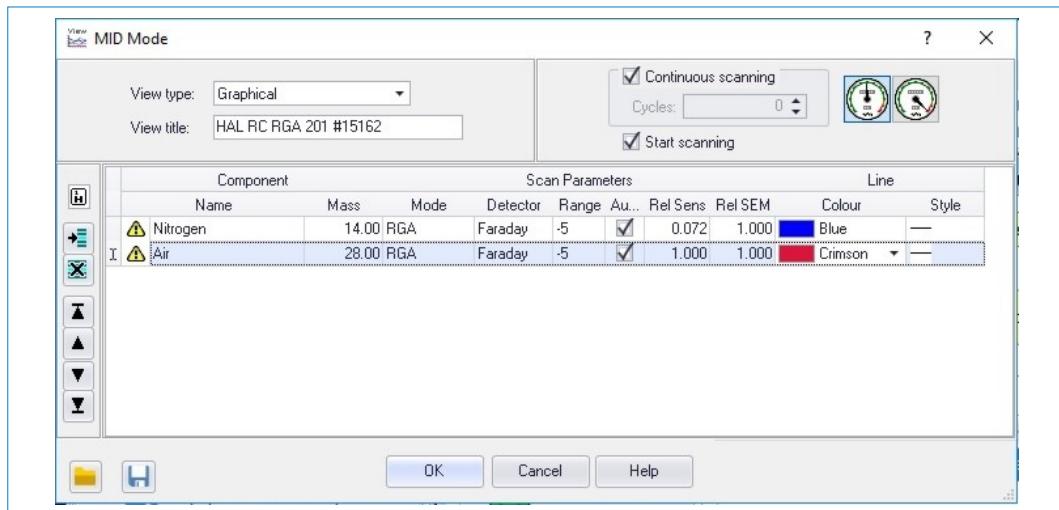
Moves the selected component to the end of the components list.

Changing the order of the scans in a scan tree is a useful technique that can be used when optimising an experiment for speed. In order to facilitate this there are a number of controls on the MID, auto-tune and auto-mass align dialog boxes that can be used to reorder the components in the table.

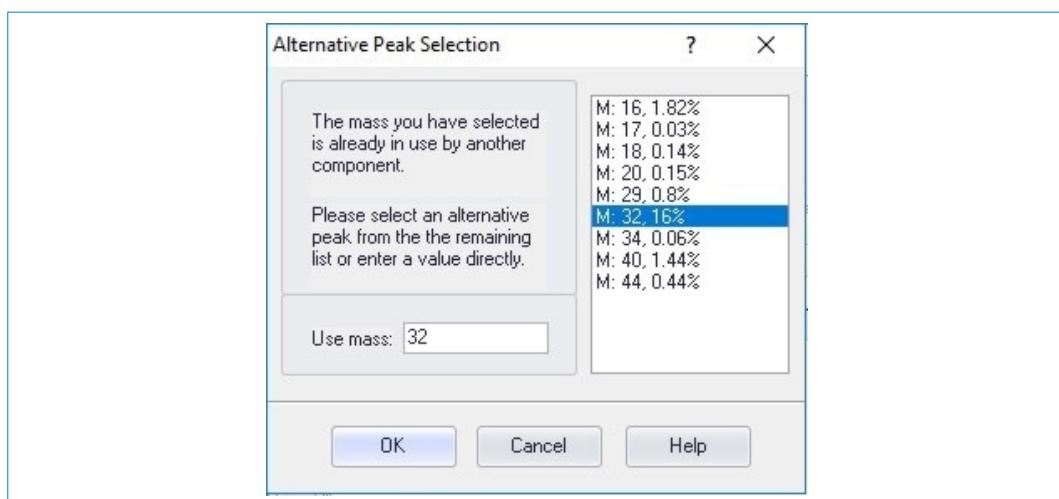
Possible conflicts due to overlaps in the cracking patterns of components are indicated in the



Component name column by a yellow warning triangle . This is displayed when two or more components have a common mass. In the figure below both air and nitrogen will give peaks at mass 14 and mass 28.



If the chosen mass for a selected component has already been added to the table the Alternative Peak Selection dialog is displayed from which an alternative can be selected.



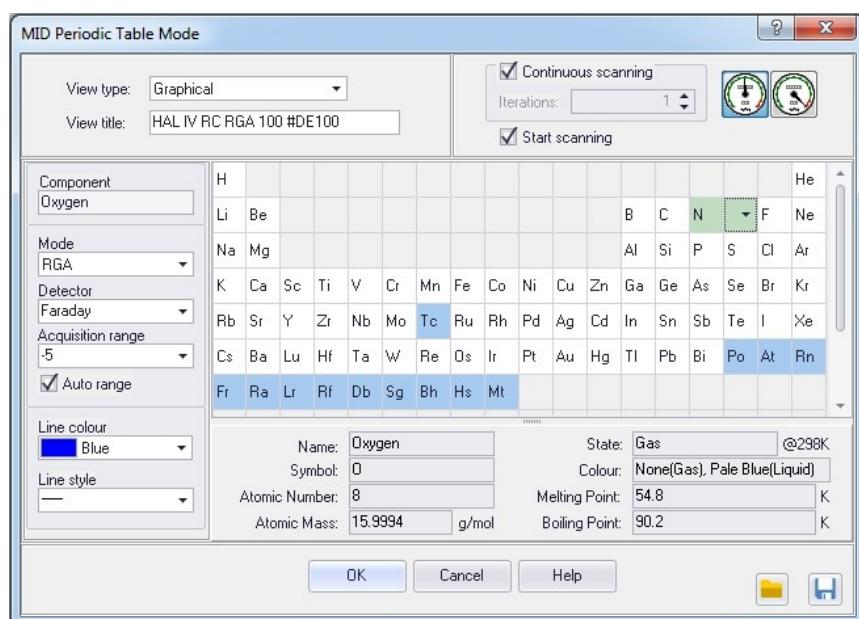
Some of the dialog items in the **MID Mode** dialog are common to other scan mode dialogs.

See also:

[Common dialog items](#)

MID Periodic Table Mode

Clicking the **MID Periodic Table Mode** button of the **Easy Scans** tab in the Control Tabs frame opens the **MID Periodic Table Mode** dialog box which allows multiple MID scans to be created choosing elements from the Periodic Table to select isotopes.



The elements to be monitored are selected by clicking on the element on the periodic table. A popup menu of associated isotopes is displayed, from which you choose the isotope to be monitored. The blue text indicates the main peak for the isotope.

After the element is selected it will change colour from white to green to indicate that it has been chosen. Elements that do not have a stable isotope appear blue and cannot be selected.

To deselect an element select (None) from the list of isotopes.

Just below the periodic table is a panel that provides information about the element currently selected, this includes amongst other things the name, symbol and atomic number.

This panel can be opened or closed by clicking the splitter bar at the top of the panel.

Select the required, **Mode**, **Detector**, **Acquisition range**, **Line colour** and **Line style** from the controls on the left hand side of the dialog box.

The other items in the **MID Periodic Table Mode** dialog are common to other scan mode dialogs.

See also: [Common dialog items](#)

[Easy Scans](#)

MID speed optimisation

An MID scan may be optimised to scan at high speed to acquire as much data as possible in a given time. This can be useful in fast gas reaction studies for example.

MID spreadsheet control

The tabular view contains a spreadsheet with a vertical scroll-bar which allows any part of the data to be viewed. Scrolling the visible rows of data in the spreadsheet can also be achieved using the mouse wheel and using the arrows keys.

Other key presses allow paging through the displayed data

Page Down Displays the next page of data.

Page Up Displays the previous page of data.

Home Displays the first row of data.

End Displays final row of data.

The first row of titles in the table is selectable which can be used to set up a different range of statistical markers for different data columns.

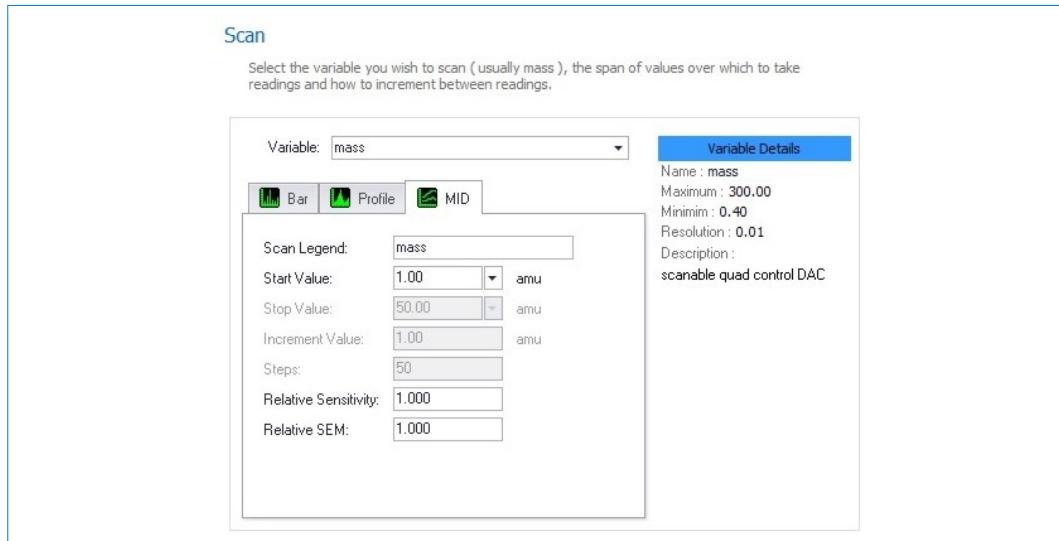
By left clicking with the mouse pointer in a cell within the spreadsheet a row of the visible data can be selected. Also when left clicking and dragging with the mouse, a range of data rows can be selected, which are highlighted in blue. The highlighted range of data may be copied to the clipboard or set as the marked range for statistical analysis.

It is also possible to select a range of data by selecting a row in the spreadsheet, then pressing SHIFT key and while still pressing the SHIFT key clicking on another row in the spreadsheet, then releasing the SHIFT key.

See also:

[MID tabular view statistics](#)

MID tab



The MID tab creates a scan which takes a single measurement at the value specified by the **Start Value:** setting. The default view created is a trend view of measurements against time.

This type of scan is typically used to create a scan tree that measures one or more masses of interest and monitors the change in these masses against time.

Scan Legend: Allows the scan legend name on views to be edited; the required name is typed into this box; up to 32 characters (including spaces) may be used. This name also appears on the **Scan** box. The scan legend defaults to the contents of the **Variable:** box.

Start Value: The scan start value for the variable selected in the **Variable:** list box.

Stop Value: Not applicable to MID scans.

Increment Value: Not applicable to MID scans.

Steps: Not applicable to MID scans.

Relative Sensitivity: Relative Sensitivity is a measure of the probability of ionising a molecule; the acquired intensity is divided by this value to give the reported value. The value for a particular ionising mode and parent molecule can be obtained from the appropriate library and, if the **Scan Gallery** or the Library button are used to set up an **MID** scan, the correct value is automatically inserted.

The reported intensity = (acquired intensity)/(relative sensitivity).

Relative SEM:

Relative SEM is similar to **Relative Sensitivity**; it is a divider which can be used to compensate for the inherent discrimination of the SEM detector. No standard values exist for this variable and a suitable value must be obtained by experiment. If a suitable value is not known, **Relative SEM** should be set to **1.00**.

Only one input device may be specified for each simple, co-variant or multi-variant scan group.

MID tabular view

A MID Tabular View displays trend view data in the form of a spreadsheet table; in addition to the basic data, statistical data for any part of the trend data can also be displayed.

This view can be created by highlighting a MID scan within the Scan Tree and selecting the **MID Tabular View** option from the Views Menu or clicking on the MID Tabular View



button on the toolbar. Alternatively a view can be created via the **Graphical/Tabular View Editor** displayed using the **New Trend View...** option of the Views Menu.

When a tabular view is created or while a **MID Tabular View** is the active window, the Views Menu options change to include options unique to the **MID Tabular View**.

A typical tabular view (without statistical data) is shown below.

The screenshot shows a software window titled "MID Tabular view C:\Projects\107765\MASsoft\bin\MID2040.exp View:4". The window contains a spreadsheet table with three columns: "Elapsed time" (in hours, minutes, and seconds), "Scan 1 : mass 20.00" (in Torr), and "Scan 2 : mass 40.00" (in Torr). The first few rows of data are as follows:

	Elapsed time	Scan 1 : mass 20.00	Scan 2 : mass 40.00
1	00:01.196	1.006e-07	7.260e-07
2	00:01.374	8.944e-08	6.791e-07
3	00:05.696	9.003e-08	6.918e-07
4	00:10.023	9.045e-08	6.990e-07
5	00:14.346	9.052e-08	7.005e-07
6	00:18.675	9.073e-08	7.030e-07
7	00:22.998	9.073e-08	7.041e-07
8	00:27.323	9.050e-08	6.915e-07
9	00:31.379	8.905e-08	6.837e-07
10	00:35.703	8.850e-08	6.766e-07
11	00:40.025	8.806e-08	6.781e-07
12	00:44.350	8.817e-08	6.863e-07
13	00:48.676	8.808e-08	6.797e-07
14	00:52.976	8.811e-08	6.881e-07
15	00:57.276	8.803e-08	6.746e-07
16	01:01.596	8.782e-08	6.755e-07
17	01:05.921	8.788e-08	6.726e-07
18	01:10.247	8.796e-08	6.790e-07
19	01:14.540	8.779e-08	6.722e-07
20	01:18.864	8.753e-08	6.791e-07
21	01:23.161	8.755e-08	6.773e-07
22	01:27.485	8.742e-08	6.855e-07
23			

The tabular view contains a spreadsheet with a vertical scroll-bar which allows any part of the data to be viewed. In the example given the tabular view has three columns displaying the elapsed time since the start of the scan (in hours, minutes and seconds) and the trends (in Torr) for the two mass values, 20 amu and 40 amu.

Columns within in the tabular view are assigned a default size dependant on the width of text displayed within the column. However, column width can be changed by moving the mouse cursor to the table columns title bar and using the left mouse button to click and hold on the boundary between two columns. The cursor can then be dragged to change the boundary to the required position.

The icon in the top right hand corner of the view determines how the scroll bar behaves



during data acquisition. When Real Time button is clicked the data will automatically scroll to the final point during data acquisition. Otherwise when Historical



button is selected then the scroll bar automatic scrolling is stopped and historic data can be looked at while collecting new data.

If any **Visible Parameters** have been checked then statistics appear above the data values.

An option is available to display a plot in a panel above the spreadsheet. Any combination of the data displayed in the columns of the spreadsheet can be plotted against one another in this simple X-Y graph.

See also:

See also:

[MID spreadsheet control](#)

[MID tabular view menu options](#)

[MID tabular view statistics](#)

[Scan tree](#)

[Views menu](#)

[MID Tabular Plot](#)

MID tabular formulas

Optionally, formulas can be added to a **MID Tabular View** by enabling the **Formulas** option of the **Additional Columns** and entering valid formulas in the **Formulas** table of the **MID Tabular View Options** dialog.

The **Formulas** table is the list of the formulas, the mathematic result of which be displayed within the table in columns, in the order entered within this table. The table is initially empty, and has two columns; the first is the name which will be displayed in the data columns title, and the second is for the formula itself. Formulas should be added to the top of the table working down, as any formulas following a gap in the table will be ignored.

Formula are added as mathematical expressions including the basic arithmetic operations +, -, /, * and ^, and the following list of valid arithmetic functions.

Mnemonics	Operand Type	Example	Explanation
ABS	One argument of double type.	ABS(C)	Returns the absolute value.
ACOS	One argument of double type.	ACOS(C)	Returns the arccosine.
ACOSH	One argument of double type.	ACOSH(C)	Returns the inverse hyperbolic cosine.
ACOT	One argument of double type.	ACOT(C)	Returns the principal value of the arccotangent, or inverse cotangent, of a number. The returned angle is given in radians in the range 0 (zero) to pi.
ACOTH	One argument of double type. The absolute value of the argument must be greater than 1.	ACOTH(C)	Returns the inverse hyperbolic cotangent of a number. If the absolute value of the argument is less than 1, ACOT returns the #VALUE! error value.
ASIN	One argument of double type.	ASIN(C)	Returns the arcsine.
ASINH	One argument of double type.	ASINH(C)	Returns the inverse hyperbolic sine of the argument.
ATAN	One argument of double type.	ATAN(C)	Returns the arctangent.

ATAN2	Two arguments of double type.	ATAN2(C, D)	Returns the arctangent using x- and y- coordinates.
ATANH	One argument of double type.	ATANH(C)	Returns the inverse hyperbolic tangent.
BASE	Two arguments of integer type: the first is greater than 0 and less than 2^{53} ; the second (radix) must be greater than or equal to 2 and less than or equal to 36. Third argument is optional, which must be greater or equal to 0.	BASE(A1, Radix[Min_length])	Converts a number into a text representation with the given radix (base). If A1, Radix, or Min_length are outside the minimum or maximum constraints, BASE returns the #NUM! error value. If A1 is a non-numeric value, BASE returns the #VALUE! error value. Any non-integer number used as an argument is truncated to an integer. If the Min_length argument is included, leading zeros are added to the result if the result would otherwise be shorter than the minimum length specified. For example, BASE(16,2) returns 10000 but BASE(16,2,8) returns 00010000.
CEILING	Two argument of double type	CEILING(2.5, 1)	Rounds the first argument up to the nearest multiple based on the significance specified by the second argument.
COS	One argument of double type	COS(C)	Returns the cosine.
COSH	One argument of double type	COSH(C)	Returns the hyperbolic cosine.
COMBIN	Two arguments of integer type. Non-integer numeric arguments are truncated to integers.	COMBIN(number, number_chosen)	Returns the number of combinations for a given number of items. Use COMBIN to determine the total possible number of groups for a given number of items. If either argument is non-numeric, COMBIN returns the #VALUE! error value. If either argument is negative, COMBIN returns the #NUM! error value.

COMBINA	Two arguments of integer type. Non-integer numeric arguments are truncated to integers.	COMBINA(number, number_chosen)	Returns the number of combinations (with repetitions) for a given number of items. If the value of either argument is outside of its constraints, COMBINA returns the #NUM! error. If either argument is a non-numeric value, COMBINA returns the #VALUE! error value.
COT	One argument of double type, which should be more than 0 and less than 2^{27} .	COT(number)	Returns the cotangent of an angle specified in radians. If the argument is outside its constraints, COT returns the #NUM! error value. If the argument is a non-numeric value, COT returns the #VALUE! error value. COT(0) returns the #DIV/0! Error value.
COTH	One argument of double type, which should be less than 2^{27} .	COTH(number)	Returns the hyperbolic cotangent of a hyperbolic angle. If Number is outside its constraints, COTH returns the #NUM! error value. If Number is a non-numeric value, COTH returns the #VALUE! error value.
CSC	One argument of double type, which should be less than 2^{27} .	CSC(number)	Returns the cosecant of an angle specified in radians. If Number is outside its constraints, CSC returns the #NUM! If Number is a non-numeric value, CSC returns the #VALUE! error value. CSC(n) equals $1/\text{SIN}(n)$.
CSCH	One argument of double type, which should be less than 2^{27} .	CSCH(number)	Returns the hyperbolic cosecant of an angle specified in radians. If Number is outside its constraints, CSC returns the #NUM! If Number is a non-numeric value, CSC returns the #VALUE! error value.
DEGREES	One argument of double type that specifies angle in radians	DEGREES(PI()/2)	Converts radians to degrees.

EVEN	One argument of double type	EVEN(-1)	Rounds the argument up to the nearest even integer.
EXP	One argument of double type	EXP(C)	Returns the exponent value of the argument.
FACT	One non-negative argument. If a number is not an integer, it is truncated.	FACT(2)	Returns the factorial of the argument.
FACTDOUBL E	One non-negative argument. If a number is not an integer, it is truncated.	FACTDOUBLE(num ber)	Returns the double factorial of a number. If the number is non-numeric, FACTDOUBLE returns the #VALUE! error value. If the number is negative, FACTDOUBLE returns the #NUM! error value.
FLOOR	Two arguments of double type	FLOOR(-2.5, -2)	Rounds the first argument down, towards zero, to the nearest multiple of the significance specified by the second argument.
INT	Argument of type double	INT(C)	Rounds the argument down to the nearest integer.
LN	One argument of double type	LN(C)	Returns the natural logarithm.
LOG	Two arguments: the number and the base	LOG(100, 10)	Returns the logarithm of a number to the specified base.
LOG10	One argument of double type	LOG10(1000)	Returns the base-10 logarithm of the argument.
MOD	Two arguments: a number and divisor	MOD(4,3)	Returns the remainder after the number is divided by the divisor.
MROUND	Two arguments: the value to be rounded, and the multiple to which you want to round the value.	MROUND(number, multiple)	Returns a number rounded to the desired multiple. MROUND rounds up, away from zero, if the remainder of dividing the number by the multiple is greater than or equal to half the value of the multiple.
ODD	One argument of double type	ODD(3.5)	Rounds the argument up to the nearest odd integer.

PI	No arguments required	PI()	Returns the value of Pi.
POWER	Two arguments of double type: the number and the power	POWER(A1,4)	Raises the number to the base.
QUOTIENT	Two arguments: the dividend and the divisor.	QUOTIENT(numerator, denominator)	Returns the integer portion of a division. Use this function when you want to discard the remainder of a division.
RADIANS	One argument of type double that specifies angle in degrees.	RADIANS(180)	Converts degrees to radians.
RAND	No arguments required	RAND()	Returns a random number between 0 and 1.
RANDBETWEEN	Two arguments of integer type: bottom that specifies the smallest returned value, and top that specifies the largest returned value.	RANDBETWEEN(bottom, top)	Returns a random integer between the numbers you specify. A new random integer is returned every time the worksheet is calculated.
ROUND	Two arguments: the number of double type and the number of digits	ROUND(20.57, 1)	Rounds the first argument to the specified number of digits.
ROUNDDOWN	Two arguments of double type	ROUNDDOWN(2.75,0)	Rounds the argument toward zero. The first argument specifies a number to round up. The second argument defines the number of digits to which you want to round the first argument.
ROUNDUP	Two arguments of double type	ROUNDUP(-3.42, 1)	Rounds the argument toward infinity. The first argument specifies a number to round up. The second argument defines the number of digits to which you want to round the first argument.

SEC	One argument of double type. Number is the angle in radians for which you want to calculate the secant.	SEC(number)	Returns the secant of an angle. The absolute value of the argument must be less than 2^27. If the argument is outside of its constraints, SEC returns the #NUM! error value. If the argument is a non-numeric value, SEC returns the #VALUE! error value.
SECH	One argument of double type. Number is the angle in radians for which you want to calculate the hyperbolic secant.	SECH(number)	Returns the hyperbolic secant of an angle. The absolute value of the argument must be less than 2^27. If the argument is outside of its constraints, SECH returns the #NUM! error value. If the argument is a non-numeric value, SECH returns the #VALUE! error value.
SIGN	One argument of double type	SIGN(C)	Returns the sign.
SIN	One argument of double type	SIN(C)	Returns the sine.
SINH	One argument of double type	SINH(1)	Returns the hyperbolic sine.
SQRT	One argument of double type	SQRT(C)	Returns the square root.
SQRTPI	One argument of double type.	SQRTPI(number)	Returns the square root of (number * pi). If the argument is negative, SQRTPI returns the #NUM! error value.
SUM	A list of arguments	SUM(C:D)	Sums the values in the columns from the first to last. In this example from column C to column D.
TAN	One argument of double type	TAN(C)	Returns the tangent.
TANH	One argument of double type	TANH(0)	Returns the hyperbolic tangent.
TRUNC	One argument of double type	TRUNC(PI())	Returns the integer part. Compare this with the Int function, which returns a double

The arguments which are used in the formula are extracted from the data values in the columns, where the columns are indexed by the spreadsheet column headers, i.e. A, B, C, D, E,...AA,AB..., etc. Note that column A is always used for the row indexes and column B displays by default with the Elapsed Time , which contains data which is not a valid argument for formulas. Columns A and B are therefore not normally used in formulas. For a column index to be a valid argument for a Formula, the column must exist and must have numerical data assigned to it in the spreadsheet.

Matched brackets can be used to ensure the operations are carried out in the correct sequence.

An example of a very simple formula is C+D, which will add the value found in column C to that of column D, for each row of data in the spreadsheet.

Some more examples of formula which have been entered into the Formulas table are given below.

Formulas		
	Name	Formula
1	Formula#1	C+D
2	Formula#2	SUM(C:D)
3	Formula#3	C / (C+D)
4	Formula#4	LOG(C)
5		
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		

The output of which for our example MID Tabular View is shown here.

MID Tabular view C:\Projects\107765\MASsoft\bin\MID2040.exp View:4

A	B	C	D	E	F	G	H	I
	Parameters/Scans:	Scan 1 : mass 20.00	Scan 2 : mass 40.00	Formula#1	Formula#2	Formula#3	Formula#4	
	Elapsed time	torr	torr	C+D	SUM(C:D)	C / (C+D)	LOG(C)	
1	00:01.011	1.006E-07	7.26E-07	8.266E-07	8.266E-07	0.12170336	-6.997402	
2	00:01.196	8.984E-08	6.791E-07	7.6894E-07	7.6894E-07	0.11683616	-7.0465303	
3	00:01.374	8.949E-08	6.902E-07	7.7969E-07	7.7969E-07	0.11477639	-7.0482255	
4	00:05.696	9.003E-08	6.918E-07	7.8183E-07	7.8183E-07	0.11515291	-7.0456127	
5	00:10.023	9.045E-08	6.99E-07	7.8945E-07	7.8945E-07	0.11457344	-7.0435914	
6	00:14.346	9.052E-08	7.005E-07	7.9102E-07	7.9102E-07	0.11443453	-7.0432555	
7	00:18.675	9.073E-08	7.03E-07	7.9373E-07	7.9373E-07	0.11430839	-7.0422491	
8	00:22.998	9.073E-08	7.041E-07	7.9483E-07	7.9483E-07	0.1141502	-7.0422491	
9	00:27.323	9.05E-08	6.915E-07	7.82E-07	7.82E-07	0.1157289	-7.0433514	
10	00:31.379	8.905E-08	6.837E-07	7.7275E-07	7.7275E-07	0.11523779	-7.0503661	
11	00:35.703	8.85E-08	6.766E-07	7.651E-07	7.651E-07	0.11567115	-7.0530567	
12	00:40.025	8.806E-08	6.781E-07	7.661E-07	7.661E-07	0.11495683	-7.0552213	
13	00:44.350	8.817E-08	6.863E-07	7.7447E-07	7.7447E-07	0.1138456	-7.0546792	
14	00:48.676	8.808E-08	6.797E-07	7.6778E-07	7.6778E-07	0.11472036	-7.0551227	
15	00:52.976	8.811E-08	6.881E-07	7.7621E-07	7.7621E-07	0.1135131	-7.0549748	
16	00:57.276	8.803E-08	6.746E-07	7.6263E-07	7.6263E-07	0.1154295	-7.0553693	
17	01:01.596	8.782E-08	6.755E-07	7.6332E-07	7.6332E-07	0.11505004	-7.0564066	
18	01:05.921	8.788E-08	6.726E-07	7.6048E-07	7.6048E-07	0.11555859	-7.05611	
19	01:10.247	8.796E-08	6.79E-07	7.6696E-07	7.6696E-07	0.11468655	-7.0557148	
20	01:14.540	8.779E-08	6.722E-07	7.5999E-07	7.5999E-07	0.11551468	-7.056555	
21	01:18.864	8.753E-08	6.791E-07	7.6663E-07	7.6663E-07	0.11417503	-7.0578431	
22	01:23.161	8.755E-08	6.773E-07	7.6485E-07	7.6485E-07	0.11446689	-7.0577438	
23	01:27.485	8.742E-08	6.855E-07	7.7292E-07	7.7292E-07	0.11310356	-7.0583892	

It is possible to use Formula values as arguments for other Formulas, however given these columns must already exist in the spreadsheet, a two-step process is required. If we take the example above, where we have already created the formula columns, then we can add a new formula (Formula#5) to the table using column E which is the result of an earlier formula.

Formulas

Name	Formula	
1	Formula#1	C+D
2	Formula#2	SUM(C:D)
3	Formula#3	C / (C+D)
4	Formula#4	LOG(C)
5	Formula#5	C / E
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		

Delete Delete All

The result of Formula#5 will be the same as Formula#3, as we see here

MID Tabular view C:\Projects\107765\MASsoft\bin\MID2040.exp View:4

A	B	C	D	E	F	G	H	I
	Parameters/Scans:	Scan 1 : mass 20.00	Scan 2 : mass 40.00	Formula#1	Formula#2	Formula#3	Formula#4	Formula#5
	Elapsed time	torr	torr	C+D	SUM(C:D)	C / (C+D)	LOG(C)	C / E
96	06:42.343	8.113E-08	6.22E-07	7.0313E-07	7.0313E-07	0.11538407	-7.0908185	0.11538407
97	06:46.668	8.111E-08	6.157E-07	6.9681E-07	6.9681E-07	0.11640189	-7.0909256	0.11640189
98	06:50.992	8.109E-08	6.102E-07	6.9129E-07	6.9129E-07	0.11730243	-7.0910327	0.11730243
99	06:55.316	8.111E-08	6.178E-07	6.9891E-07	6.9891E-07	0.11605214	-7.0909256	0.11605214
100	06:59.641	8.108E-08	6.085E-07	6.8958E-07	6.8958E-07	0.11757882	-7.0910863	0.11757882
101	07:03.936	8.081E-08	6.047E-07	6.8551E-07	6.8551E-07	0.11788304	-7.0925349	0.11788304
102	07:08.261	8.081E-08	6.094E-07	6.9021E-07	6.9021E-07	0.11708031	-7.0925349	0.11708031
103	07:12.558	8.082E-08	6.124E-07	6.9322E-07	6.9322E-07	0.11658637	-7.0924812	0.11658637
104	07:16.883	8.067E-08	6.223E-07	7.0297E-07	7.0297E-07	0.11475596	-7.0932879	0.11475596
105	07:21.206	8.088E-08	6.005E-07	6.8138E-07	6.8138E-07	0.11870028	-7.0921589	0.11870028
106	07:25.534	8.063E-08	5.988E-07	6.7943E-07	6.7943E-07	0.11867301	-7.0935033	0.11867301
107	07:29.860	8.071E-08	6.05E-07	6.8571E-07	6.8571E-07	0.11770282	-7.0930727	0.11770282
108	07:34.157	8.067E-08	6.158E-07	6.9647E-07	6.9647E-07	0.11582696	-7.0932879	0.11582696
109	07:38.484	8.066E-08	6.106E-07	6.9126E-07	6.9126E-07	0.11668547	-7.0933418	0.11668547
110	07:42.811	8.052E-08	6.013E-07	6.8182E-07	6.8182E-07	0.11809569	-7.0940962	0.11809569
111	07:47.136	8.053E-08	6.086E-07	6.8913E-07	6.8913E-07	0.11685749	-7.0940423	0.11685749
112	07:51.432	8.053E-08	6.068E-07	6.8733E-07	6.8733E-07	0.11716352	-7.0940423	0.11716352
113	07:55.760	8.042E-08	6.054E-07	6.8582E-07	6.8582E-07	0.11726109	-7.0946359	0.11726109
114	08:00.084	8.038E-08	6.022E-07	6.8258E-07	6.8258E-07	0.11775909	-7.094852	0.11775909
115	08:04.412	8.038E-08	6.11E-07	6.9138E-07	6.9138E-07	0.11626023	-7.094852	0.11626023
116	08:08.740	8.045E-08	6.036E-07	6.8405E-07	6.8405E-07	0.11760836	-7.094474	0.11760836
117	08:13.062	8.03E-08	5.986E-07	6.789E-07	6.789E-07	0.11827957	-7.0952845	0.11827957
118	08:17.391	8.03E-08	5.99E-07	6.793E-07	6.793E-07	0.11820992	-7.0952845	0.11820992

A formulas column index values do not change to take account of new columns being added, or existing columns being removed to the spreadsheet. Care should, therefore, be taken when adding or removing columns from the table as either can result of formulas changing or become invalid.

It should also be noted that formulas use values as displayed within the table, not the raw data values, in their calculation. Therefore it is recommended that **Max decimal places** be set at its maximum value. If formulas are used as inputs into other formulas number precision rounding will inevitably occur.

Also see:

[MID tabular view](#)

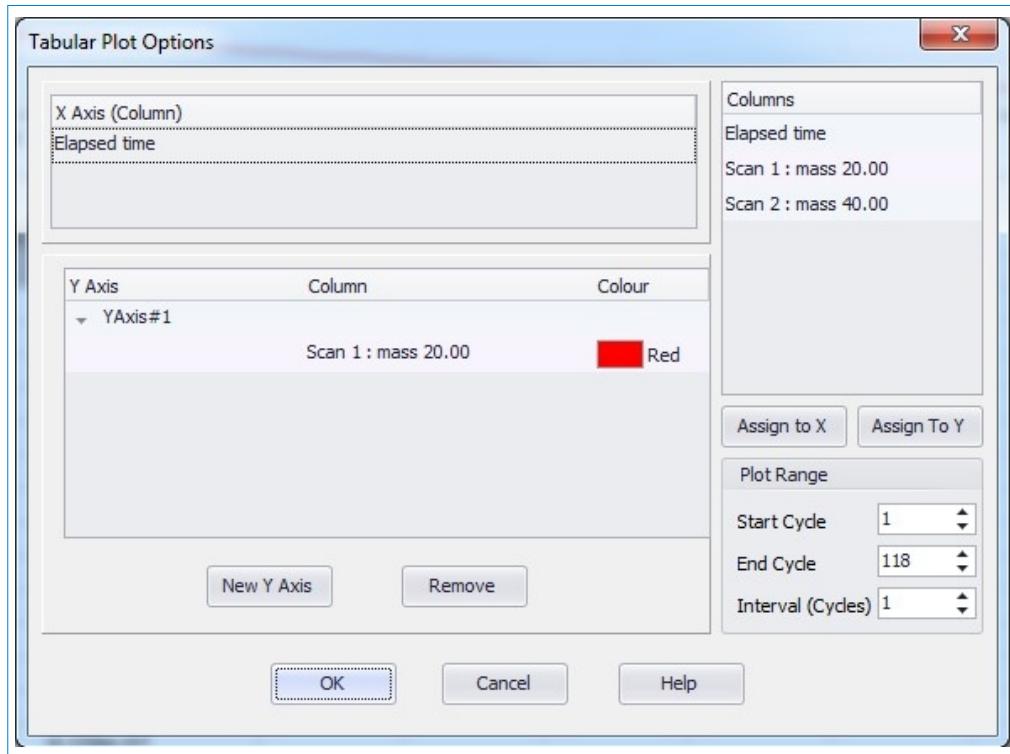
[MID tabular view options](#)

Tabular Plot

Any combination of the data displayed in the columns of the MID Tabular View can be plotted against one another on a simple X-Y graph using the optional **Tabular Plot**.

The plot is initially hidden from view, hence when a MID Tabular View is first created only the spreadsheet displaying the data for each MID scan, which has been added to the view, is displayed. To display the Tabular Plot choose the **Tabular Plot | Show Plot** option from the **Views** menu, or from the right-click popup menu. This displays a panel containing the plot above the spreadsheet. Initially the plot displays no data.

To add data to a plot choose **Tabular Plot | Plot Options** to display a dialog allowing you to choose which columns are displayed on the plot.



The **Columns** box lists all the columns of the spreadsheet, except the first header column which indexes the data rows.

The **Columns** list always starts displaying Elapsed time or Cycle, depending on whether the column is labelled in the Spreadsheet Options as Elapsed Time, Real Time or Cycle Number. Elapsed time is displayed on the plot if Real Time is selected. The other columns are those taken from the spreadsheet including data columns, the sum column, multi-variant value columns and formulas.

By default the first column (Elapsed time or Cycle) is added to the plot X Axis and the first data column added to columns added to the first Y Axis, labelled Y Axis#1.

X Axis (Column)

Only one column can ever be assigned to the X Axis, which can be any of the **Columns** in the list. To change which column is assigned to the X Axis, highlight a column in the **Columns** list and press the **Assign to X** button.

To change which column is assigned to the X Axis, highlight a column in the **Columns** list and press the **Assign to X** button.

Y Axis

Multiple columns can be added to the Y Axis, and multiple Y Axes can be created. To add a column to a Y axis, highlight the Y axis you wish to add it to and then highlight a column in the **Columns** list and press the **Assign to Y** button. Each data column can only be added once to each axis.

The first column (Elapsed time or Cycle) in the **Columns** list cannot be added to a Y axis.

To rename a Y axis, then right click over the selected axis and choose the **Rename Selected Y axis** option which displays a dialog allowing you to rename the axis.

When a new column is added a Y axis it is assigned a default colour used for that data line on the plot. The colour can be changed by clicking on the colour control and choosing a new colour.

There are no in-built restrictions on what unit types, or value ranges can be assigned to the same Y axis, therefore the user is required to choose sensible combinations (with the same units) to assign to the same Y axis.

New Y Axis

A new Y axis can be created by selecting the **New Y Axis** button, which prompts for a name of the new axis. The second Y Axis will be plotting on the right-hand axis of the plot. If a third Y axis is added the plot Y axis will stack, first on the left and then on the right.

Every Y axis must have at least one column. When a new Y axis is created the currently selected column is added to the Y axis. If no column is selected you are required to select one before creating a new Y axis.

Remove

A Y axis can be removed by highlighting the selected axis and pressing the **Remove** button, which prompts whether you wish to carry out the operation. Alternatively a column assigned to a Y axis can be removed, by selecting the column and pressing the **Remove** button.

A Y axis must have at least one column assigned to it, therefore deleting the last column of an axis deletes the Y axis.

There must always be at least one Y axis, so it is not possible to delete the first Y axis.

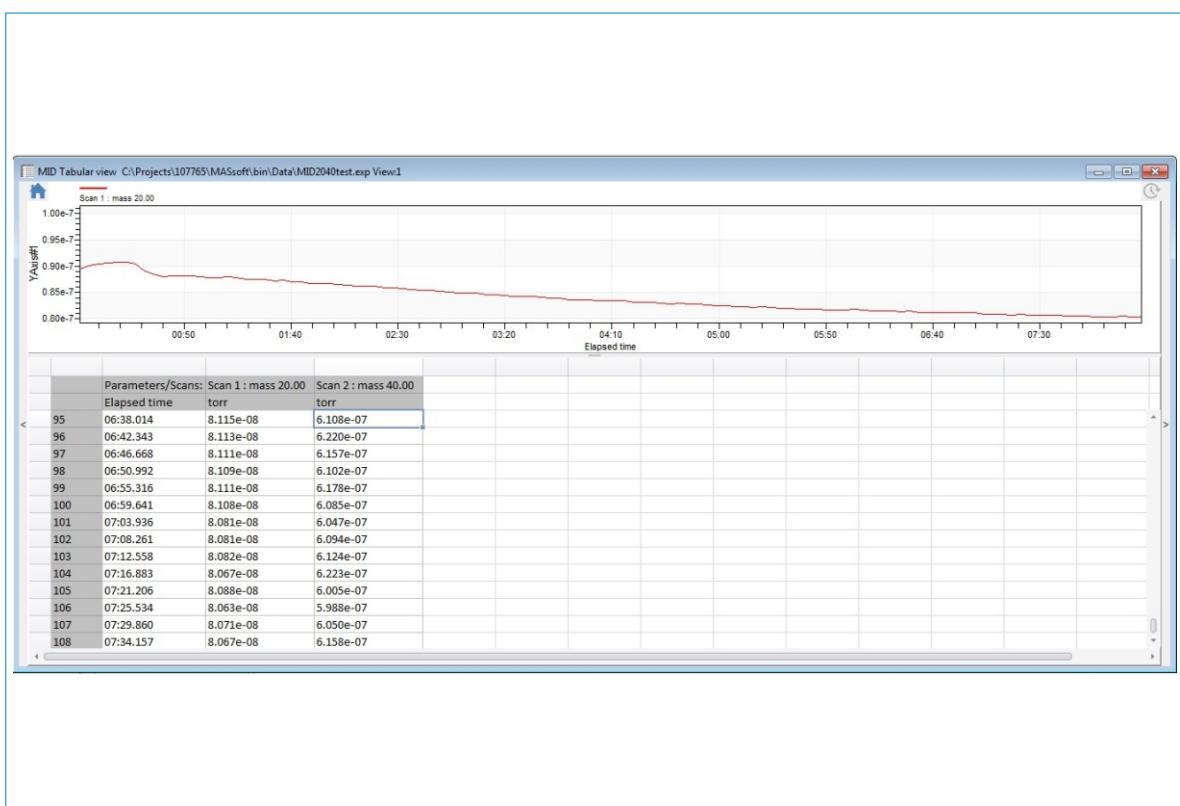
Plot Range

The Plot Range determines the range of points which will be plotted on the tabular plot. Data from the **Start Cycle** to **End Cycle** is plotted. The **Interval (Cycles)** field determines the interval between points plotted on graph.

*If a tabular plot displays columns containing **Formula** values, **Multivariant** values or the **Sum** column the process of extracting the data value from the spreadsheet is relatively slow. This is because the values are extracted from the spreadsheet, not directly from the data, and hence for each data point a value must be added to a spreadsheet and then read back from it – which is computationally slow. Therefore if a plot was displayed displaying a large number of data points which included **Formula** columns, the plot would be very slow to plot. Increasing the interval between data points, and therefore reducing the number of data points plotted means the plot will not be as slow to update.*

The default plot interval is set to display a maximum of between 500 to 1000 data points on the plot.

Pressing **OK** will add the selected data columns to the tabular plot. An example plotting mass 20 on Y axis against Elapsed Time on X axis is shown below.



The right-click popup menu displayed on the MID Tabular View includes a **Tabular Plot** sub-menu with the following options:

Show Plot	The Show Plot option is used to show or hide the Tabular Plot. When visible the Show Plot option is ticked on. Selecting the option when the plot is visible unchecks the Show Plot option and closes the plot panel.
Plot Options	To add data to the plot, when the plot is visible, choose Tabular Plot Plot Options to display a dialog allowing you to choose which columns are displayed on the plot.
Selected Data To Plot	The Selected Data To Plot option of the Tabular Plot is a submenu of the MID Tabular View menu items. This adds or replaces the current range of data displayed in the plot, with the range of data currently highlighted in the spreadsheet. To select all data choose Select All , and the Selected Range To Plot option.
Print Tabular View	This option displays a Printing Chart dialog which allows the plot to be printed via the built in print method of the plotting module. Note that the plot is currently printed via the File menu Print... option.
Copy	If the plot option is visible, then the Copy option will copy the current graphic of the plot to windows clipboard as well as the spreadsheet data.

Zooming

Left-clicking and dragging with the mouse within the plot area will zoom in on the selected area of the plot. Double click to return the plot to its starting range.

Changes to the Spreadsheet Columns

Any changes to the columns displayed in the spreadsheet, via the **MID Tabular View Options** dialog or the **Edit Trend View** options will potentially affect the data displayed in the tabular plot.

*A column index which is being displayed on the tabular plot, does not take account new columns being added, or existing columns being removed from the spreadsheet. Care should, therefore, be taken when adding or removing columns from the table. Any changes to the columns displayed in the spreadsheet, via the **MID Tabular View Options** dialog or the **Edit Trend View** options will potentially affect the data displayed in the tabular plot.*

If columns are removed, such that the index of a column being plotted is greater than the number of columns currently displayed, then those columns will be removed from the plot.

Comparison to the **Graphical Trend View plot**

The Tabular Plot offers a simple method to plot data displayed in the spreadsheet without first exporting that data to for example Excel. It allows plotting of data which is not possible to plot in the **Graphical Trend View** plot. For example, to plot normalised values, formula, or columns on the x axis other than time / cycles. However, it is not designed to replace the Graphical Trend View plot, which has considerably more features.

Data points will be added to the Tabular Plot if it is visible when scanning.

See also:

[MID tabular view](#)

MID tabular view menu options

Edit trend view...	Opens the Tabular View Editor allowing new data columns to be added to the current MID Tabular View .
Options	Opens the MID Tabular View Options dialog which controls the format and contents of the tabular view.
Set First Statistics Marker / Set Last Statistics Marker	Allows the selection of a range of data for statistical analysis.
Select All	Selects all the data in the spreadsheet (highlighting it in blue). The selected range of data may be copied to the clipboard or set as the marked range for statistical analysis.
Set Statistic Markers From Selected Range	Sets the selected range of data for statistical analysis.
Clear Statistics Markers	Clears the statistics markers.
Source View	Designates the MID Tabular view as the “source” view for the Background subtract function. A tick mark beside Source view indicates whether a selected view is the source view.

Background Subtract	Designates the MID Tabular view as the “target” view for the Background subtract function, then subtracts the data values in the “source” view from the data values in the selected “target” view. The result displayed in the “target” view. An operations window, describing the operation that has been performed, is displayed by default in the “target” view.
Show Operations	Toggles the operations panel on and off in the Background subtract “target” window.
Copy	This option only appears on the right-click popup menu. It copies the selected range of data to the Windows clipboard, allowing it to be pasted into another application such as Excel.

See also:

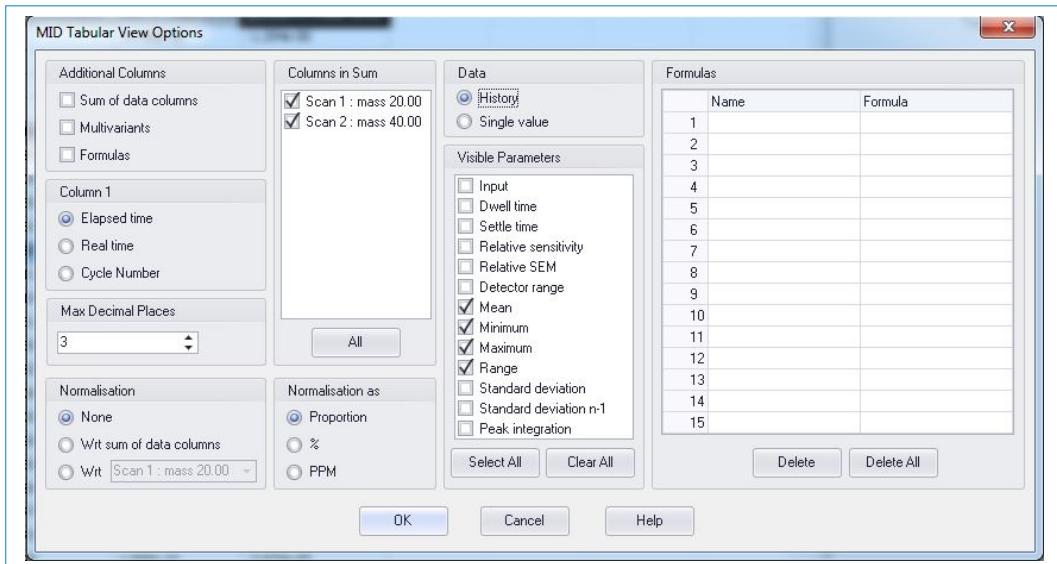
[Background subtraction](#)

[MID tabular view options](#)

[MID tabular view statistics](#)

MID tabular view options

When a tabular view is first created only basic data are displayed. The **MID Tabular View Options** dialog allows customisation including addition of formula and normalisation of the data displayed in the table.



The following options are available.

Additional Columns

Optional columns, which are displayed after the data columns, can be added to the data displayed in the table by checking on or off the following.

Sum of data columns

Displays a column of the sum of data values of each row, where which columns are included in the sum is determined by the **Columns in Sum** list.

Multivariants

If a multi-variant scan structure is being used, then columns are added which display the multi-variant values for each scan.

Formulas

If formulas have been entered into the **Formulas** list, then this displays an additional column for each formula. If this option is selected then the spreadsheet headers are displayed with letter headings which are used to reference columns within formula. If switched off the spreadsheet headers are blank.

Column 1

This controls the format of the data displayed in the first column of the table. Options are:

Elapsed time

Displays the time elapsed since the start of acquisition. This is the default display format.

Real time	Displays the actual time of acquisition.
Cycle number	Displays the cycle number in the acquisition.
Max decimal places	Selects the number of decimal places to which the data is displayed.
Normalisation	This controls if the data displayed in the table is normalised and how it is normalised. Options are:
None	The data are not normalised.
Wrt the sum of data columns	The data is normalised with respect to the sum of data columns. Where data is included in the sum is determined by the Columns in Sum list.
Wrt	The data is normalised with respect to the data in the column selected from the list of data columns.
Columns in Sum	Each of the data columns within the table is listed here, and this allows choice as to which are included in the sum of columns by checking on or off their contribution to the sum. Some data columns may not be required in the sum because they are of a different data type or duplicate columns may have been added via the Graphical/Tabular View Editor []. Only one sum is allowed per View, therefore if a second sum over different columns is required then another view must be created
Normalisation as	Determines whether the normalised data is displayed as a Proportion, % or PPM .
Data	This controls whether the data is displayed as :
History	The view will contain a continuous record of the acquired data. A scroll bar allows the data to be scrolled for viewing as required.
Single value	The view contains a single data line; this automatically updates during data acquisition.
Visible Parameters	This controls the parameters for which statistics are displayed, above the data columns in the table.
Formulas	This contains a list of the formulas for which the mathematic result of which be displayed as an additional columns within the table.

Click the **OK** button to update the tabular view with the selected options.

Also see:

[Multi-variant scan](#)

[MID tabular view statistics](#)

[MID tabular formulas](#)

MID tabular view statistics

A region displaying Statistics is displayed in the **MID Tabular View** above the trends data for any selected **Visible Parameters**. By default when first created these statistics apply to the full range of data. An example of a spreadsheet containing statistics is displayed below for the spreadsheet with mass 20 and 40, for the **Mean**, **Min**, **Max** and **Range** parameters is shown below.

Parameters/Scans:	Scan 1 : mass 20.00	Scan 2 : mass 40.00
Mean	8.425e-08	6.425e-07
Min	8.030e-08	5.986e-07
Max	1.006e-07	7.260e-07
Range	2.025e-08	1.274e-07
Elapsed time	torr	torr
1	00:01.011	1.006e-07
2	00:01.196	6.791e-07
3	00:01.374	8.949e-08
4	00:05.696	9.003e-08
5	00:10.023	9.045e-08
6	00:14.346	9.052e-08
7	00:18.675	9.073e-08
8	00:22.998	9.075e-08
9	00:27.323	9.050e-08
10	00:31.379	8.905e-08
11	00:35.703	8.850e-08
12	00:40.025	8.806e-08
13	00:44.350	8.817e-08
14	00:48.676	8.808e-08
15	00:52.976	8.811e-08
16	00:57.276	8.803e-08
17	01:01.596	8.782e-08
18	01:05.921	8.788e-08
19	01:10.247	8.796e-08

The range data from which statistics are generated can be changed by selecting a column, then changing the data range for which statistic markers apply.

To select a column click on the columns title (the first row of the table in the required column). The selected column will be highlighted in dark grey. If statistic markers for that column have already been set then those data rows will be displayed with a dark grey index in the first column.

There two ways of changing which rows of data are to be included in the selected data columns statistics markers.

The first method of selecting the statistic markers is to locate the first data row you wish the statistics to apply, click on the row in the spreadsheet to select it, then choose **Set First Statistics Marker** from the Views menu. This will highlight the row index in the first column in blue and marks this as the first data point of the range we wish to generate statistics for. Then locate and click on the row of data you wish the statistics range to span to. Now select **Set Last Statistics Marker** from the Views menu.

The selected range of data is assigned as having statistics markers which are shown with dark grey row indexes, and the statistics change to apply to the selected range of data. The selected column is prepended with **(S)** to show it has statistics assigned to it. The first column will also say **Locked** above the index values for the visible data rows, to show that the statistics for this data column are now locked.

An example where the statistics markers have been set to data rows 1 to 15 for the data column **Scan 2: mass 40** of the table is shown below.

The screenshot shows a software window titled "MID Tabular view C:\Projects\107765\MASSoft\bin\MID2040.exp View:4". The spreadsheet contains two header rows under the "Parameters/Scans" column, followed by 19 data rows numbered 1 to 19. The data columns are "Elapsed time" and "torr". Rows 1 through 15 are highlighted in blue, indicating they are selected as statistics markers. The first two rows are standard headers, while rows 10 through 15 correspond to the data from the previous example.

	Parameters/Scans:	Scan 1 : mass 20.00	(S) Scan 2 : mass 40.00
	Locked	Elapsed time	torr
1		00:01.011	1.006e-07
2		00:01.196	8.984e-08
3		00:01.374	8.949e-08
4		00:05.696	9.003e-08
5		00:10.023	9.045e-08
6		00:14.346	9.052e-08
7		00:18.675	9.073e-08
8		00:22.998	9.073e-08
9		00:27.323	9.050e-08
10		00:31.379	8.905e-08
11		00:35.703	8.850e-08
12		00:40.025	8.806e-08
13		00:44.350	8.817e-08
14		00:48.676	8.808e-08
15		00:52.976	8.811e-08
16		00:57.276	8.803e-08
17		01:01.596	8.782e-08
18		01:05.921	8.788e-08
19		01:10.247	8.796e-08

The second method for selecting statistic markers is to highlight (in blue) a range of spreadsheet data rows by left dragging with the mouse (or using SHIFT key), see Spreadsheet control. The selected range of data can then be assigned as statistics markers by choosing **Set Statistics Markers to Selected Range** from the Views menu.

If a range of statistics markers has already been set for a data column then you will observe a message warning that statistics are locked. If you wish to proceed then press the **Yes** button which will replace any existing statistics markers with the new ones.

The statistics for the selected column can be cleared by choosing **Clear Statistics Markers** from the Views menu.

A different range of statistic markers can be used for different data columns.

The first column labelled **Parameters/Scans** has a special use where setting statistics markers for this column, sets a new default range of markers for all data columns which have not had their own range of statistics markers set. If no column headers are selected then a change to the statistic markers occurs by default to the **Parameters/Scans** column, as if this column had been selected. In the example below statistic markers have been set to data rows 10 to 15 for the **Parameters/Scans** column, of the previous example.

The screenshot shows a software window titled "MID Tabular view C:\Projects\107765\MASsoft\bin\MID2040.exp View:4". The window contains a table with two header rows: "(S) Parameters/Scans" and "Scan 1 : mass 20.00 (S) Scan 2 : mass 40.00". Below these are four statistic rows: Mean, Min, Max, and Range. The main body of the table has 19 rows, each containing a number from 1 to 19 in the first column, followed by "Elapsed time" and "torr" in the second and third columns respectively. Rows 10 through 15 are highlighted with a dark gray background, indicating they are selected. The entire table is enclosed in a light gray border.

(S) Parameters/Scans		Scan 1 : mass 20.00	(S) Scan 2 : mass 40.00
Mean		8.833e-08	6.821e-07
Min		8.806e-08	6.766e-07
Max		8.905e-08	6.881e-07
Range		9.890e-10	1.149e-08
Locked	Elapsed time	torr	torr
1	00:01.011	1.006e-07	7.260e-07
2	00:01.196	8.984e-08	6.791e-07
3	00:01.374	8.949e-08	6.902e-07
4	00:05.696	9.003e-08	6.918e-07
5	00:10.023	9.045e-08	6.990e-07
6	00:14.346	9.052e-08	7.005e-07
7	00:18.675	9.073e-08	7.030e-07
8	00:22.998	9.073e-08	7.041e-07
9	00:27.323	9.050e-08	6.915e-07
10	00:31.379	8.905e-08	6.837e-07
11	00:35.703	8.850e-08	6.766e-07
12	00:40.025	8.806e-08	6.781e-07
13	00:44.350	8.817e-08	6.863e-07
14	00:48.676	8.808e-08	6.797e-07
15	00:52.976	8.811e-08	6.881e-07
16	00:57.276	8.803e-08	6.746e-07
17	01:01.596	8.782e-08	6.755e-07
18	01:05.921	8.788e-08	6.726e-07
19	01:10.247	8.796e-08	6.790e-07

While either the **Parameters/Scans column** or the **Scan 1: mass 20** column (which has had no statistics markers set) is selected then statistics for the range 10 – 15 are displayed. Whereas if the **Scan 2: mass 40** column is selected then statistics are displayed in the range 1 to 15.

See also:

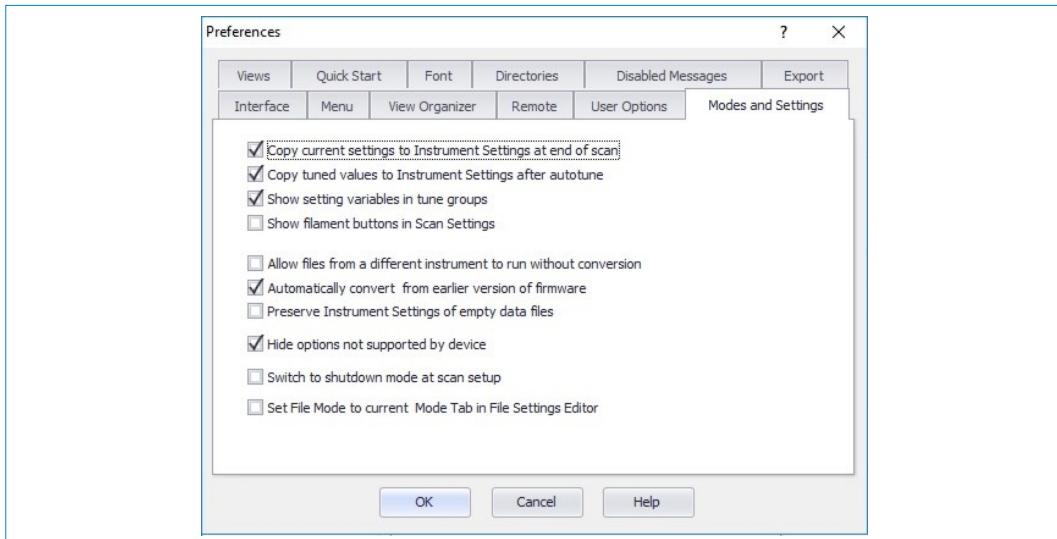
[Home window views menu](#)

[MID spreadsheet control](#)

[MID tabular view](#)

[MID tabular views menu options](#)

Modes and settings



To view the Modes and Settings preferences select **Preferences..** on the **Edit** menu then select the **Modes and Settings** tab. The options are explained below.

Copy current settings to Instrument Settings at end of scan

If this option is checked then at the end of the scan the values in the Scan's File Settings are copied to the Mass Spectrometer's Instrument Settings.

This allows the Instrument Settings to be updated to include any values that have been altered or tuned. Instrument Setting values whose **Default** option is set will not be altered. Values in the File Settings that do not have their **Default** option set are not copied. The result of this is that if a new file is created using **File, New** or via the Easy Scans it will inherit the File Setting values of the last file run. This behaviour is the same as previous versions of MASsoft.

Copy tuned values to Instrument Settings after autotune

This option is complementary to the “**Copy current settings to Instrument Settings at end of scan**”.

Auto-tuning relies on **Copy current settings to Instrument Settings at end of scan** to copy the tuned values to the Instrument. However, some users may choose to have all the tuned values derived from the Instrument Settings in which case they may opt to de-select **Copy current settings to Instrument Settings at end of scan** to avoid these values being modified by files with exceptions set in the File Settings; to allow auto-tuning to work as intended **Copy tuned values to instrument after autotune** should be checked. The values of the tuned devices are saved to the Instrument Settings in the same way as importing a .tun file to the Instrument Settings does, that is:

The tuned values over-write values in the Instrument Settings even if their **Use** option is set, and the **Use** option is set for those values that were copied.

Show settings variables in tune groups

If this option is enabled the setting editors group the variables according to their tune group. If this option is disabled the tune group is shown as a separate column. Devices not in a tune group are shown as "none".

Show filament buttons in Scan Settings

Un-checking this option will hide the filament buttons in the **Scan Settings** dialog. RGA users should not switch the filaments in the scan settings but SIMS analysis requires the filaments to be switched off to analyse neutrals.

Allow files from a different instrument to run without conversion

Normally, MASsoft requires the user to convert a file that was created on a different instrument before it can be run. Conversion will delete any variables in the file's environments that are not present on the current instrument and use default values from the Instrument Settings for any missing variables. The scan's input and output devices are also checked.

If this option is selected MASsoft will run files without requiring them to be converted. Variables in the file's settings that are not present on the current instrument will produce an "Unknown logical device" error, missing variables will have an undefined value.

Incompatible input and output devices will cause errors and MASsoft may not be able to display the data. This behaviour is the same as previous versions of MASsoft.

Use of this option is NOT recommended.

Automatically convert from earlier version of firmware

If this option is selected files without data that were created using an earlier version of the instrument's firmware are automatically converted when the file is opened. Files with data are automatically converted if the file is run.

Preserve Instrument Settings of empty data files

This option should be set if other users' files need to be examined. Values with **Use** un-checked will display the file's Instrument Settings value not the mass spectrometer's current Instrument Settings value.

This option is intended for use by Hiden support personnel or by supervisors when editing files off-line.

Hide options not supported by device

If a device does not support a particular capability the associated control will be hidden. This can be overridden by deselecting the **Hide options not supported by device** option. This option is selected by default.

Switch to shutdown mode at scan setup

This option is not described in this version of the manuals. Please contact Hiden Analytical for a manual update.

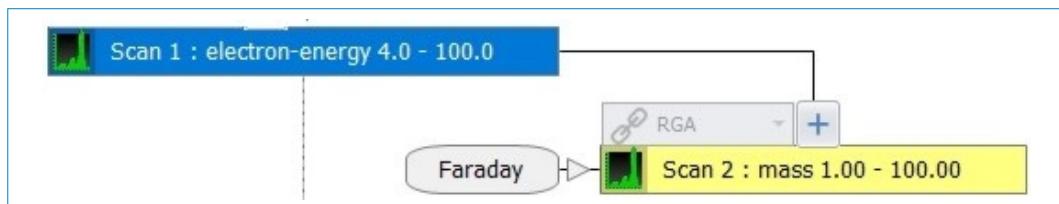
Set File Mode to current Mode Tab in File Settings Editor

This option is not described in this version of the manuals. Please contact Hiden Analytical for a manual update.

Monitored devices

This option is not described in this version of the manuals. Please contact Hiden Analytical for a manual update.

Multi-variant scan



A multi-variant scan sets the output variable in Scan 1 (electron energy in the case above) to its Start value and then performs Scan 2. Scan 2 sets its output variable (mass in the above case) to its Start value, reads the input variable (the Faraday detector) and then steps the output variable by its Increment value and repeats the read, continuing this cycle until its Stop value is reached.

Scan 1 then steps its output variable (electron energy) by its Increment value and performs Scan 2 again, repeating this until its Stop value is reached.

Multi-variant scans can be nested to any depth required, limited only by the memory required to store multi-variant data in the mass spectrometer's control unit. If Scan 1 and Scan 2 both have 100 steps this requires the storage of 10,000 data points. Adding another nesting level would increase this to 1 million data points - nesting scans rapidly uses memory.

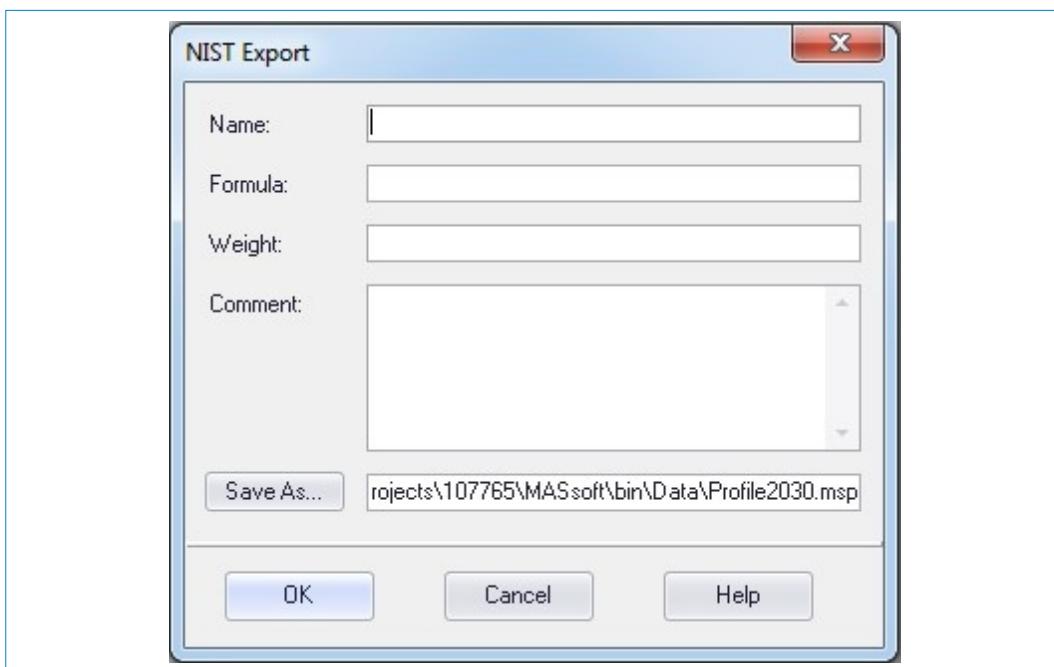
Note that a multi-variant scan can have several levels of hierarchy but only one input device, which is always attached to the lowest scan in the hierarchy to indicate that the input is only read after the last scan's output variable is set. There may be several scans in the lowest hierarchy level, and each may have an input device.

A multi-variant scan is created by selecting the appropriate **Scan** box and then clicking the Multi-variant scan button, or by pressing **Shift + Ins** or by right clicking on the scan and selecting **Insert Multi-variant**. The new scan will be added to the scan tree and will have the focus.

NIST export

The **Export| NIST...** option is available from the **File** menu when a graphical view of a Profile or Bar scan is selected. The scan must have data for the option to be enabled. Only scans with the scanned device set to mass can be exported into a NIST library.

The NIST Export Dialog will appear as shown below.



Name	Enter the default spectrum name.
Formula	If known, the formula for the substance producing the spectrum should be entered. This can be left blank.
Weight	If known, the molecular weight in atomic mass units (amu) for the substance producing the spectrum should be entered.
Comment	An area to enter any text that may be useful.

Save As...

Pressing **Save As...** opens a standard Windows Save dialog to choose the name of the NIST library file. The default file name is that of the current experiment file name with the.msp extension. The file name can be edited.

If the NIST library file already exists then the spectrum will be added to the spectra already contained that file. Otherwise if the library does not exist a new NIST library file will be created.

Pressing **OK** will validate the spectrum name and the NIST library file. The scan is converted into NIST library format and added to the NIST library.

See also:

[File menu](#)

[Exporting](#)

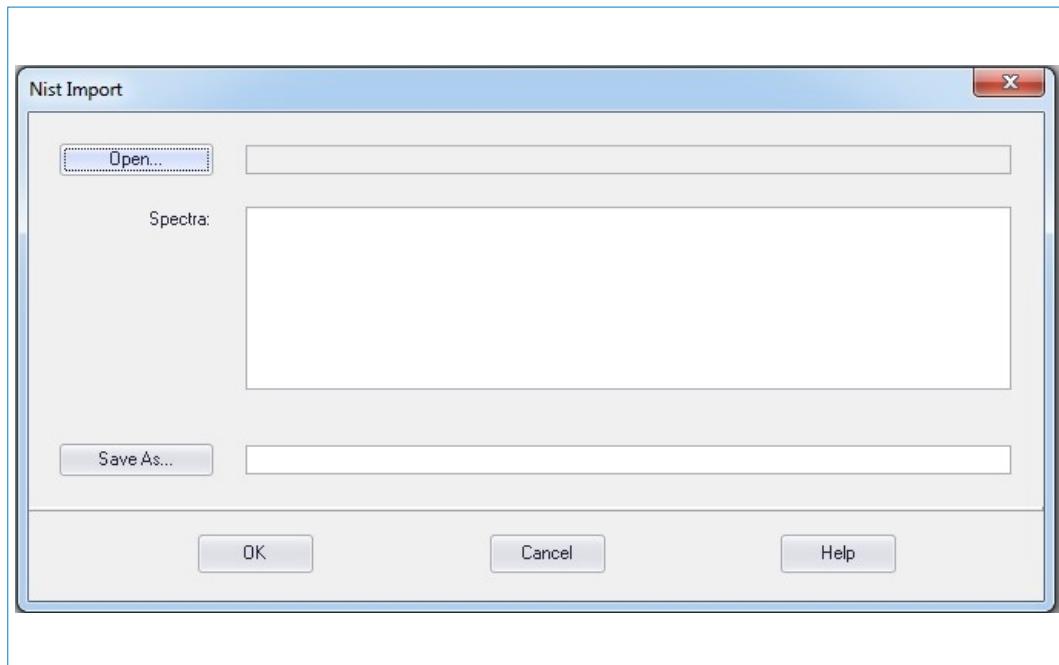
NIST import

The **Import| NIST...** option is available from the **File** menu. This feature can be used to import a scan from a NIST library into MASsoft.

When this is used a Bar scan, with scanned device set to mass, of the data contained in the NIST spectra is created. Data values set to the cracking pattern of the spectra within the NIST library file

Scans set to mass can be imported from a NIST library.

The NIST Import dialog as shown below is displayed.



First press the **Open...** button to display a dialog to select a NIST library file (with .msp extension).

The selected NIST library file may contain more than one spectra. The Spectra box will lists all the named spectra found within the selected NIST library file. Highlight the spectra you wish to import.

A default name for the MASsoft experiment file will be automatically displayed in the Save As... box, where the name matches that of the selected spectrum. This can be modified.

Press OK to validate the selected file name and NIST spectra. The NIST library spectra is converted into Bar scan file over the range of the current instrument where data peaks are added to match the NIST spectra. If the NIST contains peaks which go beyond the scan range of the current instrument then a warning message is displayed.

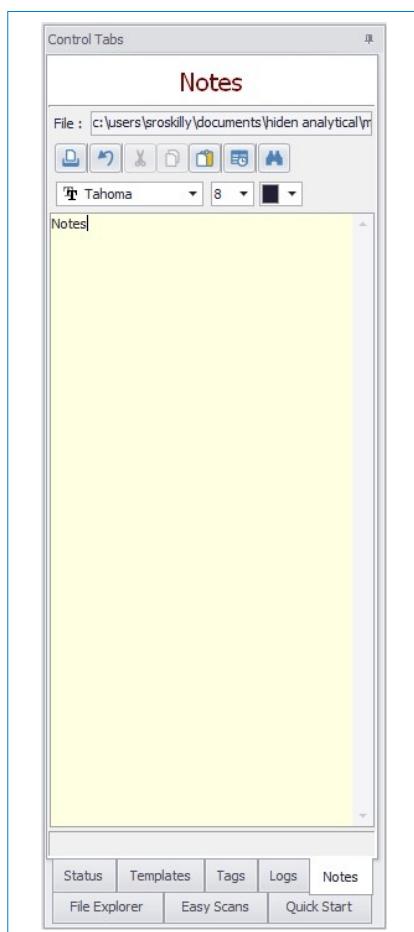
Note that the data displayed is that imported from the NIST. If a scan was started, collecting data from the current instrument the data is likely be completely different to that imported.

See also:

[File menu](#)

Notes

The **Notes** tab of the Control Tabs frame provides a method of writing optional notes associated with the current experiment file. When no experiment files are open the notes section is greyed out. When a new file is created or an existing experiment file is opened the notes tab is displayed as below.



Type your notes into the yellow box. These are automatically associated with the currently active experiment file which will be saved when the file is closed, and restored when that file is reopened.

Right-clicking displays a popup menu with the following options:

Undo Undo the last text typed in.

Cut Cut the highlighted text.

Copy	Copy the highlighted text.
Paste	Paste text into the notes at the current cursor position.
Delete	Delete the highlighted text.
Find	Open a dialog to enter what text you wish to find.
Refresh	Refresh the templates list.
Select All	Select all the text
Time/Date	Insert the current time and date into the text.

Some of these features are also available via the iconised toolbar above the text entry field. The font style, size and colour can be changed using the controls below the toolbar.

See also:

[Easy Scan](#)

Operation modes

The operating mode determines what sort of ions will be monitored, and where they originate. The possible acquisition modes include:

RGA

positive ion SIMS

negative ion SIMS

negative-ion RGA.

In RGA mode, the analyser creates ions in an internal electron impact ionisation source and extracts positive ions for monitoring. All Hiden Analytical mass spectrometers are capable of operating in this mode.

In positive ion SIMS mode, the ionisation source is normally switched off (although it does not have to be) and positive ions created outside the analyser (e.g. in a plasma or secondary ions from a surface) are monitored. The polarity of the ion transport variables only allow positive ions to be transmitted from the extractor to the detector. Not all Hiden Analytical mass spectrometers are capable of operating in this mode. Typically, EQS, EQP, PSM and IMP instruments use the positive ion SIMS mode (+SIMS).

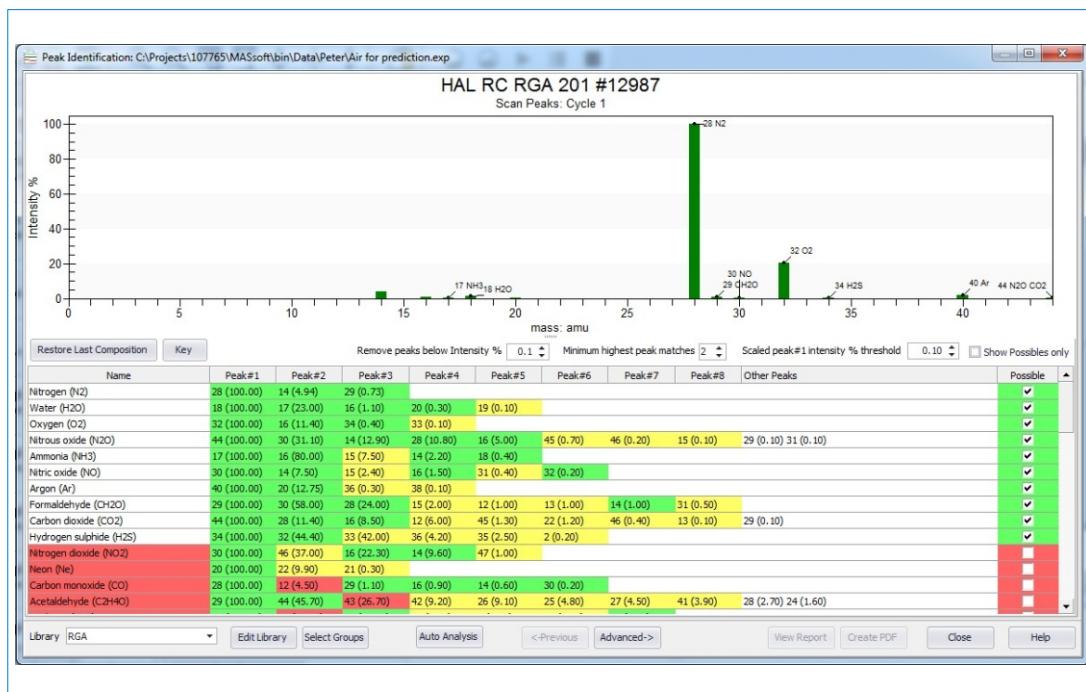
In negative ion SIMS modes, the ionisation source is normally switched off (although it does not have to be) and negative ions created outside the analyser (e.g. in a plasma or secondary ions from a surface) are monitored. The polarity and values of the ion transport variables allow only negative ions to be transmitted from the extractor to the detector. Not all Hiden Analytical mass spectrometers are capable of operating in these modes. Typically, the negative ion SIMS mode (-SIMS) is an option with EQS, EQP and PSM instruments.

In negative-ion RGA mode, negative ions created in an internal electron impact ionisation source are extracted for monitoring. Not all Hiden Analytical mass spectrometers are capable of operating in this mode.

Peak Identification

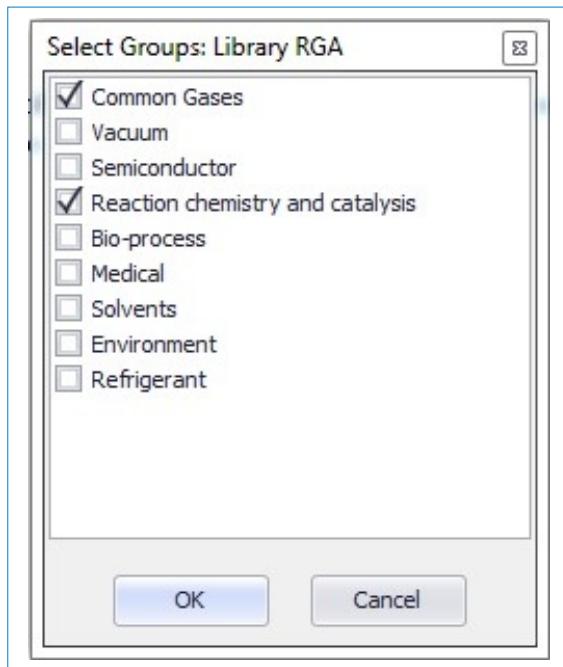
The **Peak Identification...** and **Auto Analysis...** options are available from **Analysis** sub menu of the **Views** menu when viewing a Bar or Profile Graphical view, where the scan has occurred against mass. The options are also available on the right-click popup menu.

Choosing the **Peak Identification...** option displays the **Peak Identification** view.



This view functions as a wizard, which steps through the **Possible Components Page**, then the **Analysis Pages** and finally the **Results Page**.

When this view is first displayed, a dialog appears in which you can choose which groups associated with the current library are selected. An example of the dialog for the default Hiden MS Library is shown below where the Common Gases and Vacuum groups are selected. The groups which are initially selected in this dialog are those which have been set as selected by default for peak identification in the current library.



Groups which you know to be not relevant to the chemistry of your scan should be checked off. By restricting the groups which are used, only those species in the selected groups will be considered as possible components in the spectrum, and only those groups are listed in the **Possible Components Table**. Any changes to the selections made within this dialog are saved to the current user directory.

Peak identification is used on historical data, and cannot be carried out while collecting data.

Possible Components Page The first page of this view displays a labelled plot of the selected scan. Below this is listed all the species of the selected groups in the current library. The bar at the bottom of the view has buttons to allow the library and groups to be changed, as well as moving onto the next page.

Library Options If there are more than one **MASsoft** library you can change which library is being used by selecting your choice from the pull down list box in the bottom left of the view. By default the Hiden MS Library will be used.

If your scan contains species which are not in the **MASsoft** library you are using, then you will not be able to identify them in the scans data.

Edit Library	The library editor can be accessed by pressing the Edit Library button. This displays the Library Editor allowing you to edit the species included in each library. Note that changes to the Unselect or Select default for Peak Identification options for the groups, only come into effect the next time you enter the Peak Identification dialog. Use the Select Groups option below to change the groups within the Peak Identification dialog.
Select Groups	The Select Groups button displays the dialog listing all the groups associated with the current library. Selected groups can be checked on or off within this dialog.
Possible Components Table	The lower half of the first page of the Peak Identification view displays a table with all the components within the selected MASsoft library. The first 8 peaks of each component are displayed. Peak positions which match a peak position within the scan are shown with a green background. Peak positions which do not match are shown in either red or yellow. Those marked in yellow are ignored, these include peaks out of scan range, the special case of mass 1 and those below the Scaled peak intensity % threshold .
Remove peaks below Intensity %	<p>Increasing this value removes small peaks from the spectrum. This simplifies the spectrum and may remove noise. When left at its default value of 0.1 no peaks are removed from the spectrum, this is because the intensity values displayed on the plot always scale to a range from 100% to 0.1%. NIST intensity values range from 1000 to 1, therefore peaks below 0.1% are not observed in a NIST spectra. If the value is changed the Scaled peak#1 intensity threshold % is automatically set to equal the new value and the Minimum highest peak matches is set to 1, as explained below.</p> <p>Note that some legitimate peaks used to differentiate between different species may be removed as the Remove peaks below Intensity % value is increased.</p>

Scaled peak intensity#1 % threshold

A weighting factor for a given species is calculated from the signal level measured at peak#1, relative to the highest level in the spectrum. If the intensity of a peak in that species cracking pattern multiplied by this weighting factor falls below the Scaled peak#1 intensity threshold % value, then if they are found to be missing from the recorded data they are ignored and marked yellow. If any peaks are above the % threshold, they are not ignored and the peaks which are missing from the recorded data are marked in red, otherwise when found they are marked in green.

If this value is increased then more missing peaks, marked red, are shown as yellow ignored peaks.

The intensity threshold default is 0.1%.

If the **Remove peaks below Intensity %** value is changed then the **Scaled peak#1 intensity threshold %** is automatically set to equal the new value. The **Scaled peak#1 intensity threshold %** should be equal or greater than then **Remove peaks below Intensity %** value.

An example is with air spectrum. The peak at mass 28 has the largest intensity of 100. Nitrogen's primary peak#1 is at mass 28. The scaling factor is therefore 1.0 (100/100) and a secondary Nitrogen peak at mass 14 of intensity 5 would be well above the threshold of 0.1. Whereas for Carbon Dioxide if the intensity of the scan at its primary peak of 44 was 0.3. The scaling factor is 0.003 (0.3/100). The carbon dioxides peak at mass 12 with intensity 6 would be weighted by scaling factor of 0.003 making it 0.018, which is below the threshold. If a peak is not found in the spectrum at peak 12, it is ignored for Carbon Dioxide and hence shown in yellow, not red. An example is shown below where the peaks at 12, 45, 22, 46 and 13 are not located in the scan, but all fall below the threshold and hence are ignored.

Carbon dioxide (CO₂)

44 (100.00) 28 (11.40) 16 (8.50) 12 (6.00) 45 (1.30) 22 (1.20) 46 (0.40) 13 (0.10)

Minimum highest peak matches

An additional constraint on which components are possible is the applied by the **Minimum highest peak matches** number. This is minimum number of green matching peaks which must be found starting from the primary peak of the species and then the next highest etc., from left to right in the possible components list. The default value of 2 means that the primary and secondary peaks must be found in the spectrum hence marked in green, for the component to be labelled as possible.

Components marked Possible	Species which have green and or yellow peaks within their first 8 peaks are considered as possible components found within the scan. The text of species which are not possible are shown with a red background. Each green matching peak adds a positive weighting to a species, the higher intensity peaks add a greater weight than lower peaks. Whereas each red not matching peak subtracts from the weighting associated with the species. The species are listed in order of weighting, with Possible components checked on. Changing the Scaled peak intensity threshold %, Minimum highest peak matches or restricting the groups of components used to a subset of those in the current library, will potentially change which species are labelled as possible components.
Show Possibles only	When this is checked on only possible species are listed in the Components Table .
Labelled Scan Peaks Plot	Above the components table is a plot showing the mass versus intensity scan on a linear scale across the scan range. Peaks are displayed as bars. Small peaks (below 0.1%) and noise are eliminated, , as NIST intensity values have a maximum 1000 to 1 ratio. If the source is a profile plot then data is divided to data bars. Peaks are labelled with their mass and with the formula of any possible species found within the selected library and groups with a primary peak at that mass. The peak or label may be clicked on with the mouse left-button to display the list of possible components which have peaks at that mass. In this case all peaks are listed, not just the primary peak. The title bar also displays the intensity of the peak in the scan as shown below

Library RGA: Possible at Mass 28 (100.00)		
Name	Formula	Intensity
Nitrogen	N2	100
Carbon dioxide	CO2	11.4

If the possible peaks change then the labels and list of components may change.

Restore Last Composition

The **Restore Last Composition** button allows the components found in the composition of the previous Peak Identification analysis which was carried out to be restored. This restores the library used in the previous analysis, and only components which were found to contribute to the composition are added to the table. This feature should only be used when you know that a gas sample contains the same components, although their percentage contribution may have changed.

Key

Pressing the **Key** button displays a dialog which explains the colour coding, and the meaning of the controls displayed on this page of the Peak Identification dialog.

Auto Analysis

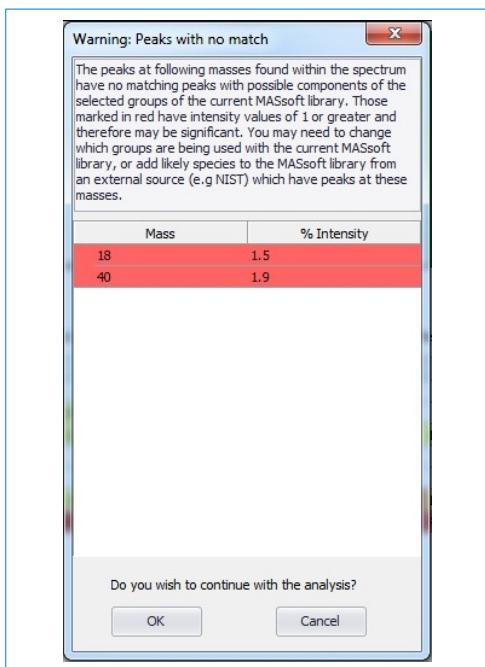
If you wish to carry out an analysis quickly using the currently selected groups, without preceding through the advanced options you can press the **Auto Analysis** button. This will automatically start the optimisation, displaying the **Optimisation Progress...** dialog. Components which either do not add to, or add insignificantly to the contribution are then automatically eliminated. After the optimisation has completed the **Results** page is displayed.

Alternatively, the components which are included in the optimisation can be adjusted manually. Using the **Advanced->** button, as described below, will step through the procedure.

Advanced->

Pressing the **Advanced->** button will move onto the next page of the view. Prior to moving to the next page it is possible to manually check on or off which components are possible. In most cases you are not going to choose select a component as possible if the scan does not have the required peaks to match that component. However you may know that a particular component labelled as possible from its peak positions, is not likely to be present in reality.

When you move onto the next page, either using the **Advanced->** or **Auto Analysis** buttons a check is made whether the currently selected possible species have peaks in their cracking patterns matching all the significant peaks in the spectrum we are analysing. If any of the peaks with % Intensity of 1.0 or above have no match to the peaks in the selected possible components the warning message shown below is displayed. You may need to select more groups or add new species to your library in order to match these peaks.



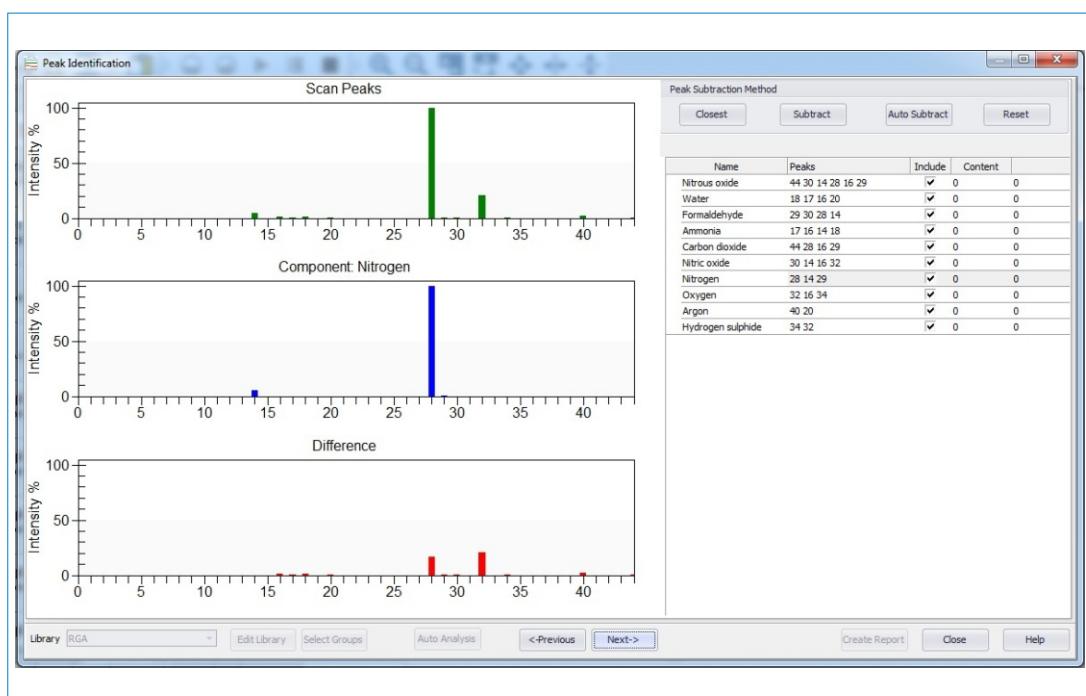
Auto Analysis... from a Bar or Profile Graphical view

If the **Auto Analysis...** option is selected from a Bar or Profile Graphical view, then an analysis is automatically started without displaying the first page of the **Peak Identification** dialog. The selected groups which are included are determined by the default groups of the current Library. The optimisation automatically starts displaying the **Optimisation Progress...** dialog. When complete the **Results** page is displayed (see below) with the analysis predicting the contents of the spectrum. If the results are not good, then you may need to change the selected groups or carry out the analysis step by step via the **Peak Identification** dialog.

Subtraction Page

The second page of the **Peak Identification** view shows three plots on the left and a number of option buttons in the top right panel labelled **Peak Subtraction Method**. The list of possible components determined from the previous page **Possible Components Page** is displayed below the buttons, in a table to the right.

Within the **Peak Subtraction Method** panel are four buttons, **Closest**, **Subtract**, **Auto Subtract** and **Reset**.



List of Possible Components

The table lists the **Name** of each possible component which the matched the peak positions in the previous page. For each component the **Peaks** which have not been ignored are listed. The **Include** check box allows for including or excluding the given component from the analysis. The final two columns are initially titled as **Content** and displayed blank respectively.

Peak Subtraction Method

The use of the **Peak Subtraction Method** to determine which components are present is optional.

The peak subtraction method subtracts components from the spectrum one by one, in an attempt to determine which are present. It is a useful tool for determining which components add significantly to component mixture, but the technique has limitations.

When subtracting a component from the spectrum the cracking pattern found within the current *MASsoft* library determines what will be removed. The primary peak of the cracking pattern is matched to the equivalent peak in the spectrum and the intensity of that peak used to determine a scaling factor to apply to the other peaks in the cracking pattern. An attempt can then be made to subtract the scaled matched pattern from the current spectrum. How much component can be removed is limited by the restriction that subtraction occurs across all peaks which have not been ignored in the cracking pattern. The fraction of component removed is multiplied by the scaling factor and determines the content of that component in the spectrum.

If a peak within a cracking pattern of a component has already been eliminated then it is not possible to subtract that component from the spectrum.

The method is limited by requiring that the cracking patterns of the components must be accurate for the instrument you are carrying out the analysis on. Also it does not work well when there are overlapping peaks in the spectrum.

It is therefore likely that subtraction will tell you some, but not all, of the components which are present in the spectra. However it is still a useful tool which can be used to determine which components should be included in the optimisation used to predict the spectrum's composition (on the next page of the view).

Peak Subtraction Plots

Three plots are shown on the left hand side of the screen.

The top plot shows the scan peaks (titled **Scan Peaks**). After a component is subtracted it will update to display the peak intensities after the subtraction (titled **Subtracted Scan Peaks**). Each subsequent subtraction will remove more intensity from the plot.

The middle plot shows the cracking pattern of the selected component in the list to the right, in the current library. Selecting a new component will update to show the peaks associated with that species.

The bottom plot shows the scan peaks after subtracting the middle plot (selected component) from the top plot (subtracted scan peaks). This temporarily shows the effect of removing the selected component from the spectrum.

A subtraction does not actually occur until the **Subtract** button is pressed.

Clicking on a component in the list will change the middle and bottom plot, but does not affect the top plot.

Left-clicking on a data bar in any of the plots will display the list of the possible components which have peaks at that mass.

Closest

Pressing the **Closest** button will automatically find the best match between the top plot (subtracted scan peaks) and all the components in the table which have not been previously subtracted, or eliminated. This will temporarily update the middle and bottom plot to show the effect of subtraction, but you will need to press the **Subtract** button to carry out the subtraction.

Subtract

Pressing the **Subtract** button will carry out a subtraction if it is possible. The peaks of the currently selected component (the middle plot) are subtracted from the scan peaks (the top plot). After subtraction occurs the top plot will change to reflect that the subtraction has occurred. The list of components will be updated with the **Content** of that component in the scan.

The **Content** values are not a percentage contribution or a normalised value. The value gives a value which can be considered relative to other content values of components which have been successfully subtracted. The maximum content value a component can have is 1. The sum of content of all components can exceed 1.

As an example, if the primary peak of a component was located at the intensity 100 peak in the scan, and subtraction removed all that peak and all the other peaks in the cracking pattern then that would have content 1.

Following a subtraction, the **Include** field of those components which can no longer be subtracted are now unchecked. This will be the case if any of the components peaks in its cracking pattern have been eliminated.

An attempt to subtract a component which cannot be subtracted will return a message informing which mass cannot be removed.

Auto Subtract

Pressing the **Auto Subtract** ^ button will automatically subtract components from the scan one by one, in order of which component removes the largest content. The list of components will be updated with the content of all the subtracted components in the scan.

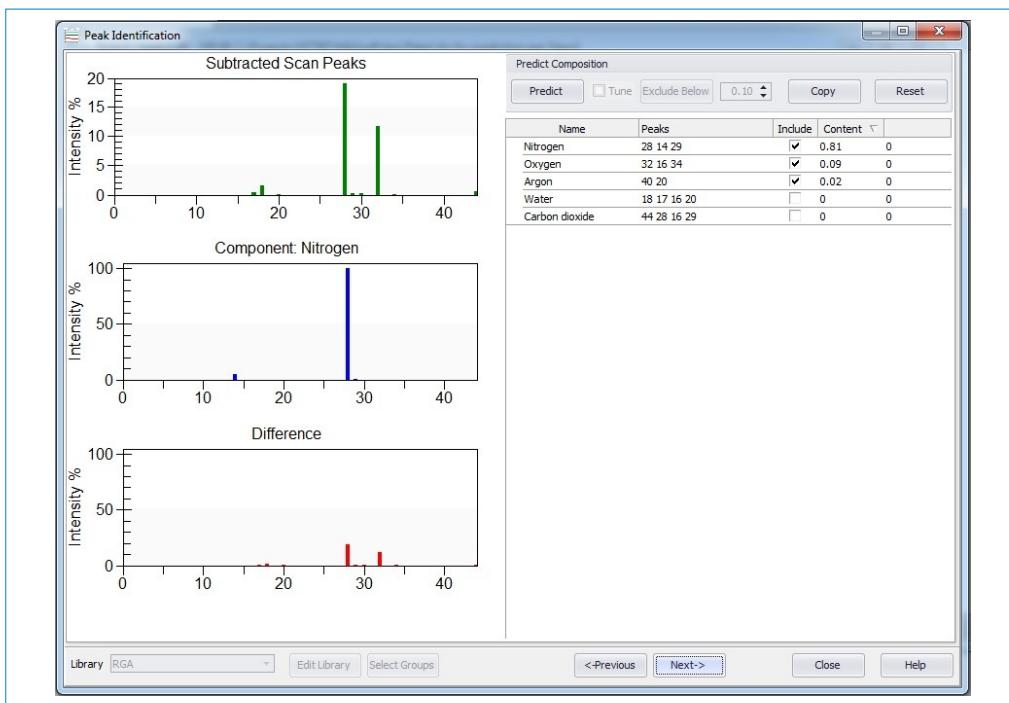
Predict Composition Page

When first entering the **Predict Composition Page**, the plots on the left and the table with the **List of Possible Components** will be unchanged, however the buttons in the **Predict Composition** panel in the top right will change.

If the **Peak Subtraction Method** has been used then only some of the possible components will be ticked on in the **Include** in column. Otherwise by default all the components will be included (ticked on). Included components can be clicked on or off manually.

An optimisation method is used to predict composition of the components which are included (which have **Include** is checked on). This method must be carried out in order to move onto the next page displaying the identified peaks.

The example of this page for the Air spectrum is given below.



Predict Composition Buttons

Within the **Predict Composition** panel are the **Predict**, **Exclude Below**, **Copy** and **Reset** buttons.

Predict

Pressing the **Predict** button will carry out the optimisation, starting from a random percentage contribution of the included components. This is the only optimisation option available initially. While optimising the **Optimisation Progress...** dialog tracks the progress of the optimisation. The length of time the optimisation takes is proportional to the number of components which have been included in the optimisation.

The optimisation automatically changes the percentage contribution of each of the included components to optimise the match between the predicted scan intensities and the actual scan intensities. This occurs over a number of iterations where the best solutions are evolved.

After an optimisation the list of components is updated to display the **%** contribution of each included component and **% (RS)** contribution corrected with their Relative Sensitivity (RS) value.

The **%** contribution values returned are estimated based on the selected species of the current library. The values should not be considered as accurate quantitative values of gas composition. They can, however, be used to determine which components likely to be present.

The three plots on the left hand side of the screen are updated with the prediction results.

Prediction Plots

These plots allow you to determine how well the optimisation has worked, and which masses have the largest errors associated with them. Examples are shown below after predicting with Nitrogen, Oxygen and Aragon included.

The top plot shows the actual scan spectrum.

The middle plot shows the predicted scan spectrum returned by the optimisation. This predicted scan spectrum should be very similar to the top plot displaying the actual scan spectrum if the optimisation has been successful.

The bottom plot shows the difference between the actual and predicted plots. The Y-axis displaying Intensity % is scaled to fill the plot. Differences of up to one or two percent are normally expected.

Left-clicking on a data bar in any of the three plots will display the list of possible components which have peaks at that mass.

If there is a large difference at a particular mass then try clicking on the mass to see the list of possible components at that mass. If a component with has been eliminated from the optimisation at that mass, then try re-optimising after including that component.

Mean Squared Error (MSE) value

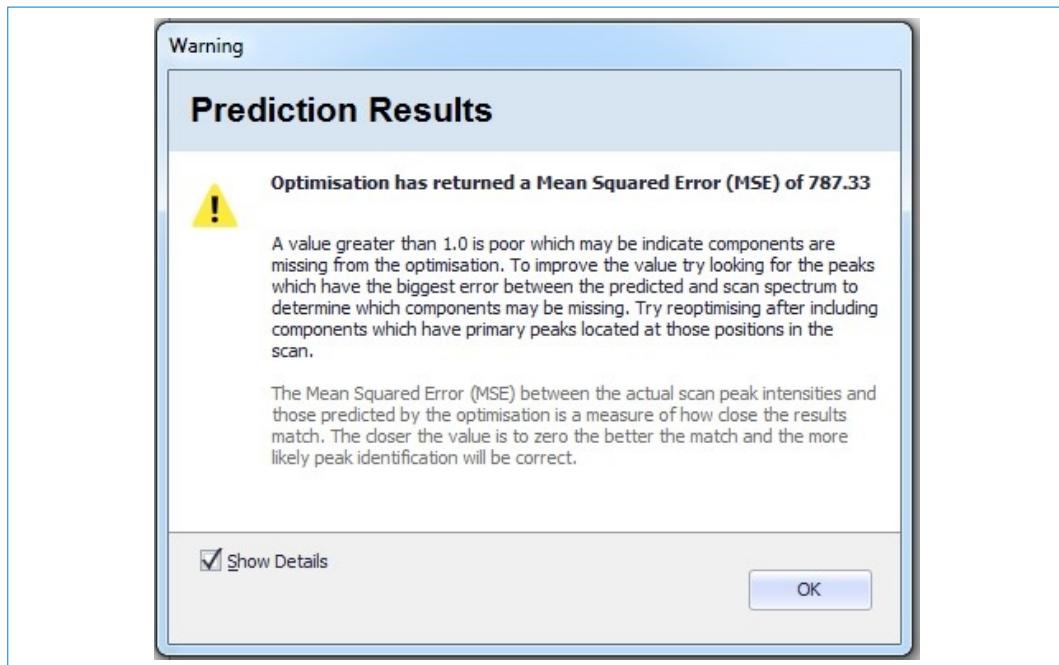
Below the **Predict Composition** panel is displayed a panel with the Mean Squared Error (MSE) value.

Mean Squared Error (MSE) value gives an idea as to how good the match is between the predicted and actual spectrum. In general the closer to zero the MSE value is, the better, and the more likely peak identification will be correct. A value of zero would indicate a perfect match, although this is highly unlikely in reality.

A mean Squared Error greater than 1.0 is poor which may indicate that components are missing from the optimisation. To improve the value try looking for the peaks which have the biggest error between the optimised and scan spectrum to determine which components may be missing. Try re-optimising after including components which have primary peaks located at those positions in the scan.

If the cracking patterns deviate significantly from those in the **MASsoft** library, or if a large number of possible components are included in an optimization it is possible to obtain false identification where the components which fit the spectrum may not be present in reality.

After pressing **Predict** if the Mean Squared Error (MSE) value of the optimisation is poor, a message will warn you of the case. An example is shown below where Nitrogen was removed from the Air prediction (by checking off **Include**), which returns a very poor MSE.



The optimisation may not be able to make a sensible match if components found in the spectrum are not located in the **MASsoft** library, or if the cracking patterns deviate significantly from those in the **MASsoft** library.

Fine-tune

After optimising for the first time the **Fine-tune** check box is enabled. Checking on this and pressing the **Predict** button will continue the optimisation from the start point of the current component contributions. This optimisation is much quicker than starting from random starting values. Typically this is done after eliminating insignificant components following the first optimisation.

Exclude Below

The **Exclude Below** button is enabled after an optimisation has taken place. Pressing this will automatically exclude any components which have contribution below the given threshold which is by default 0.1%.

After eliminating insignificant components, a new optimisation must be carried out, with or without using the **Tune** option.

Care should be taken when eliminating components since it is possible that components which are present in reality (at low contribution levels) may be eliminated by a poor optimisation. Some trial and error may be required to find which components are present.

Reset

The **Reset** button can be used to clear results following the **Optimisation**. The **Content** is reset back to 0 and all components are included. Use the **Reset** button to start from fresh.

Next ->

Moves to the **Results** page displaying the results of the optimisation. The composition must have been predicted before you can move onto the next page. Pressing the **Next->** button before predicting the composition will display a message with an option to automatically carrying out the optimisation.

<-Previous

The **<-Previous** button returns to the **Peak Subtraction** page. If an optimisation has been carried out and not reset, then the **Peak Subtraction** buttons are disabled until the optimised results are reset.

Results Page

The Results page has four tabs for displaying the results in a number of different ways. The **Identified Scan Peaks** tab is displayed first when moving onto this page. The example of this page for the Air spectrum is given below, where Nitrogen, Oxygen, Aragon, Water and Carbon Dioxide was included in the prediction.

The screenshot shows a software window titled "Peak Identification: C:\Projects\107765\MASsoft\bin\Data\Mike\file1.exp". The window contains a table with several columns: Component, Formula, %, Corrected for Relative Sensitivity, Intensity, Predicted, Difference, and Components. The table lists various gases and their relative abundances. At the bottom of the window, there are buttons for Library (RGA), Edit Library, Select Groups, Auto Analysis, <-Previous, Next->, View Report, Create PDF, Close, and Help.

Analysis Table										K	
	A	B	C	D	E	F	G	H	I	J	K
1	Component	Formula	%	% Corrected for Relative Sensitivity							
2	Nitrogen	N2	80.74	78.87							
3	Oxygen	O2	14.74	16.75							
4	Water	H2O	2.82	3.06							
5	Argon	Ar	1.2	0.98							
6	Carbon dioxide	CO2	0.49	0.34							
7											
8	Mass	Intensity	Predicted	Difference	Components						
9	2	0.30	0.00	-0.30							
10	12	0.10	0.04	-0.06	CO2						
11	14	3.30	4.93	1.63	N2						
12	15	0.10	0.00	-0.10							
13	16	1.20	2.17	0.97	H2O O2 CO2						
14	17	0.80	0.80	0.00	H2O						
15	18	3.50	3.48	-0.02	H2O						
16	20	0.10	0.20	0.10	H2O Ar						
17	27	0.60	0.00	-0.60							
18	28	100.00	99.91	-0.09	N2 CO2						
19	29	0.70	0.73	0.03	N2 CO2						
20	30	0.20	0.00	-0.20							
21	31	0.20	0.00	-0.20							
22	32	18.32	18.23	-0.09	O2						
23	34	0.10	0.07	-0.03	O2						
24	40	1.50	1.49	-0.01	Ar						
25	43	0.10	0.00	-0.10							
26	44	0.70	0.61	-0.09	CO2						
??											

Analysis Table	The Analysis Table displays a spreadsheet of the data in the prediction plots shown on the Predict Composition page.
	The list of components and formula, with non-zero the % contribution to the predicted spectrum are listed.
	For each mass peak the actual intensity, predicted intensity and difference in intensity is displayed. Also shown is the formula of all the components predicted at each mass.
	The Mean Squared Error (MSE) is shown below.
Identified Scan Peaks	This displays a labelled plot of the scan data. Each peak is labelled with the formula of each component which contributes to that mass. Left-clicking on either the data bar or the label associated with that bar displays a dialog listing all the components associated with that mass, and the predicted contribution to the total intensity at that mass. The title bar includes the actual intensity at that mass in brackets. The actual and predicted intensity will not be identical. The sum of the errors between these values contributes to the MSE value giving an indication as to how good the optimisation is. Right-clicking on this plot displays a popup menu with the options to copy the plot to windows clipboard in the JPEG graphics format, or to print the plot.
Stacked Peaks Table	This displays the same data as the Stacked Peaks Plot but in a table format. You can see which components contribute what values to the different masses.

Popup Menu Options

Right-clicking on any of the results plots or spreadsheets displays a popup menu with these options

Copy	The Copy button on a plot copies the graphic to windows clipboard in JPEG graphics format. The Copy button on a spreadsheet copies the spreadsheet contents to windows clipboard in a tab delimited format, which may be pasted into for example <i>Excel</i> .
Print	The Print button on a plot opens a dialog with options on how to print the plot. The Print button on a spreadsheet displays the print preview for the spreadsheet. Choose the Print option to print the spreadsheet.

Preview Print Report	The Preview Print Report button creates a print preview combining all four plots and spreadsheets. Choose the Print option to print the report.
	The View Report button found on the control bar along the bottom of the Peak Identification window will also create a print preview.
Create PDF Report	<p>The Create PDF Report button creates a PDF report combining all four plots and spreadsheets. A name for the PDF is automatically created, appending the current date and time. This name can be changed, but it must not already exist. This file can be opened in a PDF file Viewer of your choice.</p> <p>The Create PDF button found on the control bar along the bottom of the Peak Identification window will also create a PDF report.</p> <p>When closing the Peak Identification window after carrying out an analysis if you have not either printed any results or created a PDF report, you will be prompted if you wish to do this before closing the window.</p>

See also:

[Library](#)

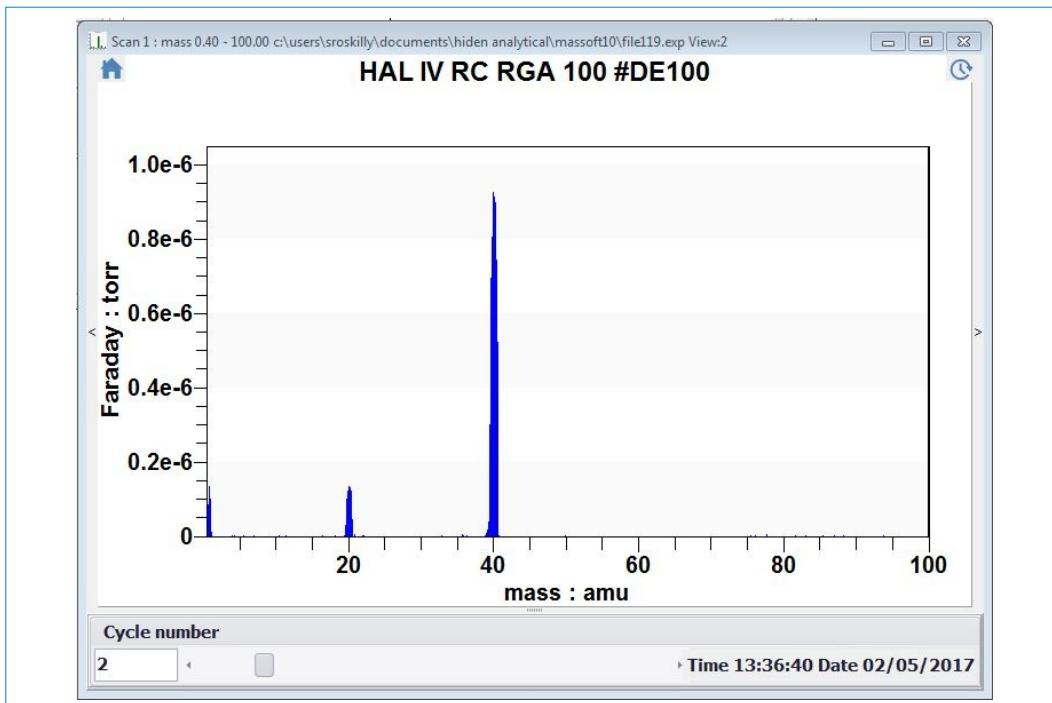
[Cracking Patterns](#)

Plot mode

The Mode is a sub menu of the **Bar/Profile Graphical Views** menu. It determines whether real time or historical is displayed.

Real time	Displays the latest cycle. If viewing data from a data file, cycle number 1 will be displayed; select Historical data to view other cycles.
Historical data	This is used to look at data already acquired. A scroll bar is added to the view which allows the time scale or cycles to be scrolled backwards and forwards, which displays the data at the given cycle. Alternatively a specific cycle number can be typed in the Cycle number text box. If the scan is of a multi-variant type then additional scroll bar are displayed for each multi-variant value allowing the data for the scan at each variable to be displayed.

An example of a View in Historical mode with a scroll bar is displayed below.



The icon in the top right hand corner of the view also determines which mode the plot is in.



displays Real time data and



displays Historical data.

Also see:

[Bar/Profile plot menu options](#)

Plotting types

The Plot Types is a sub menu of both the Bar/Profile Graphical and MID Graphical Views menu. These options control the axes scale and how the data are displayed on the plot.

Area

Fills in the area between the graph and the X-axis.

Line

Draws the graph as a line, with no fill between the line and X-axis. This is the only option available for a MID Graphical View.

Histogram

Each point on the graph is drawn as a histogram bar (a vertical line).

Bar	Each point on the graph is drawn as a two-dimensional histogram bar.
Spline	Draws a curved spline (line) fitting through the data points (as opposed to a series of straight lines). If the increment between data points on the X axis is small, there is little difference between viewing as a Spline or Line . However if there are fewer data points along the X axis, or the plot has been zoomed into on the X axis, then the smoothing effect of the spline is more noticeable. The location of data points may not be so obvious when viewing a spline, hence the Mark Points option may be helpful.
Linear	Draws the graph on a linear Y-axis.
Log	Draws the graph on a logarithmic (log10) Y-axis.

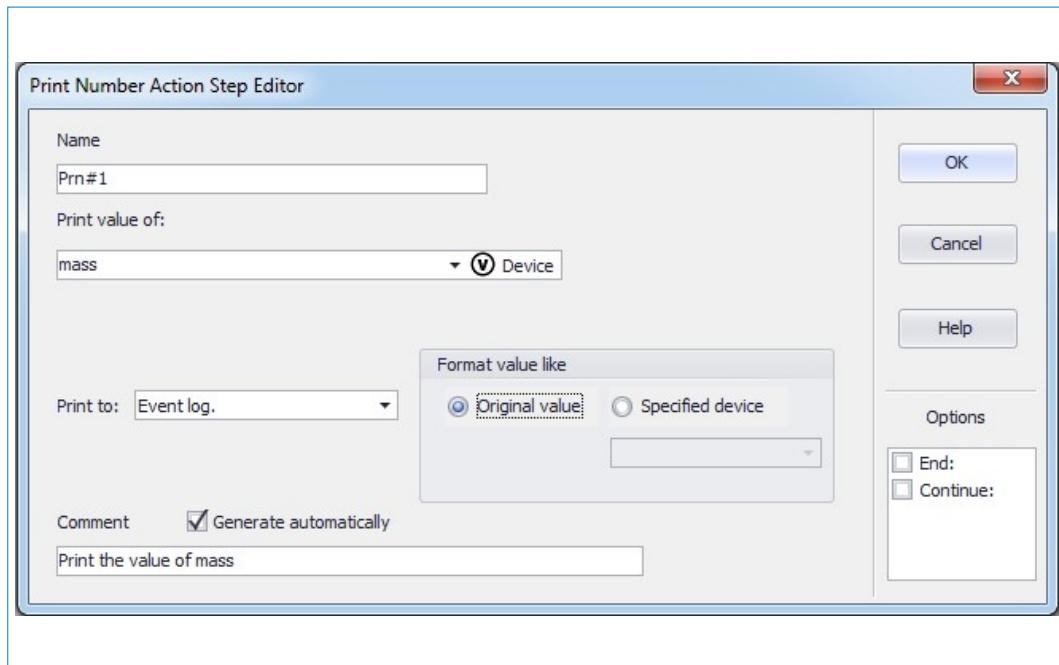
Print Number Action Step Editor

1/

The **Print Value Action**, function can be used to send a value as an ASCII string to other instruments (e.g. a process computer). A value can be taken from an input device or an event function, converted to an ASCII string using a choice of formats, and can then be transmitted on one of the IU's communications links.

The **Print Number Step Editor** is displayed when editing a **Print Value Action**.

An example of Print Number Action is shown below.



Fields **Print Number Action Step Editor** are:

Name	The name assigned to the Print Value Action.
Print value of	The value to be output can be selected. A pull down allows you to choose between Device and Action step .
Device	The value returned for the given device is output.
Action step	The value is that returned from an action is output.
Print to	An output port must be chosen from the list in this box in order to send the number. If EventLog is selected in the Print To: box in both the Print Number Editor and Print Text Editor dialog boxes, the number is appended to the message in the event log file. This field depends on the [STREAMS] entries in the HIDEN.INI file; if this section is missing the field will be blank.
Format value like	Determines the format of the value which is output. This can be Original value for the default format of the device, or Specified device to match the format of a selected device. Original value sets the format to the default input device of the instrument, i.e. SEM on a pulse counting instrument (integer), Faraday on a Faraday instrument (floating point).

Options	A list of options supported by the firmware version of the instrument is displayed. Double click on an option to select or deselect it. A selected option is ticked.
End:	The message does not continue. The next message will start on a new line.
Continue:	The message continues. The next message follow on the same line as this message. For backwards compatibility with old Action Sequences if neither End: nor Continue: are selected then the message continues; the Print Number event must be followed by a Print Text event which ends the message; failure to end the message will cause MASsoft to crash.
Comment	The comment associated with the Print Number Action. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

See also:

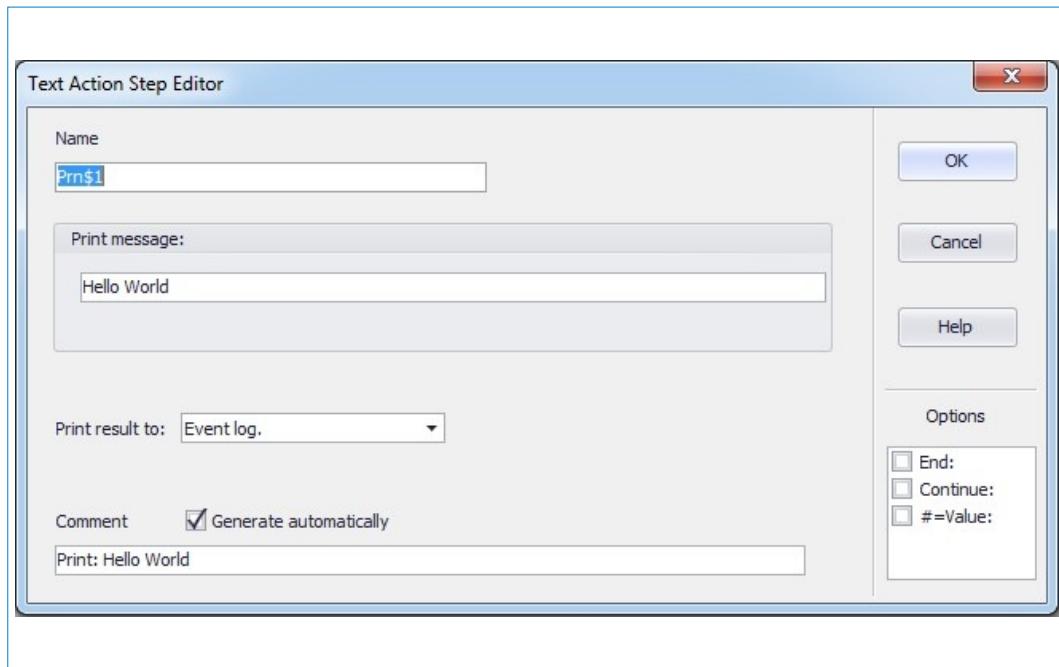
[Automation page](#)

Print Text Action Step Editor

The **Print Text Action**  can be used to make print actions. This can be used to send messages to other instruments (e.g. a process computer). A user-entered message of up to 30 ASCII characters can be defined which can be transmitted on one of the MSIU's communications links.

The **Text Action Step Editor** is displayed when editing a **Print Text Action**.

An example of Print Text Action is shown below which prints *Hello World* to the Event Log.



Fields **Text Action Step Editor** are:

Name	The name assigned to the Print Text Action.
Print message:	A message of up to 30 characters may be typed directly into this text box. The message scrolls left and right as required. Several print events may follow each other to create lines greater than 30 characters long. The last print event MUST have the <i>End:</i> option set. MASsoft may become unstable if EventLog messages are extremely long.
Print result to	This is where to send the message. An output port must be chosen from the list in this box. The message is sent to the event log file if EventLog is selected. The event log file can be displayed on the PC monitor. This field depends on the [STREAMS] entries in the HIDEN.INI file; if this section is missing the field will be blank.
Options	A list of options supported by the firmware version of the instrument is displayed. Double click on an option to select or deselect it. A selected option is ticked.
End:	The message does not continue. The next message will start on a new line.

Continue: The message continues. The next message follow on the same line as this message.

#=Value:

A # character embedded in the message will be replaced with the event's value, using the value's associated device format. Use a Set event to store the value in the Print Text event.

For backwards compatibility with old Action Sequences if neither **End:** nor **Continue:** are selected then the message must end in . (full stop), : (colon), ! (exclamation mark) or ? (question mark) to start the next message on a new line; failure to end the message will cause MASsoft to crash.

Comment The comment associated with the Print Text Action.

If **Generate automatically** is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation page](#)

Preferences

The **Preferences** dialog is a multi-tab dialog opened by selecting **Preferences..** on the **Edit** menu. It allows the user to customise MASsoft.

See also:

[Directories](#)

[Disabled messages](#)

[Export preferences](#)

[Font preference](#)

[Interface preferences](#)

[Modes and settings](#)

[Quick start preferences](#)

[Remote preferences](#)

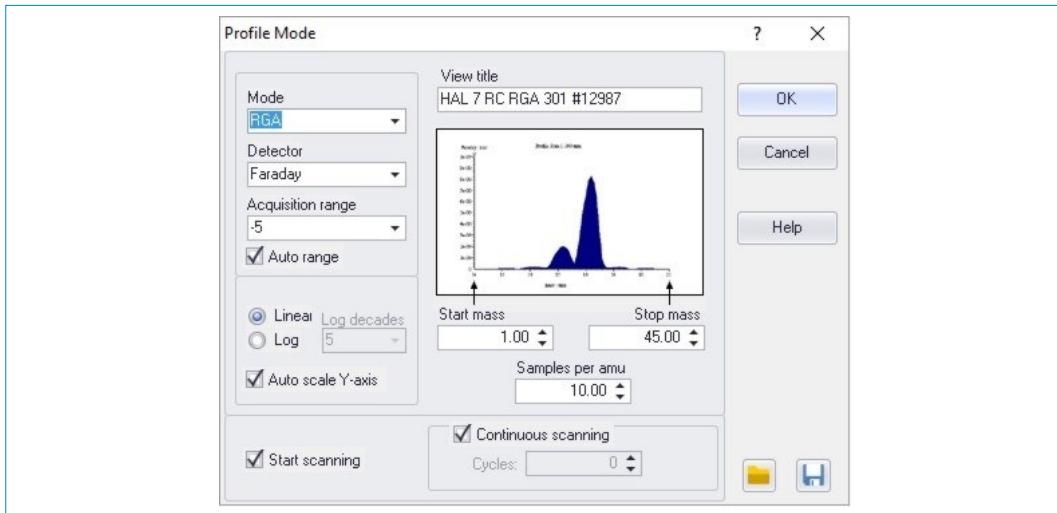
[User options](#)

[View organiser](#)

[Views preferences](#)

[Email Preferences](#)

Profile Mode dialog



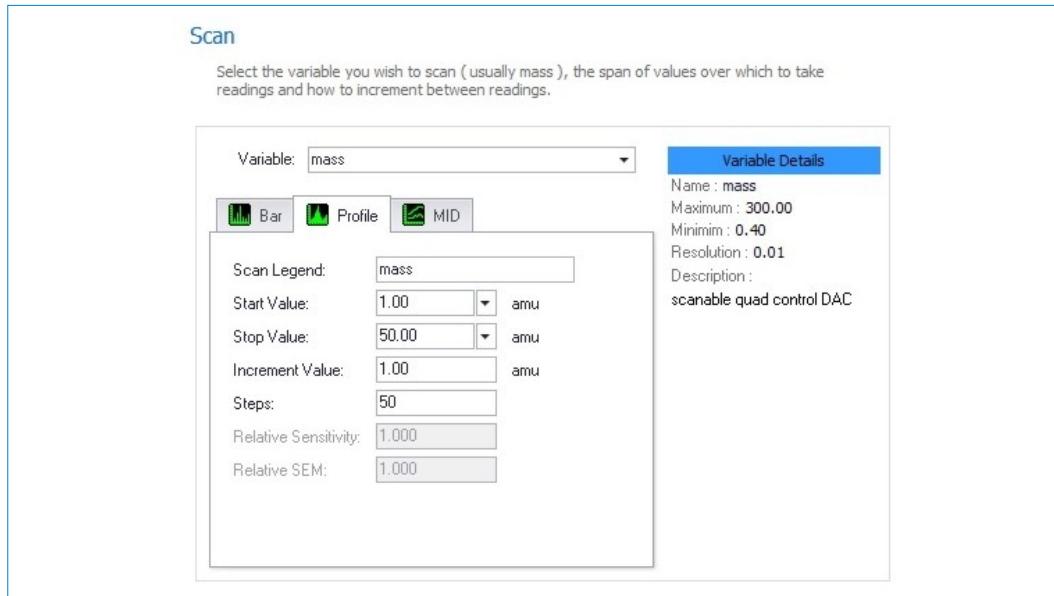
Clicking the Profile Scan button on the Easy Scans tab opens the **Profile Mode** dialog box for a simple linear mass scan. Parameters for the scan such as **Start mass** and **Stop mass** are defined in the Profile Mode dialog box.

Samples per amu Sets the increment for the scan. This will determine at how many points across a 1 amu mass span the instrument will measure the partial pressure. For instance setting **Samples per amu** to 20 will result in 20 measurement points per amu (20 points per peak) a **measurement every 0.05 amu**.

See also:

[Common dialog items](#)

Profile tab



The Profile tab creates a scan which takes measurements beginning at the **Start Value:** and increases the value by the **Increment Value:** until the **Stop Value:** is reached. It may be used to scan variables other than mass to display characteristic curves, for example if electron-energy is scanned the "appearance potential" curve can be plotted.

When scanning variables other than mass the mass at which measurements are taken is determined by the value in the Global Environment, or Local Environment if one is attached.

Profile scans are made with shorter dwell and settle times than Bar scans because of the large number of reading made by the Profile scan. A Profile scan of mass is qualitative.

A Profile scan with an increment of 1 is treated as a Bar scan.

A Profile scan of a device with a minimum increment of 1 will display as a Bar scan. The user may wish to change the view type to "Area" or "Line". The default view created for this type of scan is an "Area Graph".

A Profile scan may be used to scan the mass to inspect the shape, resolution and alignment of peaks.

Scan Legend: Allows the scan legend name on views to be edited; the required name is typed into this box; up to 32 characters (including spaces) may be used. This name also appears on the **Scan** box. The scan legend defaults to the contents of the **Variable:** box.

Start Value: The scan start value for the variable selected in the **Available to Scan:** list box. This must be within the **Minimum Value** and **Maximum Value** range for the variable.

Stop Value:	The scan stop value for the variable selected in the Available to Scan: list box. This must be within the Minimum Value and Maximum Value range for the variable.
Increment Value:	Defines the increment value for the scan; this cannot be less than Minimum Increment . Where an Increment value less than one is used, a PROFILE scan is performed which displays as an analogue graph.
Steps:	The total number of steps during the scan, for the defined Start value , Stop value and Increment is calculated and displayed in this box. However, if a value is entered in this text box, the Increment value is adjusted to suit.
Relative Sensitivity:	This is only available for MID scans.
Relative SEM:	This is only available for MID scans.

Quantitative Analysis

Quantitative Analysis is a licensed module of MASsoft including matrix inversion algorithms for accurate quantitative gas analysis. When Quantitative Analysis is licensed for an instrument and the **Advanced Interface** type is selected the **Preferences**, the **Quantitative Analysis menu** is available.

The Quantitative Analysis module provides gas analysis for known mixtures containing component gases that, due to the presence of overlapping peaks, are difficult to quantify. This is achieved through the use of a library of cracking patterns, which detail the contributions made by the constituent masses, and a series of matrix calculations to derive the levels of specific components within a known mixture. An analysis template is created, which specifies the component gases within a mixture and automatically generates a MASsoft experiment file.

The steps to creating an analysis are:

Check that each component in the analysis is an entry in the component library. The component library provides two pieces of information required by the analysis; the relative sensitivity of the mass spectrometer to the component and the cracking pattern. MASsoft supplies the **RGA** component library containing many gases. If the analysis contains components which are not found within the supplied library you will be required to enter them in the library.

The **Quantitative Analysis** menu contains commands to create a new template or open an existing template. A new analysis template is created using the **Quantitative Analysis Template Wizard**. This goes through the process step by step. From the list of components the wizard is able to build a list of masses that need to be measured. Not all the masses in each cracking pattern need to be measured; the wizard calculates a score for each mass,

awarding it points according to various criteria and will then choose a specified number from the highest scoring masses. It is important that enough masses are measured. To solve a set of simultaneous equations there must be more “knowns” than “unknowns”. If there are more than the minimum number of knowns the matrix is said to be “overdetermined”, this is usually desirable because it allows the matrix to determine a best fit when it solves the equations. It is therefore essential to measure more masses than components.

On completion the **Quantitative Analysis Template Wizard** creates the template file and a modified version of a MASsoft experiment file to measure the partial pressures. The **Home Window** shows the scan structure for the experiment, which has been created based on the parameters entered into the **Quantitative Analysis Template Wizard**. A series of MID Scans is created, one for each included mass of the analysis. The experiment can not have masses added or removed from the scan tree, although some of the other parameters can be edited. The **Quantitative Analysis Results View** is also created where the results of calibration or analysis are displayed in a spreadsheet and optional integrated plot.

Before calibrating the concentrations of gases in the mixtures in the calibration the gas bottles must be defined. The **Calibration Bottle Editor** provides an interface for adding, deleting and modifying entries in the calibration bottle library. A “calibration” gas must consist of a pure gas or of a mixture of gases whose cracking patterns do not overlap so that each mass may be uniquely assigned to a component. If the cracking patterns overlapped (i.e. had masses in common) then when those masses were measured it would not be possible to work out how much came from each component. The concentration of the components in the mixture should be high enough for the intensity of the peaks with smaller contributions to the cracking pattern to be accurately measured. To perform a calibration a list of bottles is selected from the gas bottle library. As previously noted the order of analysis is important to allow the relative sensitivities to be calculated. It is usual for the last bottle in the list to be the check gas. If the instrument is fitted with an automatic inlet each gas bottle can be assigned to an inlet as part of the library entry. The calibration procedure will then select the correct inlet as each bottle is analysed.

After the gas bottles have been specified, the calibration procedure can be carried out. Firstly a **Background gas** calibration may be considered for measuring the system background. Then a **Calibration gas** calibration to measure peak ratios in the cracking pattern of each component in the analysis. Finally a **Check gas** can be used to check and revise the RS of a component in a mixture. After each calibration the ratios of the peaks are re-calculated and the cracking patterns updated in the **Quantitative Analysis Template** file.

When the measurement of the calibration gas is complete the ratios of the peaks are re-calculated and the cracking patterns updated. If the calibration gas contains more than one component then the Relative Sensitivity (RS) may be calculated by treating the RS of one of the components as known. For instance in a mixture of argon in nitrogen the RS of nitrogen is 1 by definition so the RS of argon can be calculated relative to it. Then analysis of a mixture of carbon dioxide in argon would allow RS of carbon dioxide to be calculated as the RS of argon would already be known. The order of calibration is, therefore, important. A “check gas” contains a mixture of gases which result in overlapping peaks in the mass spectrum. The check gas is analysed by the matrix to calculate the concentration of each component. The calculated concentrations are then compared with the actual concentrations (as entered into the calibration gas library). If the calculated concentrations are not too far

from the actual concentrations (the user can specify the maximum acceptable deviation) then the relative sensitivities are revised to bring calculated and actual quantities in agreement.

Once the calibration is complete the template file can be used to analyse a sample, with the option of background subtraction. When analysed the results themselves are not stored with the analysis template, but in an experiment file created from the template. The results are displayed in a **Quantitative Analysis Results View**.

The **Directories tab** of the **Preferences** dialog contains entries for the default file directories where Quantitative Analysis templates and analysis files will be stored.

See also:

[Component Library](#)

[Cracking Pattern](#)

[Quantitative Analysis Menu](#)

[Quantitative Analysis Template Wizard](#)

[Quantitative Analysis Results View](#)

[Calibration Editor](#)

Quantitative Analysis Menu

When Quantitative Analysis licensed for an instrument and the **Advanced Interface** type is selected, the **Quantitative Analysis menu** appears.

The **Quantitative Analysis menu** items are described below. The first two options are always available.

New Analysis...

Create a new analysis. The **Quantitative Analysis Template Wizard** is displayed in order to create a new quantitative analysis template. This wizard steps through a series of pages used to configure the analysis.

Open Analysis...

Either open an existing quantitative analysis template or a previously created analysis. A dialog is displayed allowing you to choose which **Quantitative Analysis (.xml)** file to open.

The template files are by default stored in the **Quantitative Analysis Template Files** directory and the analysis files in the **Quantitative Analysis Data Files** directory, as defined the MASsoft Preferences.

On opening a template file the experiments **Home Window** is displayed, together with the **Quantitative Analysis Results View** containing no data, and optional MID Tabular and MID Graphical Views. The menu options to calibrate and start analysis are enabled

If a previously created analysis file is opened the experiments **Home Window** is displayed, together with the **Quantitative Analysis Results View** which will contain data obtained from the analysis, and optional MID Tabular and MID Graphical Views. Note that the results from a previous analysis are stored in the associated .csv file. Only the option to **View the Cracking Pattern** is enabled after opening an analysis.

A existing quantitative analysis template or a previously created analysis can also be opened by opening the experiment file (.exp) associated with the file via the regular **File | Open** menu option of MASsoft

The following options are available in the Quantitative Analysis menu only when a template file is open.

Template / Edit Analysis Template...	Displays the Quantitative Analysis Template Wizard containing the parameters associated with currently opened template file. The parameters can be edited within the wizard. When Finish is pressed on the final page a new or revised template file is created.
Template / Save Analysis Template As...	Allows the currently open template file to be renamed.
Calibration / Background Calibrate...	Displays the Calibration Editor for Background Calibration .
Calibration/ Calibrate...	Displays the Calibration Editor to Calibrate one of the components of the analysis.
Calibration / Gas Check...	Displays the Calibration Editor for Gas Check .
Acquire / Start Analysis	Starts an analysis using the currently open template. This opens a Save As dialog box, into which you must enter the name which the MASsoft experiment file will be saved as. This will default to a file name within the Quantitative Analysis Data Files directory. The name must be different to any existing files in this directory. The experiment is created as a copy the currently open template file. Data returned from this experiment file will then be used to generate results. The analysis continues until it is stopped or aborted. If the analysis is restarted after being aborted, it always overwrites any existing data.
Acquire / Background subtraction	If a background calibration has been carried out, then if selected, the results of a background scan will be subtracted from the data acquired by MASsoft during the analysis.
Results / View Cracking pattern	Displays the Analysis Cracking Pattern Data dialog box; this shows the contributions each of the selected masses makes to the various components in the template. This also displays the relative sensitivities and whether the components have been calibrated.
Results / Reset Cracking pattern	If selected, a dialog box will be displayed asking for confirmation that you want to reset the cracking pattern. If Yes is selected then the cracking pattern data and relative sensitivities will be reset to their initial library values. Select No to retain the existing values. If the reset option is chosen then the template will need to be recalibrated.

See also:

[Quantitative Analysis](#)

[Quantitative Analysis Template Wizard](#)

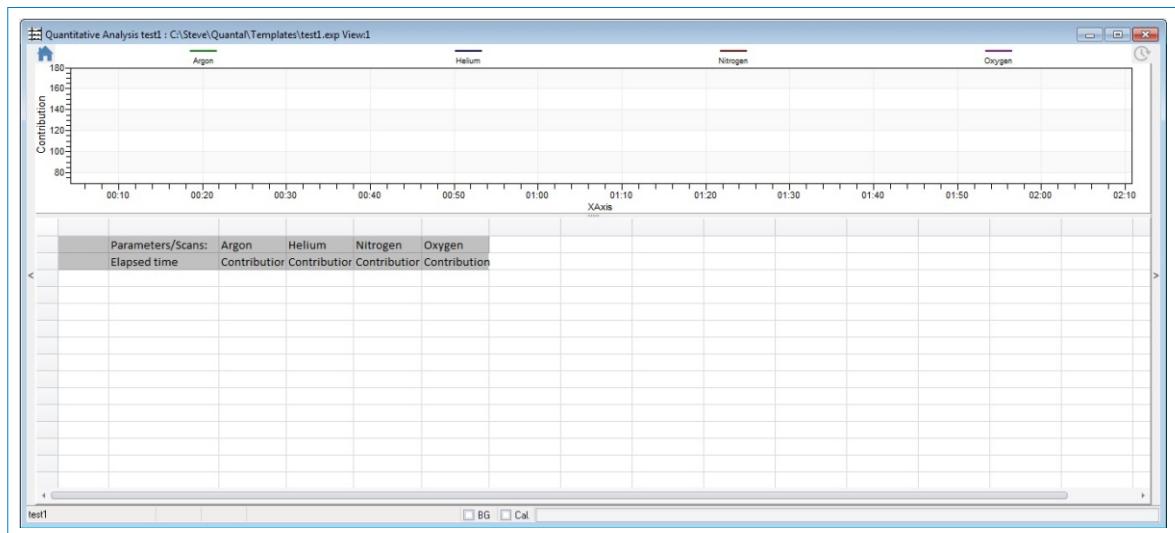
[Calibration Editor](#)

[Analysis Cracking Pattern Data Dialog](#)

Quantitative Analysis Results View

The **Quantitative Analysis Results View** displays the quantitative analysis data. It is displayed when calibrating the template or when carrying out an analysis.

A warning message is displayed if you attempt to close this view. The view is automatically closed when the Home Window of the Quantitative Analysis Template associated with the view is closed. An example is shown below.



The spreadsheet displays columns for the elapsed time, and contribution of each of the selected components in the analysis. If the optional tabular plot is visible, it displays the same data in graphical form.

At the bottom of the window is the status bar containing four panels. The first panel displays an informative text message to provide information on the state of the system. When calibrating this will display the type of calibration, and when analysing that an analysis is taking place. The **BG** and **Cal** check box panels indicate if the template has been calibrated. When background calibration has been carried out the **BG** box is ticked, and when at least one the component s has been calibrated the **Cal** box is ticked. The final panel displays a progress bar when calibrating.

When calibrating the progress bar will increment, until the point where the target number of calibration steps has occurred. At this point a message is displayed and all the data collected up to this point is re-calculated based on the results of the calibration, so that displayed in the table and graph may change.

When carrying out an analysis the results are automatically output to a csv format file.

Right-clicking on the **Quantitative Analysis Results View** brings up menu with the **Copy** and **Tabular Plot** sub menu option to **Show Plot or Print Tabular Plot**.

When clicked on a plot is shown above the data in the table. The plot shows the same results in a graphical form.

See also:

[Quantitative Analysis](#)

[Quantitative Analysis Template Wizard](#)

Quantitative Analysis TemplateWizard

The **Quantitative Analysis Template Wizard** is displayed when creating a new analysis template by selecting **New Analysis...** from the **Quantitative Analysis** menu, or when editing a previously created template via the **Template | Edit Analysis Template** option.

The **Quantitative Analysis Template Wizard** dialog steps through a series of pages which are used to create and configure the quantitative analysis.

The control panel at the bottom of the wizard dialog contains the **< Previous, Next >**, **Cancel** and **Help** buttons.

Next > Pressing the **Next >** button on any of the pages of the wizard moves onto the next page. This button is relabelled **Finish** on the final page.

< Previous Pressing the **< Previous** button on any of the pages of the wizard moves back to the previous page. This is disabled on the first page.

Cancel

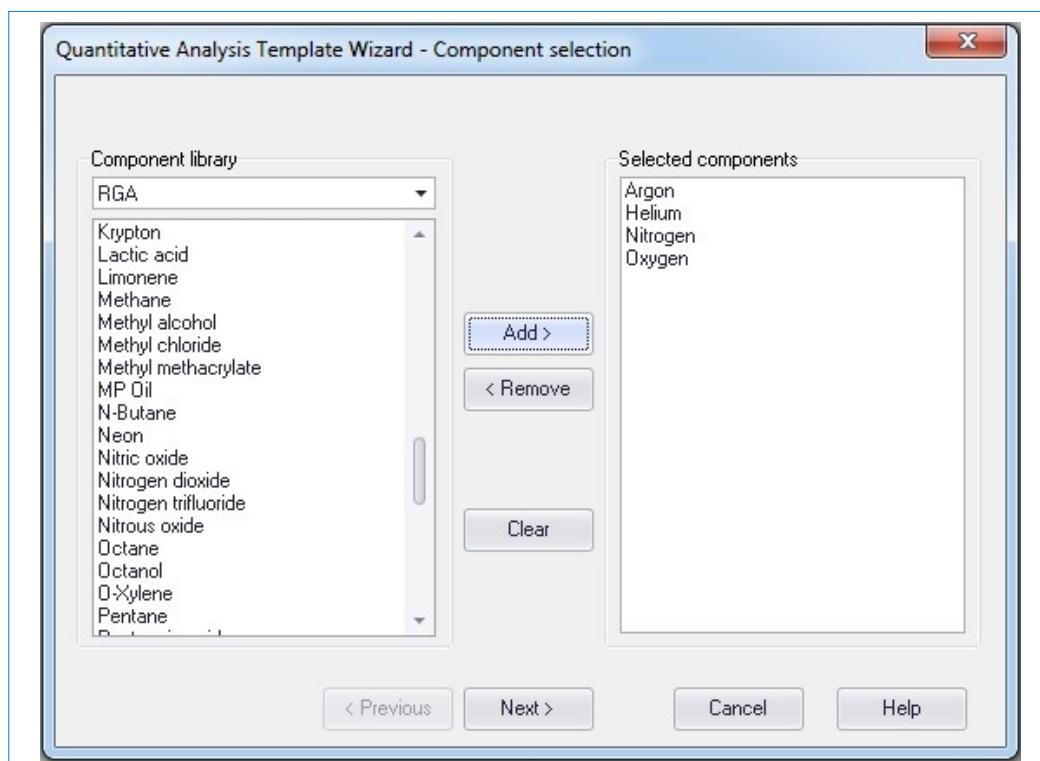
Pressing the **Cancel** button will close the wizard ignoring any changes made within the wizard dialog.

Help

Displays this help.

Component Selection

The **Component selection** is the first page displayed either when a new analysis is created, or on opening a previously created analysis. This allows the components required for the current analysis to be selected from the component library.



Component library

Lists all the component libraries used by MASsoft. By default MASsoft is supplied with the **RGA** library. If you have created your own library it can be selected from the pull-down list. All the species which are found within the selected library are displayed in the list below.

The library must contain all the components of interest in order to carry out the quantitative analysis.

The left hand list displays the contents of the component library and the right hand **Selected components** lists those components selected for inclusion in the current analysis.

Add >

Components can be included in the analysis by highlighting the required component(s) in the left hand list, then clicking the **Add >** button. The selected component(s) will then be transferred to the right hand **Selected components** list. The **Next >** button is enabled when the **Selected components** has at least one component.

< Remove

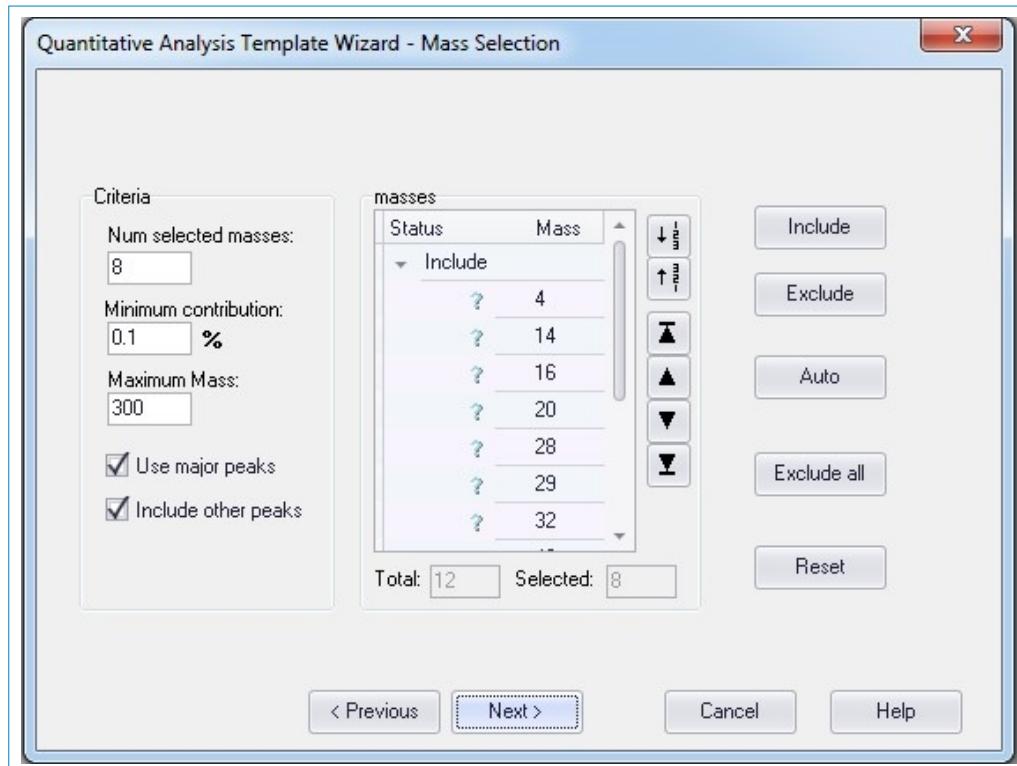
Select the component(s) in the right hand list and click the **<Remove** button to exclude it from the analysis. The selected component(s) will then return to the left hand list. If the **Selected components** list is empty then the **Next >** button is disabled.

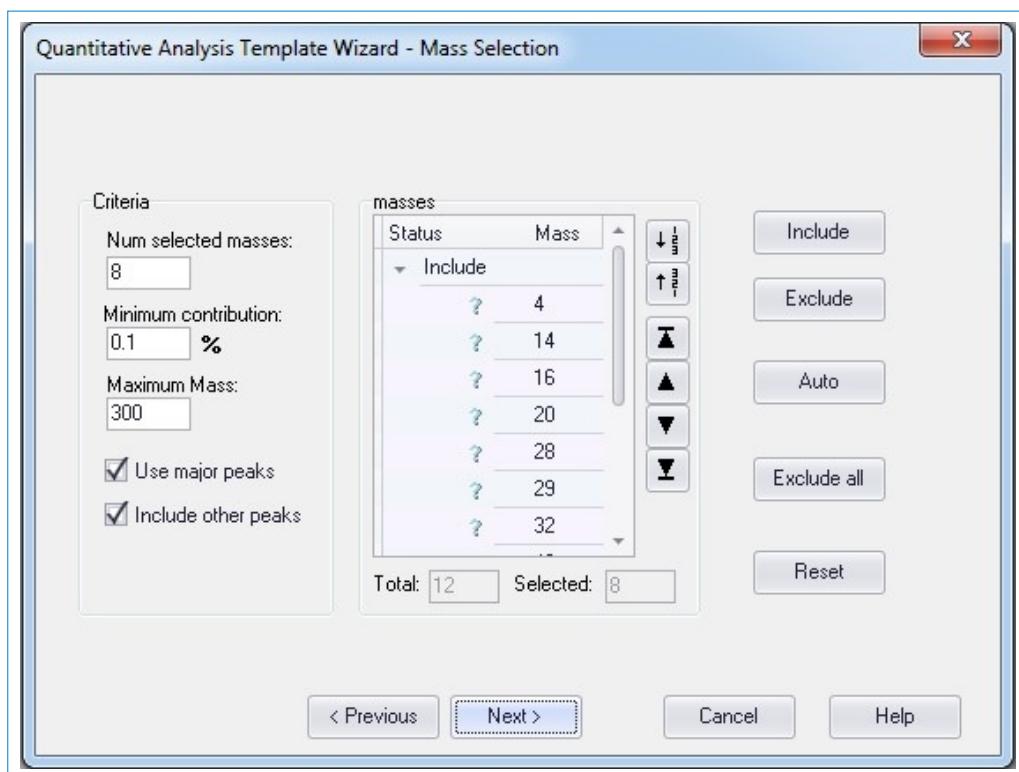
Clear

Removes all components from the selected list and returns them to the component library. The **Next >** button is disabled and remains so until components are added to the selected list. Pressing the **Next >** button will move onto the **Mass Selection** page of the dialog.

Mass Selection

The **Mass Selection** page is the second in the **Quantitative Analysis Template Wizard**. This allows the masses of interest to be defined. The wizard uses default criteria for selected masses.





The **masses** list displays all the masses of the components which were selected for the analysis in the previous page. Those that are in the **Include** section of the list are chosen for inclusion in the MASsoft template file, as determined by the various selection criteria. Those that are in the **Exclude** section are ignored.

The speed at which the results are updated is dependent on the number of masses included in the template file. Having fewer masses will provide a shorter delay between updates. Excluding masses with small contributions, whose value may be affected by noise, may provide more accurate results.

How the decision to include or exclude a mass has been made is illustrated by the ?, + and – icon in the **masses** list.

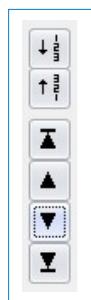
? indicates an automatically selected mass.

+ indicates manually included mass.

- indicates manually excluded mass.

Note that there must be more included masses than there are components in the analysis and there must be at least one mass from each component.

Num selected masses	This value determines the maximum number of masses that will be used to create the MASsoft template file. Reducing the number of masses will in turn decrease the time taken between readings, but some trade off against precision may occur.
Minimum contribution	Specifies the minimum partial pressure contribution a mass must make to its parent component for inclusion in the list of selected masses.
Maximum Mass	Specifies the upper limit for the masses that are included in the list of selected masses. By default this value is set to the mass spectrometer's highest value in the mass range.
Use major peaks	Toggles the inclusion/exclusion of the major peak for each of the chosen components.
Include other peaks	Toggles the inclusion/exclusion of the minor peaks for each of the chosen components.
Include	The Include button forces inclusion of the currently selected mass in the masses list, provided the maximum number of selected masses is not exceeded. The mass will be included regardless of the selection criteria defined elsewhere and appear in the Include section of the masses list with a +.
Exclude	The Exclude button forces exclusion of the currently selected mass in the masses list. The mass will not be selected for inclusion regardless of the selection criteria and appear in the Exclude section of the masses list with a -.
Auto	When the Auto button is pressed, the currently selected mass in the masses list will be automatically included if the mass meets the requirements outlined by the various selection criteria, otherwise the mass is excluded. The mass will appear in either the Include or Exclude section of the masses list with a ?.
Exclude all	Removes all masses from the Include section by setting the status for each to Exclude . This operation may be used if you wish to start by excluding all masses, then include each mass manually.
Reset	All masses will be automatically selected, returning the mass selection criteria to their original settings. The toolbar to the right of the masses list allows the mass list to be rearranged.



The toolbar affects only those masses in the **Include** section of the masses list. From top to bottom the buttons do the following:

Sort in ascending order

Rearranges the included masses in ascending order starting with the lowest.

Sort in descending order

Rearranges the included masses in descending order starting with the highest.

Move to top

Moves the selected included mass to the top of the **Include** section.

Move up

Moves the selected included mass up one position in the list.

Move down

Moves the selected included mass down one position in the list.

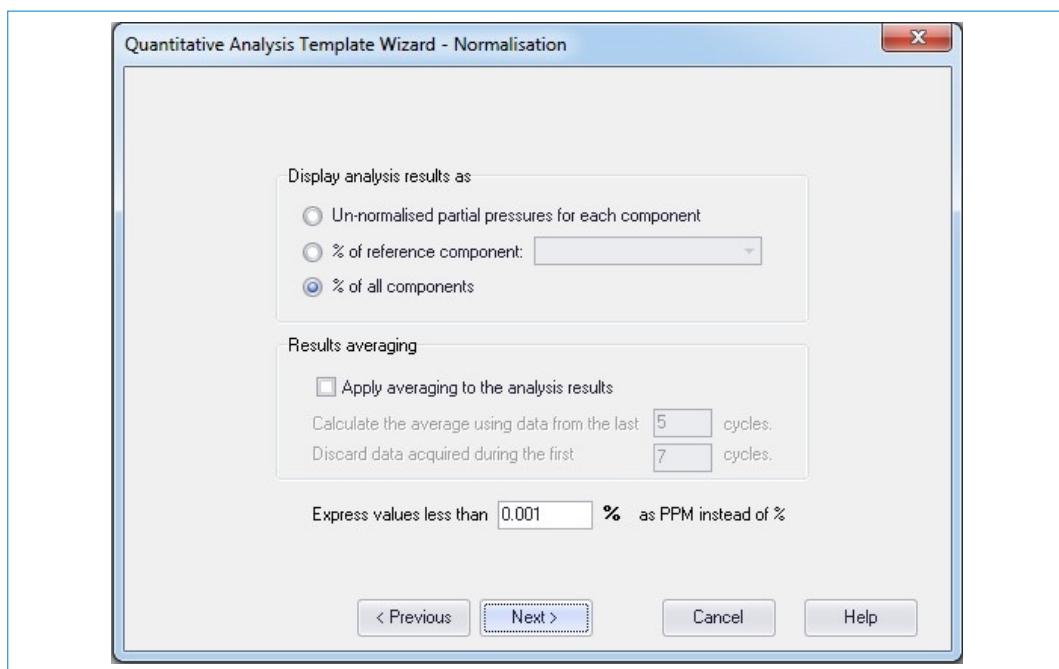
Move to bottom

Moves the selected included mass to the bottom of the **Include** section.

Pressing the **Next>** button will move onto the **Normalisation** page of the dialog.

Normalisation

The **Normalisation** page is the third in the **Quantitative Analysis Template Wizard**. This determines how the results of an analysis are presented.



Display analysis result as

Specifies the type of normalisation applied to the results of an analysis. Options are available to display data in an un-normalised form or as a percentage of either a single chosen component or all components.

Results averaging

If the results averaging check box is selected then a running average is maintained for each component for the duration of the analysis. The number of cycles used for the averaging is specified in the **Calculate the average using data from the last n cycles** (default 5). When a run starts it takes a few cycles for the signals to settle, these readings can be omitted from the average. In the **Discard data acquired during the first n cycles** field enter the number of cycles to be discarded at the start of the run (default 7).

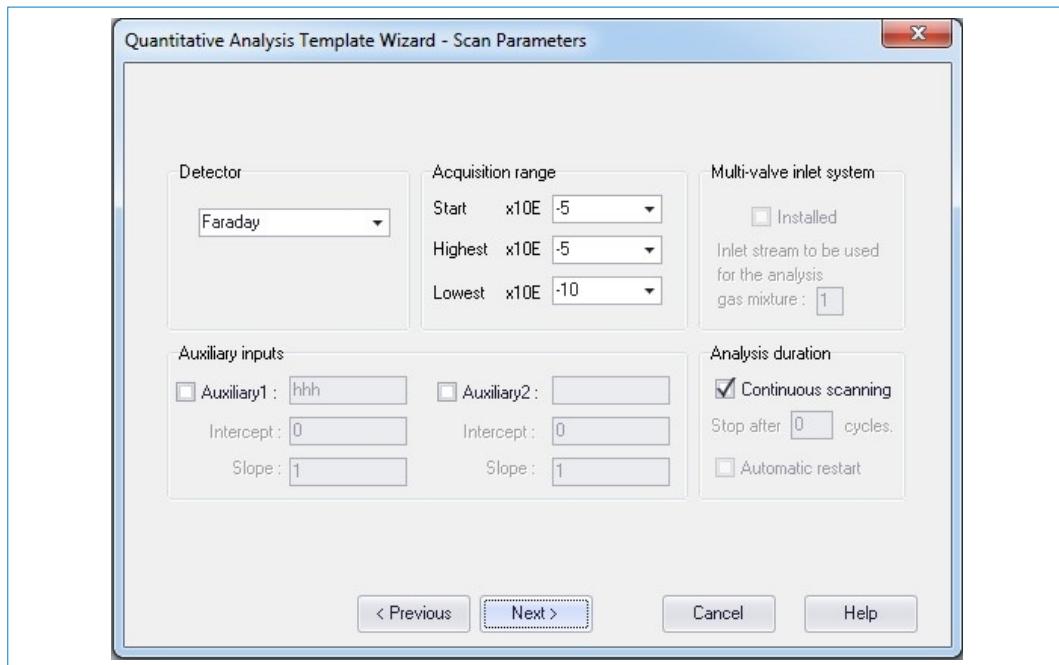
Express values less than n % as PPM instead of %

Specifies a value, below which results will be displayed as parts per million (PPM) instead of a percentage.

Pressing the **Next >** button will move onto the **Scan Parameters** page of the dialog.

Scan Parameters

The **Scan Parameters** page is the fourth in the **Quantitative Analysis Template Wizard**. This page allows detector type and ranges to be set for the quantitative analysis template.



Detector

A drop-down list contains a list of detector types for the current instrument. The default detector is automatically entered in this field. The detector will be used as the input into all mass scan created by the quantitative analysis template file. Changes to the detector type will be reflected in the limits available in the acquisition ranges.

Acquisition range

Specify the **Start**, **Highest** and **Lowest** values for the acquisition range from the pull down lists for the chosen detector type. The values available for selection will reflect the type of detector that has been chosen. The choice applies to all masses used in the creation of the quantitative analysis template file. Individual ranges can be configured from within MASSsoft once the template file has been created.

Auxiliary inputs

Data acquired via the auxiliary inputs can be displayed in the status bar at the bottom of the **Quantitative Analysis View**. A name can be assigned to each input, which then accompanies the reading in the status bar. The Mass Spectrometer accepts voltages in the range 0 to 10V. Readings can be translated to a $y=mx+c$ type curve using the slope (multiplier) and intercept (addition) values.

Multi-valve inlet system

Determines to which inlet stream the analysis gas will be connected.

Analysis duration

If **Continuous scanning** is enabled the analysis will run indefinitely. To limit the number of cycles in the analysis, uncheck the box and enter the required number in the text box to the right.

The **Stop after n cycles** field places a limit on the number of scan cycles the analysis will run for before completion. If the value zero is used then the file will run indefinitely.

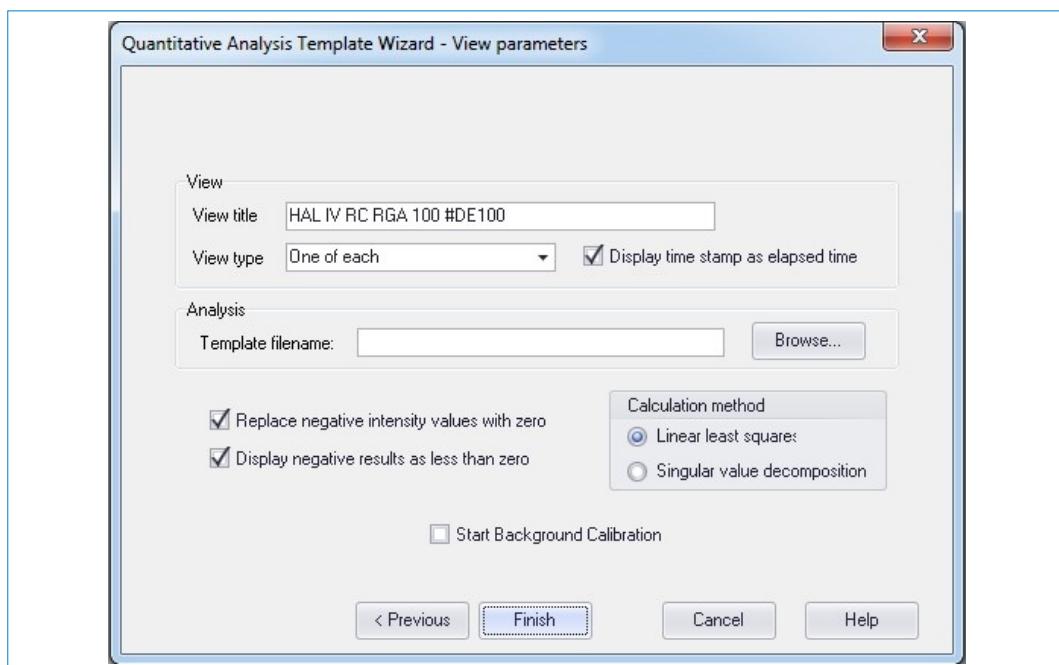
Automatic restart

If checked the user must when select the **Automatic Scan Restart** option in the **Scan Structure Cycles** dialog box that can be opened by clicking the Scan box at the bottom of the MASsoft scan tree. Quantal will then create a new trend data file each time the data file restarts.

Pressing the **Next>** button will move onto the **View Parameters** page of the dialog.

View Parameters

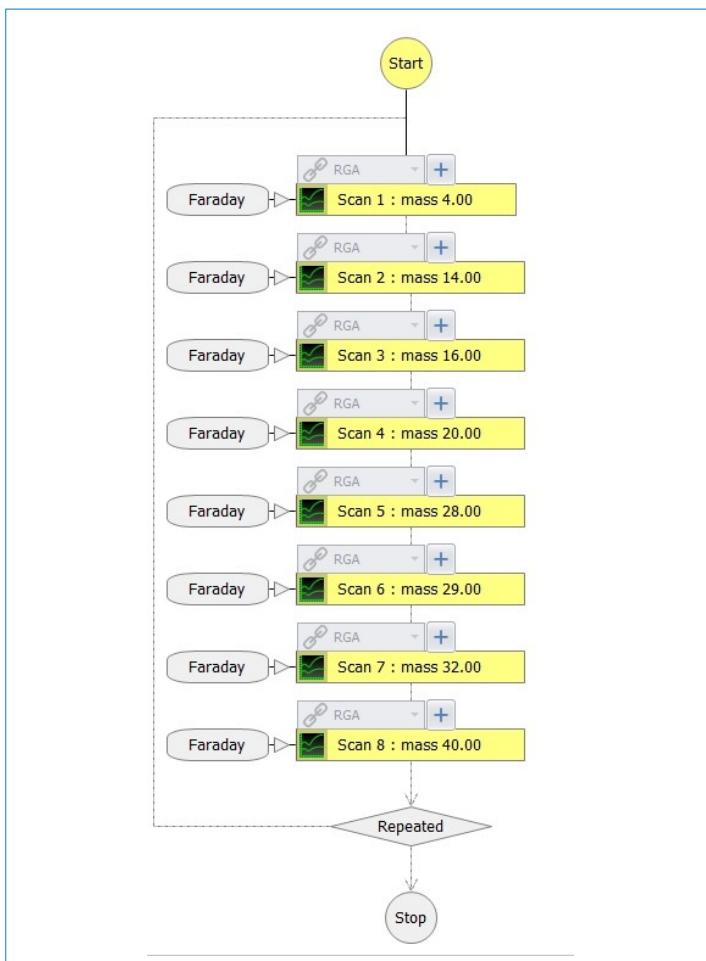
The **View Parameters** page is the fifth in the **Quantitative Analysis Template Wizard**. This allows the view type for the template file to be specified along with a view title if required.



View title

The title given to any associated views. By default the MSIU identification string is used.

View type	A drop-down list specifies the type(s) of optional views associated with the template file. This will either display a Graphical Trend View and /or a MID Tabular View of the mass peaks. A Quantitative Analysis Results View is always displayed.
Analysis Template filename	The filename of the template must be entered here. The Browse button allows a directory and filename to be specified for the template filename. The default directory where template files are stored is that specified in MASSsoft Preferences. The chosen path will be displayed in the Template filename field.
Calculation options	<p>Calculate method Select either Linear least squares fit or Singular value decomposition.</p> <p>Replace negative intensity values with zero When checked any negative results following background subtraction will be set to zero.</p> <p>Display negative results as less than zero When checked negative results are display as less than zero.</p> <p>Start Background Calibration When checked the next stage of starting a Background Calibration is initiated.</p> <p>Pressing the Finish button close the wizard dialog and create is a modified version of a MASSsoft Home Window where the scan structure is created based on the parameters entered into the wizard. A series of MID Scans is created, one for each included mass of the analysis. This differs from a normal MASSsoft Home Window in that the MID Scans cannot be edited or deleted. Neither can the Input device be changed, however individual ranges can be configured. An example of the scan structure created is shown below.</p>



A **Quantitative Analysis Results View** and the other chosen view types are created together with the Home Window.

It may be desirable to limit the ranges over which a mass can autorange when measured. It is also a good idea to select the **NoDeferAutoRange:** option in the **Scan Advanced** dialog as saturated values will cause errors in the solution of the matrix. The same template file is used for calibrating and analysing.

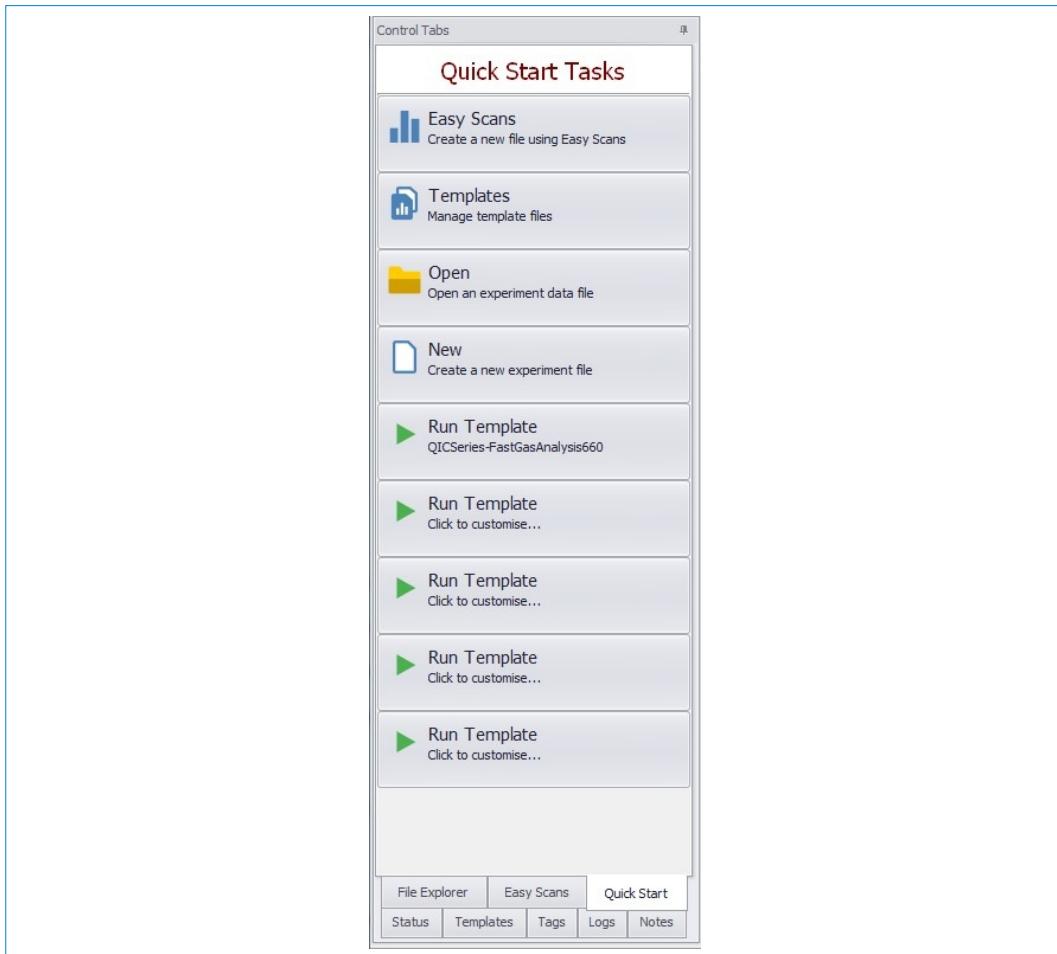
See also:

[Quantitative Analysis](#)

[Quantitative Analysis Template Wizard](#)

Quick start tab

The **Quick Start** tab of the Control Tabs frame provides access to frequently used tasks in MASsoft.



There are a number of default buttons as well as a number of customisable buttons to which templates can be assigned. Each button contains a textual description of a given task. The default buttons include:

Easy Scans Switches to the Easy Scans tab

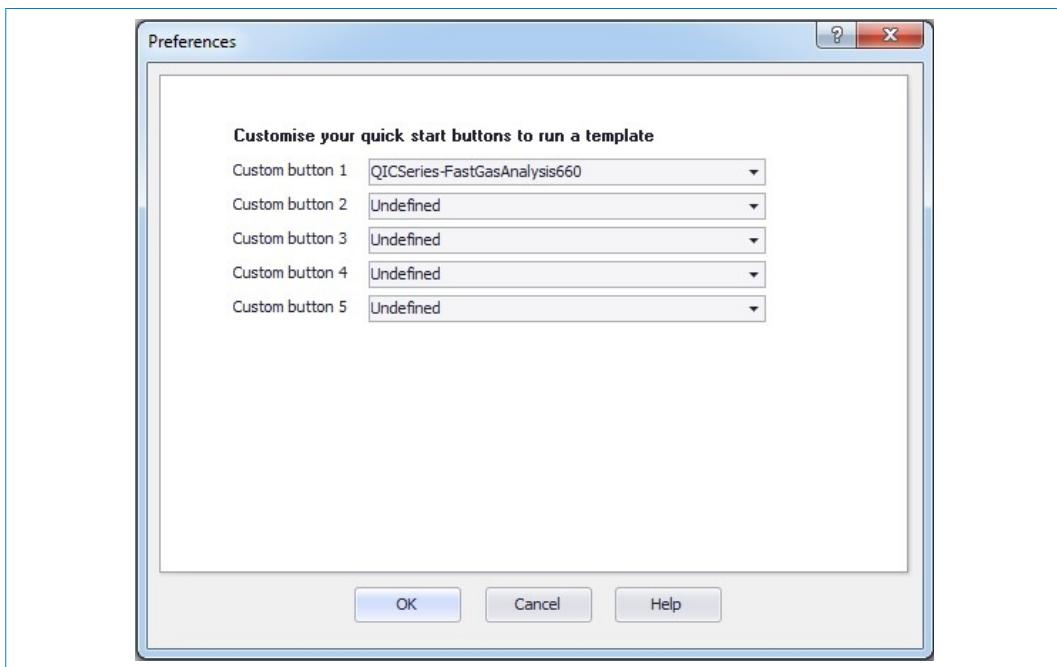
Templates Switches to the Templates tab

Open Displays a dialog to open an existing data file

New Creates a new experiment file

If a customisable template button has already been assigned a template, then clicking on it will open that template. Otherwise clicking on a button which has not yet had a template assigned allows you to customise it by assigning a template to the button. Such a button will be labelled with the description “Click to customise...”

To assign a template to a **Quick Start** button then click on button to display the dialog shown below



Click on the drop down list for the required custom button and choose the template from the drop down list. Double click on the template, or select it and press **ENTER**. Pressing the **OK** button will close the dialog updating the customisable buttons.

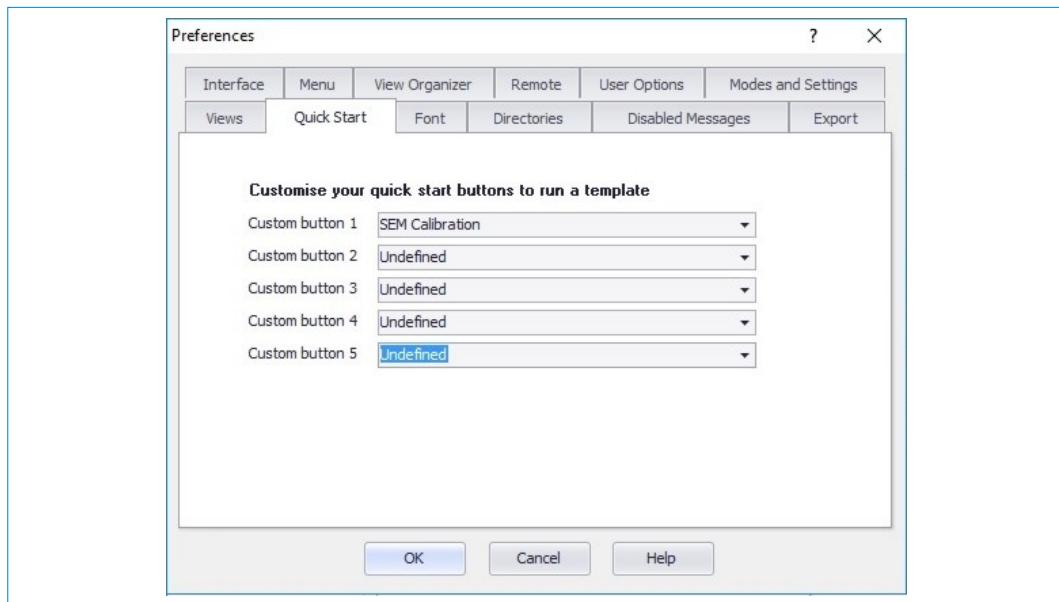
The list of Templates displayed is determined by the template files which are contained in the Template Files folder. This folder can be changed on the **Directories** tab in the **Preferences** dialog.

The customisable buttons can also be edited on the **Quick Start** tab of the **Preferences** dialog, accessed from the **Edit** menu.

See also:

[Preferences](#) [Directories](#) [Easy Scans](#)

Quick start preferences



To view the Quick Start preferences select **Preferences..** on the **Edit** menu then select the **Quick Start** tab.

Quick Start buttons when clicked automatically load and run an associated template file.

The Quick Start tab allows the user to configure the five user configurable Quick Start buttons.

One template file can be assigned to each button using the drop-down list box and selecting one file. The drop-down list is populated by using any templates files located in the designated template directory. The name on the template button will be changed to that of the template file selected.

This can also be accessed by selecting the Quick Start tab, in the Control Tabs, and then clicking the **Customise** button. However, once the button has been customized, **Edit**, **Preferences** must be used to make any further changes.

Rastering

Some of the mass spectrometers in the Hiden Analytical Limited product range (e.g. the EQS mass spectrometer) are able to support rastering with an ion or electron gun, and MASsoft allows the rastering variables to be configured. The system is intended for Hiden Analytical Limited's IG20 ion gun, but may also be used with other manufacturers' instruments.

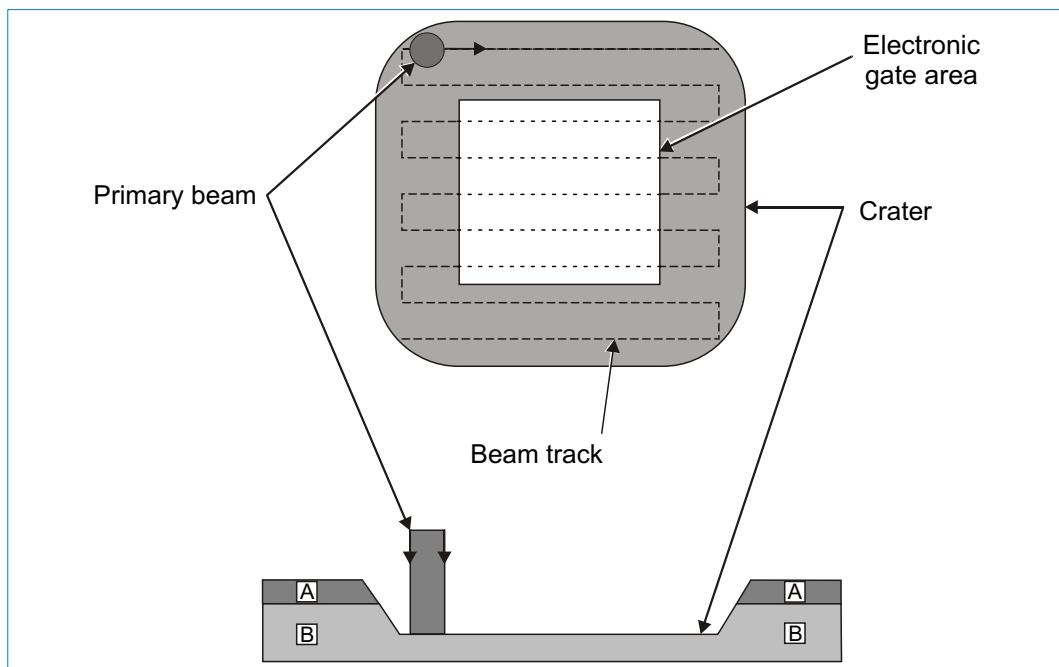


Where Rastering is available the Raster button will be visible on the Home Window.

Hiden's rastering system provides two voltages for control of the X- and Y- deflections of the gun, and an enable signal to turn the beam on and off. When activated, the outputs switch

the beam on at the required start point and start the rastering pattern as soon as the variable values in the Run environment are applied to the probe (i.e. as soon as the Run environment is executed), and switch the beam off and park it when the Shutdown environment is executed.

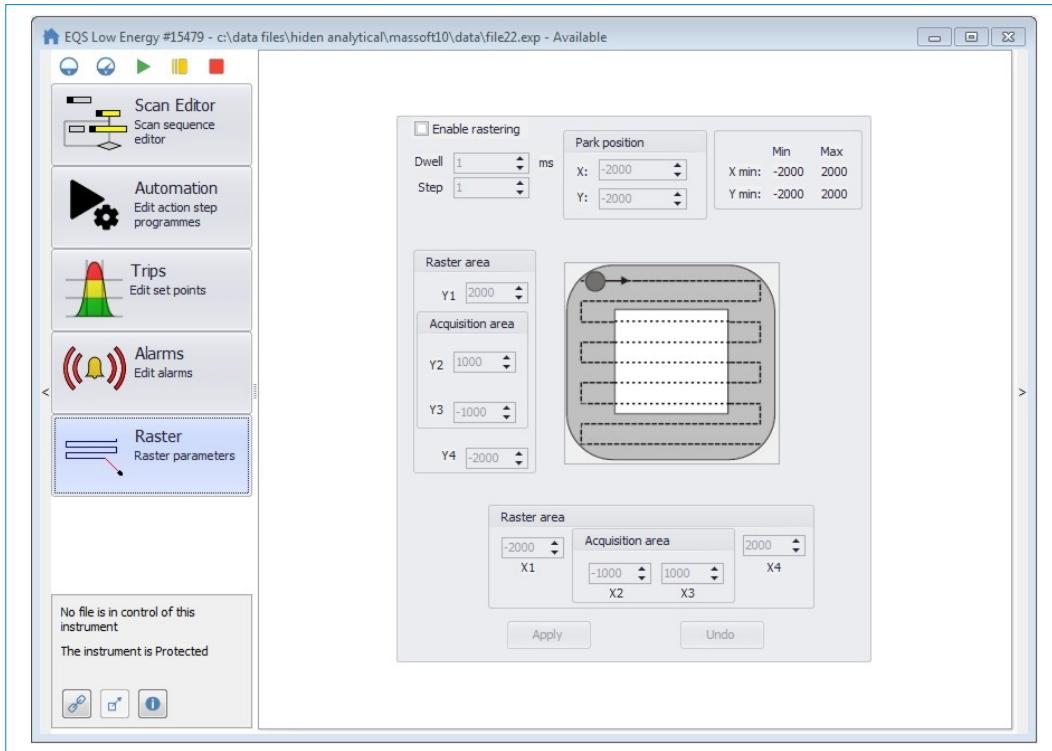
In use, the ion beam is rastered across the surface to produce a rectangular crater whilst data is acquired from the secondary ions generated at the surface. The signal from the centre of the crater plotted against time or depth for various elements is a depth-profile analysis. For good depth resolution a gating system is used to reject the signal from the edge of the crater where ions from the wall may confuse the profile. The figure below shows the primary beam spot rastering over a crater area and the track it uses to produce the crater. Data acquisition is enabled only when the spot is inside the gating area. This region is in the flat-bottomed centre of the crater so that the acquired signal is only due to particles ablated from the crater floor, with none from the crater walls.



Primary ion beam quality is an important parameter in depth-profiling SIMS applications and attention should be paid to the removal of neutral particles from the beam. These neutrals are not deflected by the ion gun deflection plates and may strike surfaces outside the gating area, resulting in low depth-profiling resolution. Neutral suppression is usually achieved by introducing a bend in the ion gun column and ensuring efficient ion source differential pumping.



Where rastering is supported, click on the **Raster** button to open the Raster dialog, shown below.



The dialog shows a series of concentric rectangles, where the outer rectangle represents the maximum possible area the gun can raster, the middle rectangle represents the actual area rastered and the inner rectangle represents the area from which data is acquired. Rectangles are scaled to a maximum of ± 2000 , which corresponds to the 12-bit DAC used to generate the X- and Y-signals. Corner points, expressed in DAC units, are used to define the limits of the rectangles and the corner co-ordinates may be entered directly into the boxes associated with each rectangle.

To enable co-ordinate entry into the corner boxes, the **Enable rastering** box must be checked, otherwise all the boxes are grayed out and inaccessible.

Text boxes **Y1** to **Y4** and **X1** to **X4** hold the rectangle corner co-ordinates in DAC steps relative to the centre of the area at 0,0. The **Dwell** box specifies the time (in milliseconds) that the beam stays on any position. The **Step** box specifies the size of the step from one position to the next, in DAC units.

The step size applies to both X- and Y-directions.

Rastering may start in any one of the corners and is selected by clicking the appropriate **Start here** radio button. When rastering is stopped, the beam is switched off and parked at the location specified by the **Park position**, **X** and **Y** boxes.

The **Enable rastering** option must be disabled when finished otherwise all subsequent scans will be gated.

Relative Sensitivity

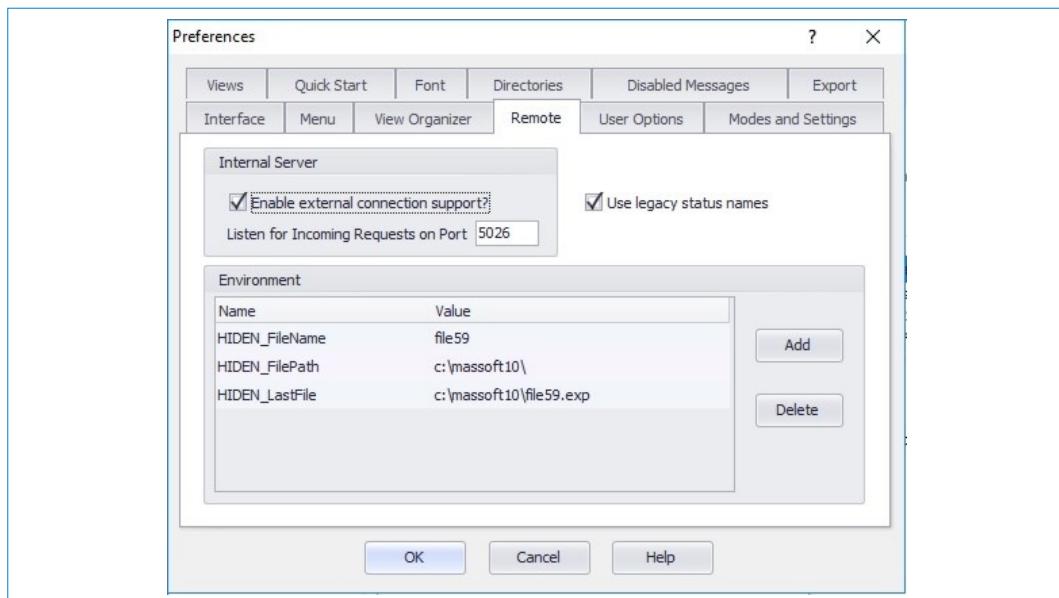
The sensitivity of the mass spectrometer to different components varies for a number of reasons; how easily the component is ionised in the source, how efficiently the resultant ion is transmitted through the mass spectrometer quadrupole filter and, if using a Secondary Electron Multiplier (SEM), how many electrons are produced when the ion hits the detector (or the probability of producing an output pulse if using pulse-counting SEM).

See also:

[Library](#)

[Quantitative Analysis](#)

Remote preferences



To view the Remote preferences select **Preferences..** on the **Edit** menu then select the **Remote** tab.

Internal Server This frame contains settings to allow external software applications to connect to MASsoft.

Enable external connection support?	If this is checked MASsoft will allow external software applications (clients) to connect to it on the specified port. Once a connection has been established, MASsoft will then be able to accept and operate on commands received from the connected client(s).
Listen for Incoming Requests on Port	The port number that MASsoft will monitor for clients attempting to connect to MASsoft. This can be any valid port number but the user will need to ensure that no other software application is currently, or will be, using this port number. Changing the Port number whilst the Internal Server is already activated will result in the Internal Server being turned off; reassigned the new port number and then turned back on again. Any clients connected to the old port number will be disconnected and will have to reconnect via the new port number.
Use legacy status names	-xStatus external connection command supports only pre version 7.29 status names. Refer to the table below.

Current	Legacy
Available	Available
Protected	Available
Tripped	Available
Unavailable	Unavailable
StoppedShutDown	StoppedShutDown
StoppedActive	StoppedActive
StartingActive	StartingActive
ScanningActive	ScanningActive
StoppingActive	StoppingActive
Degas	Degas
Disconnected	Disconnected

If clients are connected and the Internal Server is turned off the clients will be disconnected. MASsoft will display a warning message and the user may proceed or cancel.

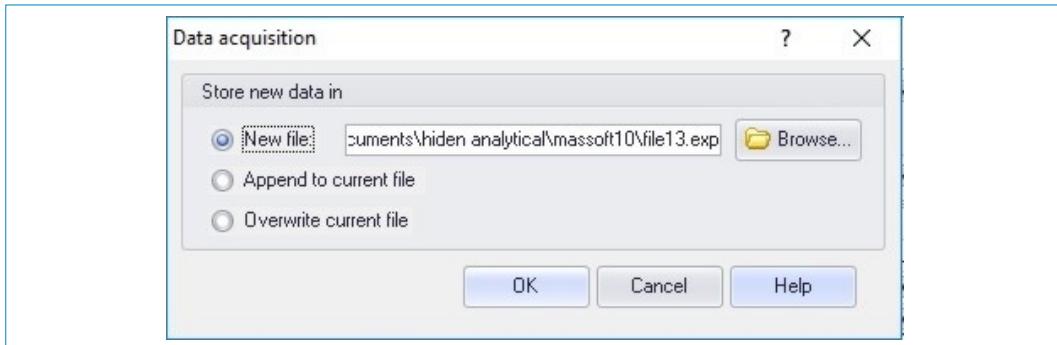
The **Environment** variables are available in MASsoft.

Add button	Inserts a new Environment variable. It will be necessary to specify the name and value of the new environment variable. This variable can then be used by external applications when specifying filenames or on the command line when starting MASsoft.
Delete button	Deletes the selected environment variable.

The environment variable *HIDEN_LastFile* is created by MASsoft automatically each time a file is saved, opened or run.

Restart

When a scan is re-started after being stopped the **Data acquisition** dialog will be opened to allow the user to specify where new data will be stored.

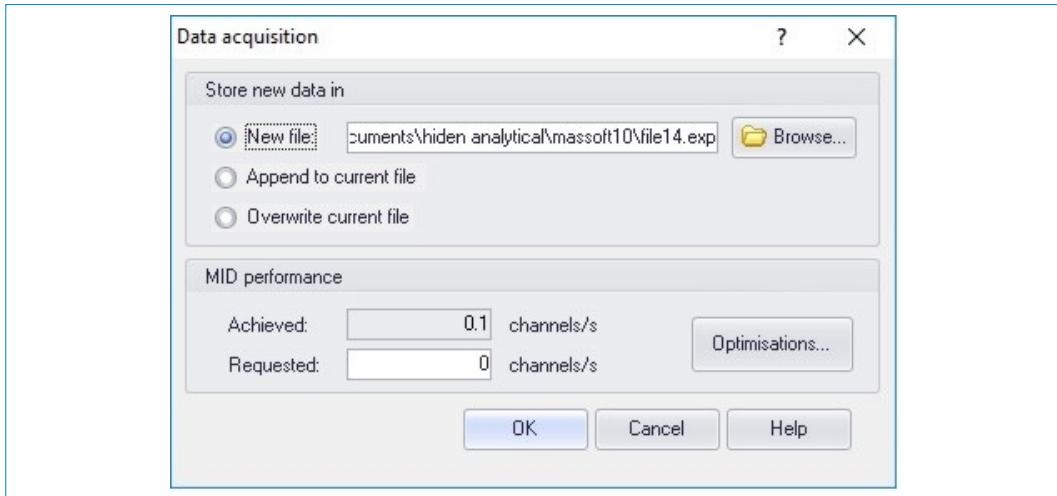


New file: When this option is selected the file name in which the new data is to be stored can be typed in the text box. A default file name is provided.

Append to current file The new data is added to the end of the contents of the current file.

Over write current file The new data replaces the contents of the current file.

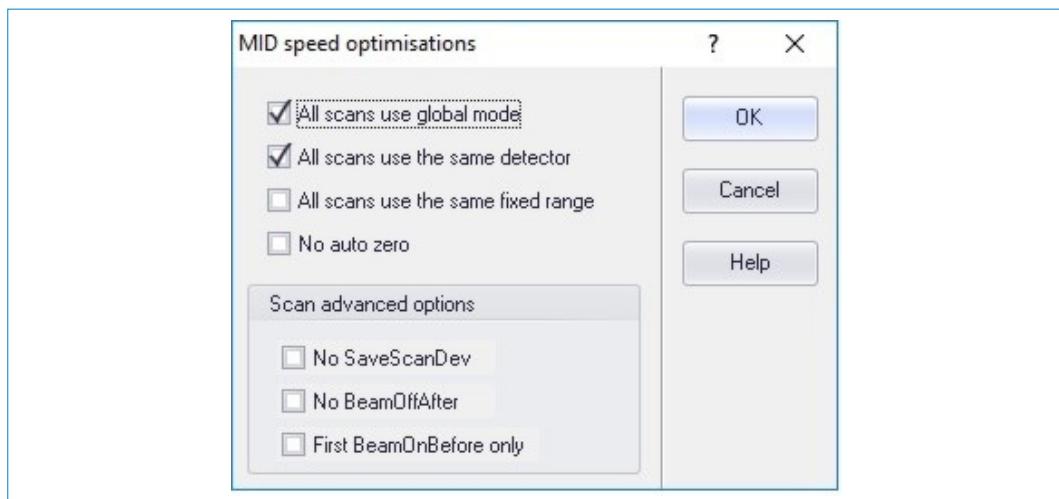
For MID mode scan there are some additional items in the Data acquisition dialog.



MID performance frame

Achieved Gives information on the performance of the MID scan before it was stopped in channels (scans) per second; this cannot be edited.

Requested	The required performance of the MID scan can be entered in the text box; MASsoft will try to optimise the scan in order to meet this performance.
Optimisations	Opens the MID speed optimisations dialog which shows which optimisation options are selected. The options can be over-ridden, as required, by checking and un-checking the appropriate boxes.



All scans use global mode	All the scans in the scan tree will use the Instrument mode selected in the Global Environment Editor dialog.
All scans use the same detector	All the scans in the scan tree will use the detector selected in the first scan in the tree.
All scans use the same fixed range	All the scans in the scan tree will use the Acquisition Range selected in the first scan in the tree.
No autozero	The analyser will not perform an automatic zeroing function at the start of each scan. No autozero only applies to analogue instruments.

Scan advanced options

No SaveScanDev	SaveScanDev is turned off; i.e. at the end of a scan the scanned variable value is not reset to what it was on starting the scan. See also: Advanced scan options .
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No BeamOffAfter **BeamOffAfter** is turned off; i.e. the ion beam is left on at the end of a scan.

See also: [Advanced scan options](#)

First BeamOnBefore only The ion beam is turned on only before the first scan.
See also: [Advanced scan options](#)

If **First BeamOnBefore only** is selected and **No BeamOffAfter** is deselected, the ion beam will be only turned on for the first scan in the scan tree.

Reviewing data

Data already recorded in a file may be viewed by opening the file by clicking **Open** on the **File** menu. The scan tree associated with the file is displayed, along with any other windows that were open when the file was last closed. All the view manipulation commands may now be used as required.

When re-opened the file will be locked to prevent inadvertent alteration of the scan parameters. The file may be modified by unlocking using the File menu, **Unlock** command or by using the unlock button. Unlocking invalidates any data in the file.

The scan and environment settings in the file may be re-used to acquire more data under the same conditions, provided the same type of mass spectrometer is used. If another mass spectrometer, possibly having different device names, is to be used, the File menu **Convert** file command must be used. The file should be inspected after conversion.

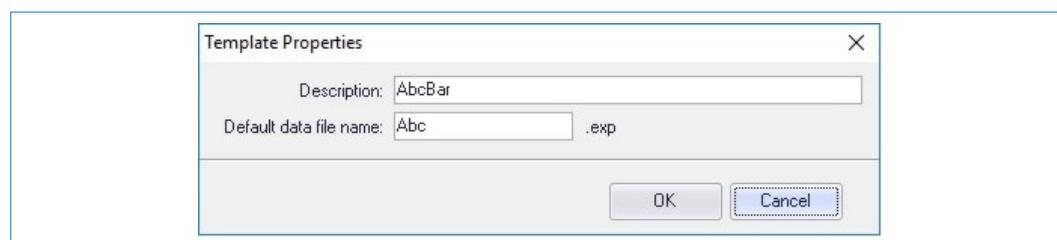
Any of the views associated with the file may be manipulated as normal; all the views associated with a file may be closed by closing the relevant mass spectrometer control window. When the file is re-opened at a later date, the views associated with it when it was closed are recreated.

It is possible to have several files open simultaneously for data review, but only one per instrument can be used at a time to acquire further data.

Data recorded in files may be viewed using the **Views, Graphical, Mode, Historical data** command.

Save as template

An experiment file may be saved as a template by selecting **Save As Template...** on the **File** menu. The **Template Properties** dialog will be displayed.



- Description:** Enter a description for the Template. This is the name that will appear on the Template control tab.
- Default data file name:** Enter a base name for all the data files created using the Template. In the above figure the first time AbcBar is run the data file will be Abc0.exp, the second time Abc1.exp, the third time Abc3.exp and so on.

See also:

[Templates](#)

Scan box

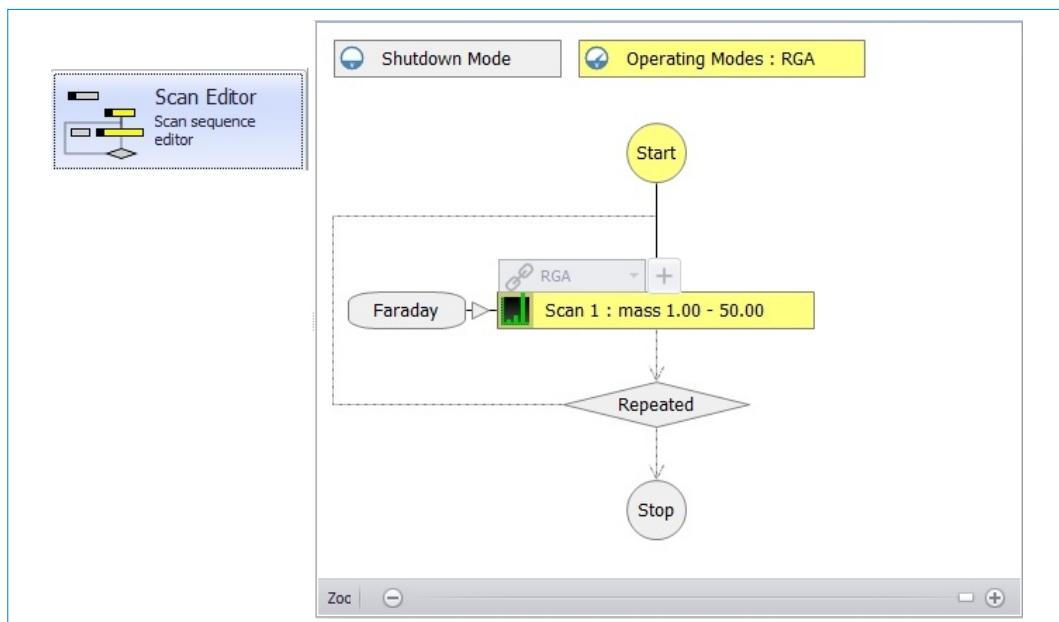
The Scan box holds the settings for the scan. Double-clicking the Scan box opens the Scan Editor dialog.

See also:

[Scan editor](#)

Scan Editor

The Scan Editor page is one of the Home Window pages displayed by clicking the **Scan Editor** button. The figure below shows the scan editor page displaying a very basic scan sequence, also known as the Scan Tree.

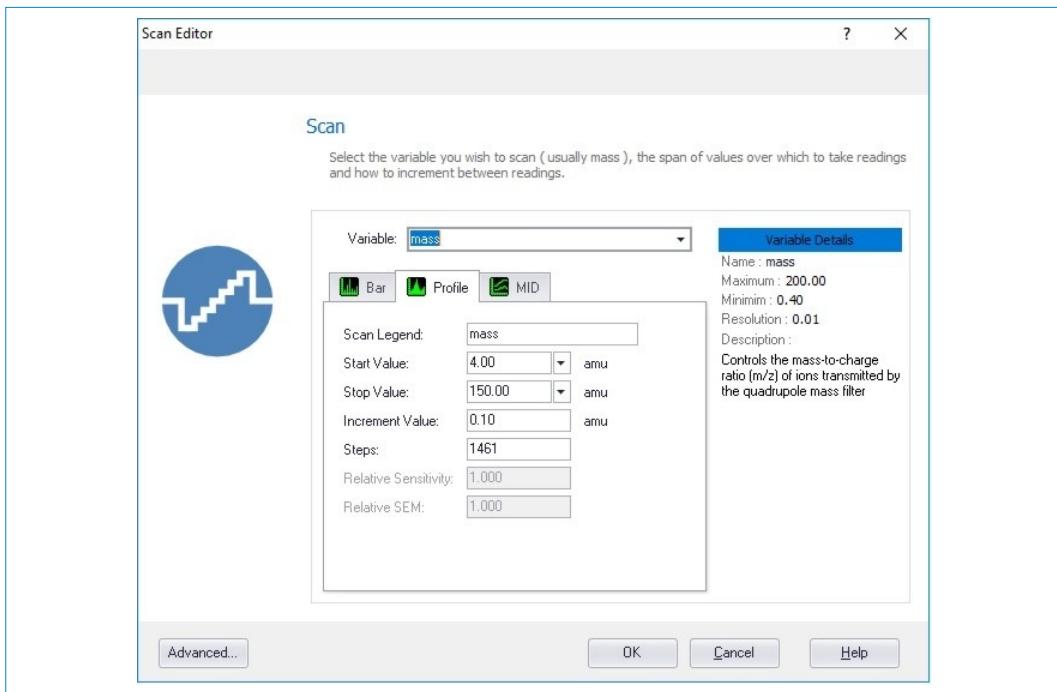


See also:

[Scan tree](#)

[Scan Editor Scan dialog](#)

Scan Editor Scan dialog



Variable

This list box defines the variable to be scanned.

The variables that are available for scanning depend on the type of instrument and the selected **Instrument mode**.

Variables that are not present in the **Variable:** list may be scanned by typing their name into the box.

The **mass** used may be set in the **Global** box or the scan's local environment.

If **energy** is scanned, an Ion Energy Distribution, or a map of the effect of this variable on the analyser performance for tuning, may be obtained.

Variable Details

Information relevant to the selected variable is displayed in the Variable Details area. The information will vary depending on the selected variable but can include; maximum and minimum values, resolution and a description of the variable.

Advanced... button

Clicking the **Advanced...** button opens the **Scan Editor Advanced** dialog.

See also: [Advanced scan options](#)

Drop-down button	The Drop-down button is available in the Start Value: and Stop Value: list boxes if on the User Settings tab of the Preferences dialog box the Period table radio button has been selected. See also: User options Clicking the Drop-down button displays a Periodic Table. Clicking on an element displays a drop-down list of mass spectral components and their relative abundances. Clicking on a component will enter the mass in the Start Value and Stop Value boxes.
Bar tab	The Bar tab creates a scan which takes a measurement at all integer values from the Start value: to the Stop value: The default view created for this type of scan is a "2D Bar Graph". Typically, this type of scan is used to survey a range of masses to identify which masses are present. Mass alignment ensures that each reading is taken close to the maximum of each individual mass peak.
Profile tab	The Profile tab creates a scan which takes measurements beginning at the Start Value: and increases the value by the Increment Value: until the Stop Value: is reached. It may be used to scan variables other than mass to display characteristic curves, for example if electron-energy is scanned the "appearance potential" curve can be plotted. When scanning variables other than mass the mass at which measurements are taken is determined by the value in the File Settings, or Scan Settings if one is attached. Profile scans are made with shorter dwell and settle times than Bar scans because of the large number of reading made by the Profile scan. A Profile scan of mass is qualitative. A Profile scan with an increment of 1 is treated as a Bar scan. A Profile scan of a device with a minimum increment of 1 will display as a Bar scan. The user may wish to change the view type to "Area" or "Line". The default view created for this type of scan is an "Area Graph". A Profile scan may be used to scan the mass to inspect the shape, resolution and alignment of peaks.
MID tab	The MID tab creates a scan which takes a single measurement at the value specified by the Start Value: setting. The default view created is a trend view of measurements against time. This type of scan is typically used to create a scan tree that measures one or more masses of interest and monitors the change in these masses against time.

Scan Legend:	Allows the scan legend name on views to be edited; the required name is typed into this box; up to 32 characters (including spaces) may be used. This name also appears on the Scan box. The scan legend defaults to the contents of the Variable: box.
Start Value:	The scan start value for the variable selected in the Available to Scan: list box. This must be within the Minimum Value and Maximum Value range for the variable.
Stop Value:	The scan stop value for the variable selected in the Available to Scan: list box. This must be within the Minimum Value and Maximum Value range for the variable. Stop Value: is not applicable to MID scans and is greyed out.
Increment Value:	Defines the increment value for a Profile scan. For a BAR scan, by definition, this is 1 and cannot be edited. For an MID scan this is not applicable and is greyed out.
Steps:	Defines the total number of steps during the scan, for the defined Start value , Stop value and Increment is calculated and displayed in this box. If it is edited the Increment Value: is re-calculated. For a BAR scan, by definition, this is 1 and cannot be edited. For an MID scan this is not applicable and is greyed out.
Relative Sensitivity:	This is only available for MID scans. Relative Sensitivity is a measure of the probability of ionising a molecule; the acquired intensity is divided by this value to give the reported value. The value for a particular ionising mode and parent molecule can be obtained from the appropriate library and, if the Easy Scans or the Library button are used to set up an MID scan, the correct value is automatically inserted. The reported intensity = (acquired intensity)/(relative sensitivity).
Relative SEM:	This is only available for MID scans. Relative SEM is similar to Relative Sensitivity ; it is a divider which can be used to compensate for the inherent discrimination of the SEM detector. No standard values exist for this variable and a suitable value must be obtained by experiment. If a suitable value is not known, Relative SEM should be set to 1.00 .

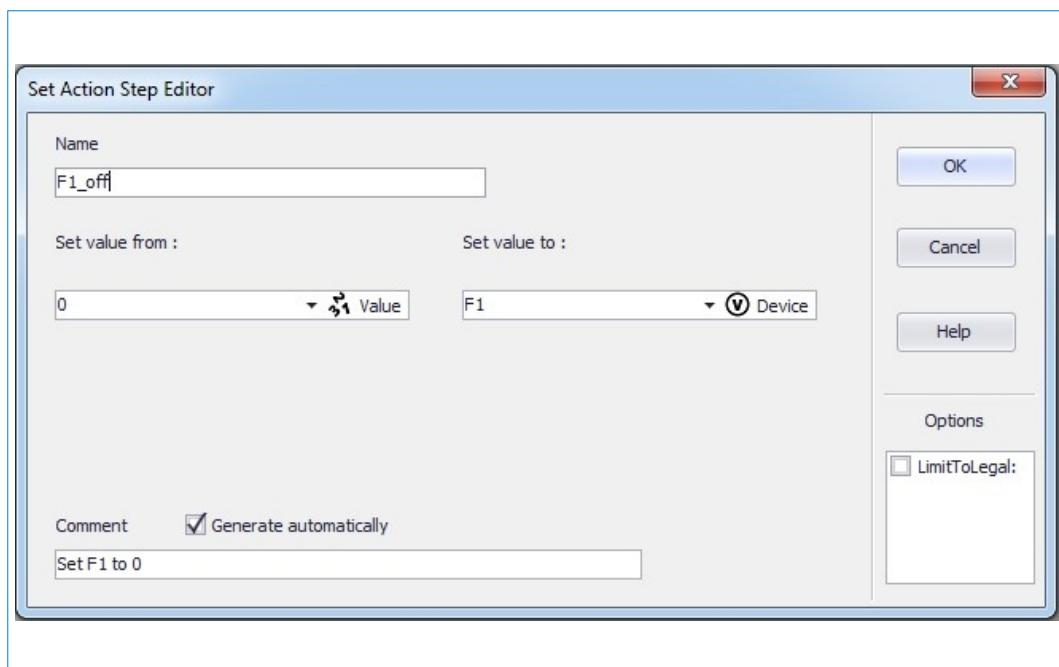
Set Action Step Editor



The **Set Action** , primary function is to set a device to a value. The “device” is usually a piece of hardware like a power supply or a relay. The power supply might drive a lens in the analyser. The relay might be an output like trip1 or might switch some of the hardware on and off, like a filament.

The **Set Action Step Editor** is displayed when editing a **Set Action**.

An example is shown below where a Set Action is setting F1 is set to 0 to switch filament 1 off.



Fields **Set Action Step Editor** are:

Name The name assigned to the Set Action.

Set value from: The source where the value is being taken from, which will be assigned to the destination in the **Set value to:** field. A pull down allows you to choose between **Device**, **Action step** and **Value**.

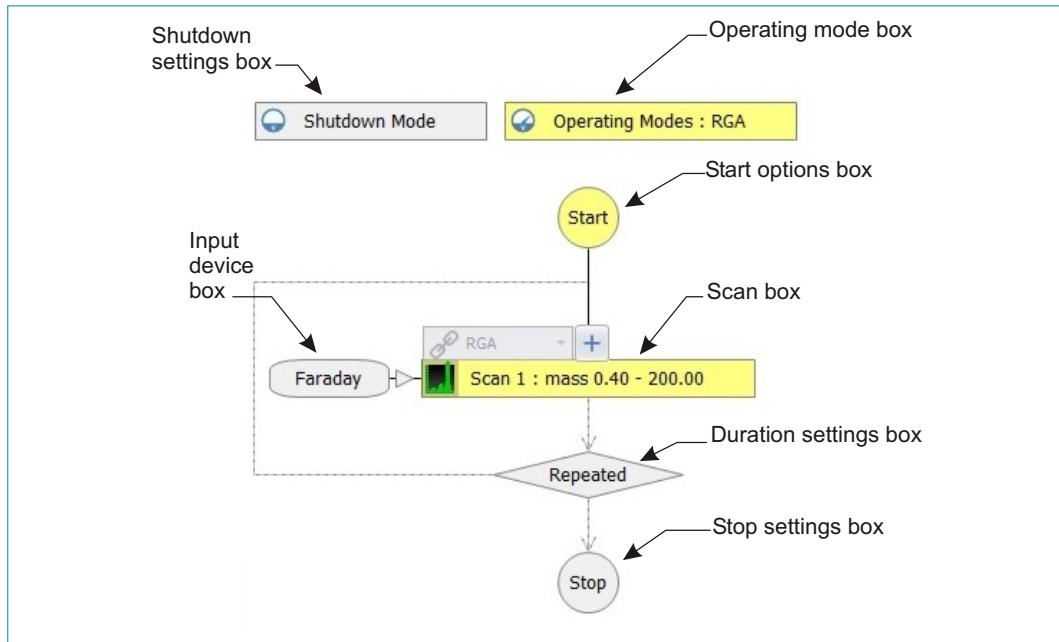
Device	A Set Action can copy a value from one device to another if both the source and destination are similar devices. It is possible, with suitably factory configured firmware, to set up dummy devices that have no physical existence or “logical” devices that affect the state of one or more other devices.
Action step	The source value can be that calculated in an action. For example it could be a value from an Evaluate Action.
Value	The source is a constant value.
Set value to:	The destination where the source value from Set value from: is stored. A pull down allows you to choose between Device or Action step
Device	The device to assign to the value in Set value from: field
Action step	A Set Action can copy a value from an action, device or constant to another action. When a value is copied from a device to an action object the action-object’s value is set to the value read from the device (i.e. the devices current setting if it is an output device or a reading from the device if it is an input device). The action’s associated device type is set to the source device itself. When a value is copied from one action to another the destination action’s value and device type are made the same as the source actions’s value and device type.
LimitToLegal Option	This ensures that the value assigned to the destination device does not exceed the devices limits. Examples of use of the set event are to copy a value to an event object when printing values using the #=>value option in Print Text events, to set Timer actions and to store the value in a “variable”.
Comment	The comment associated with the Set Action. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation page](#)

Scan tree

In MASSsoft the Scan Tree is a graphical diagram which defines the way the instrument behaves when asked to acquire data.



The Scan Tree is displayed in the Home window when the **Scan Editor** button is selected.

The total description held in the window is called an “experiment”; it comprises a series of environment, scan and scan control boxes. This description may be modified by adding extra environments and scans, and by altering their variable values. Double click on each element in the Scan Tree to open a dialog where setting may be altered.

The scan is the heart of the mass spectrometer controller; the Hiden Analytical Limited scan generators have been designed to be powerful and as flexible as possible.

Shutdown settings box

The Shutdown settings box holds the settings for Shutdown mode (normally set to reduce or turn off the source emission, turn off the SEM detector supplies, etc.). These values may be adjusted by double-clicking on the Shutdown settings box, which opens an **Edit File Settings** dialog.

See also: [Shutdown mode dialog](#)

Operating mode box

The Operating Modes box holds the File settings for all the operating modes. The File settings provide a value for all the output devices not being scanned. There are File settings for each acquisition mode which contains the current variable values for that mode. These variable values are used whenever that acquisition mode is selected for a scan, unless overridden by Scan settings associated with that particular scan.

See also: [Operating modes dialog](#)

Start options box	Double clicking the Start options box opens the Start Options dialog where the operating mode can be selected and data storage options can be set. See also: Start options dialog
Input device box	Double-clicking the Input device box opens the Input Selection dialog; this allows the selection of the input device used by a scan, if the mass spectrometer supports more than one input device. Only one input device may be selected for each simple, co-variant or multi-variant scan group. See also: Input selection dialog
Scan box	Double-clicking the Scan box opens the Scan Editor Scan dialog for that scan. In the figure above Scan 1: mass contains a description of a simple scan where the mass variable is varied. All other devices held at the values contained in the File settings. During the scan, data is read from the device described in the Input device box. Further scans may be added to extend the scan tree, with individual scans acquiring data from differing input devices, if required. Each scan in the tree uses the variable values set in the File settings, unless a Scan settings are added. Each scan in the tree also uses the default acquisition mode, set in the File settings, unless its acquisition mode is changed using the Scan Editor Scan dialog. This allows multi-mode scanning, where different scans in the tree can operate in different acquisition modes (e.g. RGA, negative ion RGA, positive ion SIMS, negative ion SIMS). Different scan types (e.g. Histogram, Multiple Ion Detection, Profile) during one acquisition cycle can also be set up by using the Scan Editor Scan dialog box. To see what is happening when data are acquired by a scan, or to replay saved data from a scan, a view window (or windows) may be attached to one or more scans. See also: Scan Editor Scan dialog
Duration settings box	Defined for how long scanning will continue in terms of time or number of scans. Double click on the box to open the Duration Settings dialog. See also: Duration settings dialog
Stop settings box	The scan sequence ends at the Stop box which describes whether the cycle is to be restarted, exported or shutdown. Double click this box to open the Completion options dialog. See also: Completion options dialog

A scan can be one of three types:

A simple scan, where a single variable is scanned by incrementing between defined start and stop values. **See also:** [Simple scan](#)

A co-variant scan, where two or more scans are linked so that each updates its output before another data point is acquired; it is used to allow variables to track one another. **See also:** [Co-variant scan](#)

A multi-variant scan, where two or more scans are linked so that subordinate scans perform a complete scan before the next higher scan in the tree updates its output. Several scans may be linked to form one multi-variant group. A multi-variant scan may be used to perform multi-variable surface mapping. **See also:** [Multi-variant scan](#)

Settle time

Settle time is the time the instrument waits having adjust the variables (for instance increased the mass setting) before making any measurements.

Higher settle times give more stable measurements but the overall scan speed will be reduced.

See also:

[Dwell and settle times](#)

Shortcut keys

The following shortcut keys are used by MASsoft.

Ctrl+S	Save
Ctrl+P	Print
Ctrl+Ins	Insert Co-variant
Shift+Ins	Insert Multi-variant
Ins	Insert Sequential
Ctrl+X	Cut
Ctrl+C	Copy
Ctrl+V	Paste
Del	Delete
Ctrl+A	Select all
Ctrl+G	Add graphical view
Shift+F4	Tile Horizontal
Shift+F5	Cascade

F1

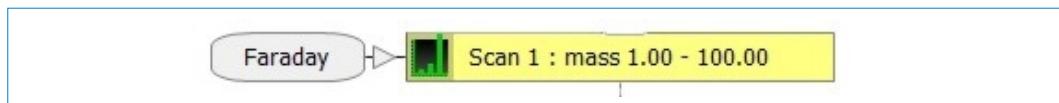
Help contents

Shutdown settings box

The Shutdown settings box holds the settings for Shutdown state. Typically in the Shutdown state the instrument may reduce the source emission or switch off the filaments and turn off the SEM detector supply. These values may be adjusted by double-clicking on the Shutdown settings box, which opens the Shutdown Mode Edit File Settings dialog **See also:**

[Shutdown mode dialog](#)

Simple scan



A simple scan sets the output variable (in the above case **mass**) to the Start value and reads the input variable (**Faraday** detector in this case). It then steps the output variable by the Increment value and reads the input again. This is repeated until the Stop value is reached.

The Scan setting may be changed in the Scan Editor Scan dialog opened by double clicking on the Scan settings box.

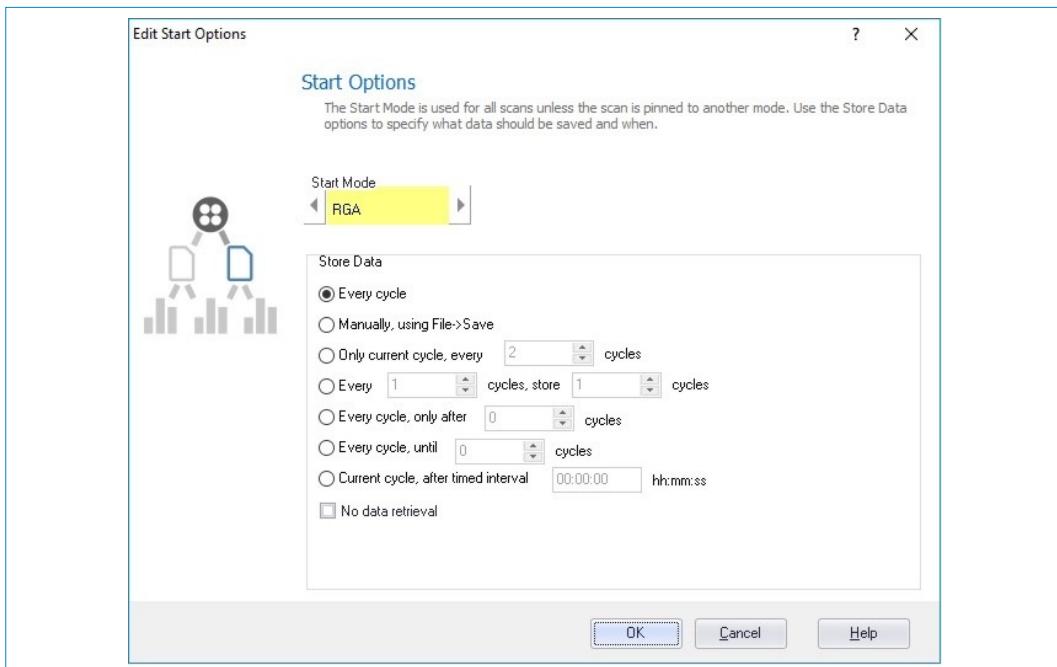
A simple scan is added to the basic scan tree by clicking a Scan settings box to select it, then clicking the Insert Sequential Scan button or by pressing the **Insert** key or by right clicking right clicking in the Scan settings box and selecting **Insert Sequence** from the pop-up menu.

The new scan will be added after the selected scan. The new scan will be highlighted to indicate it has the focus.

To remove a scan from the scan tree, select it and press the **Delete** key or right click in the Scan settings box and select **Delete** from the pop-up menu.

Each scan is given a scan number to allow it to be associated with its attached view(s) (Scan 1 in the above case). Only scans with input devices may have views attached, but several views may be attached to one scan so that the data may be presented in different ways.

Start options dialog



The **Edit Start Options** dialog allows the starting mode and data storage options to be defined.

Start Mode

Select the mode to set the instrument to at the start of the scan. Many instruments such as RGA and gas analysis (HPR20, QGA etc) only have the one, RGA, mode.

Store Data options

Every Cycle

Every complete cycle of scan data is stored.

Manually, using File -> Save

Data are not saved unless the **File**, **Save** menu command is selected during acquisition, at which time the cycle currently being acquired is saved.

Only current cycle, every n cycles

Cycles which are multiples of **n** are saved.

For example if **n**=5, then cycles 5, 10, 15, 20 and so on are stored.

Every n cycles, store m cycles

Similar to the option above, but **m** cycles are stored instead of one.

For example set **m**=3 and **n**=5. If **m** is greater than **n**, all cycles are stored.

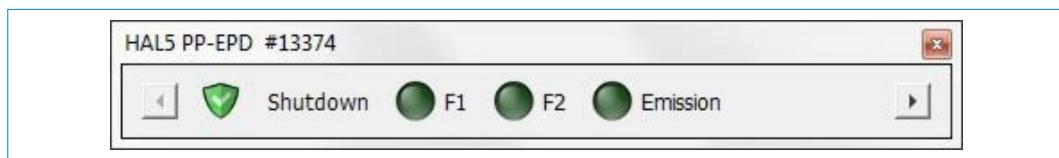
Every cycle, only after <i>n</i> cycles	The first <i>n</i> cycles are ignored, but all subsequent cycles are stored. For example if the scan is set to run for 10 scans and n=5 scans 6 to 10 will be stored.
Every cycle, until <i>n</i>	Only the first <i>n</i> cycles are stored; all subsequent cycles are ignored.
Current cycle after timed interval	The first complete cycle acquired after each time interval has expired is stored.
No data retrieval	This option stops MASSsoft retrieving data from the control unit to the PC when scanning, thus speeding up data acquisition.

Status bar

The MSIU Status Bar displays the status of all the devices being monitored by a control unit, and can exist in two states; docked or floating.



Every known control unit can have a Status Bar, with its identity being displayed either at the top of a docked Status Bar as shown in the figure above or on the caption bar of a floating Status Bar, as shown in the figure below.



By default the status bar will contain Availability, Mode, F1, F2 and multiplier.

The Availability icon shows the Availability State. The description of the state is available as a tool tip. The first figure shows an instrument in the “Available” state. The second figure shows an instrument in the “Protected” state.

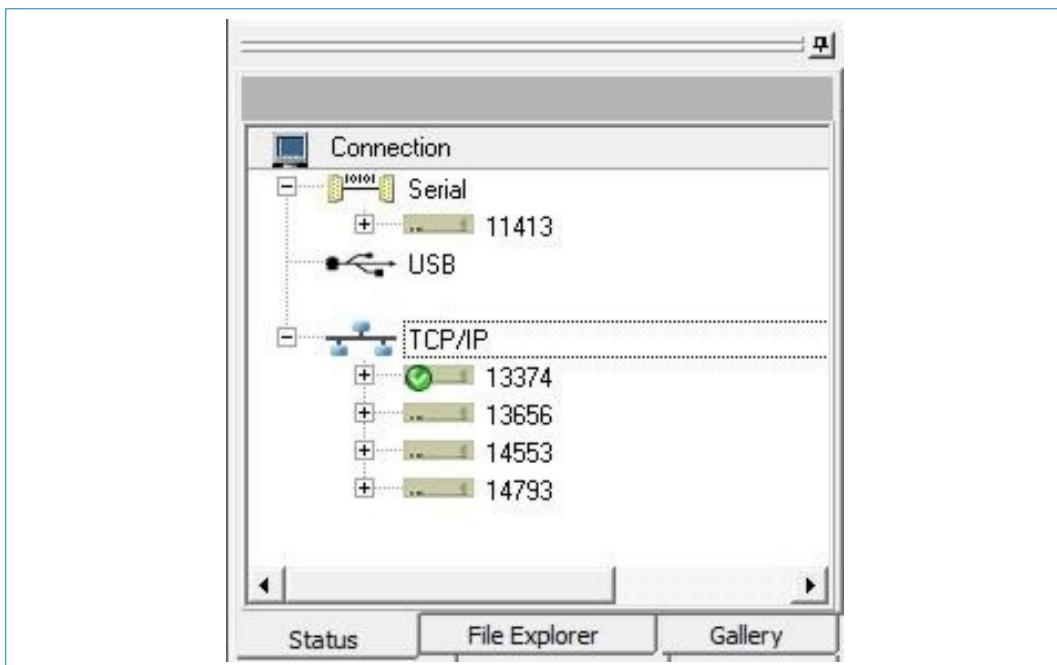
The style and size of the icons on the Status Bar may be original, small or medium, matching those on the tool bar. Medium icons are used for large and High Contrast settings. The size may be adjusted in the **Menu** tab of the **Preferences** dialog.

There is no limit on the number of control unit Status Bars that can be created. It is even possible to create more than one Status Bar for the same control unit. This is useful if there are a large number of devices being monitored on a control unit and they must all be visible.

Status tab

The Status tab shows the Connection Tree which displays all the known instruments according to the type of connection; Serial, USB or TCPIP.

To display all the instruments using a particular connection, expand the connection's node. If the connection doesn't have an expansion node there are no instruments using this type of connection.



In the figure above there are five known instruments; 11413, 13374, 13656, 14553 and 14793. Instrument “11313” is using the serial connection, there are no instruments using USB and the remaining instruments use TCP/IP.

Instruments are recognised by their Works Reference number (WR No.).

See also:

[Works reference number](#)

The active instrument is shown by this shows that it is available for use. If it

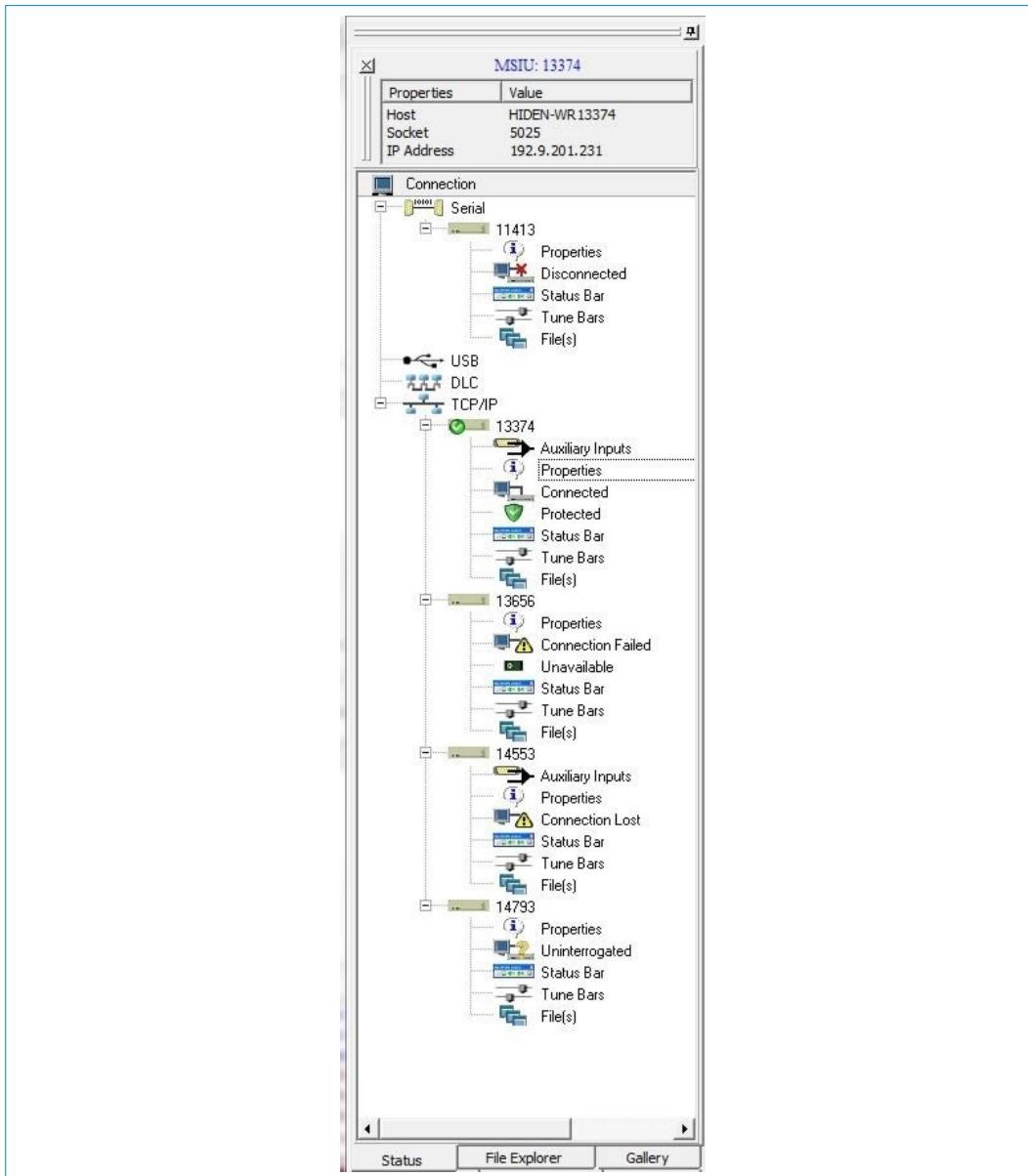
were unavailable it would be shown by .

The Active Instrument may be changed by right-clicking on a node and selecting **Make Active Instrument** in the pop-up menu, or by selecting an instrument on the **MassSpecs** menu.

The **File**, **New** and **File**, **Open** commands associate the file with the active instrument.

An Instrument's status can be displayed by expanding the instrument's node.

The figure below shows an expanded connection tree.



Right-clicking on a branch of the tree brings up a pop-up menu.

The pop-up menu may contain the commands:

Active Instrument

Edit Instrument Environment

Configure Auxiliary Inputs

Show Connection Properties

Show Status Bar

Customise Status Bar

Tune

Add New Instrument

- Import Instrument
- Export Instrument
- Connection Settings
- Connection State
- Re-interrogate
- DHCP Media Sense
- Explore
- File
 - New
 - Close
 - Save
 - Save As
 - Save as Template

The Instrument Status consist of up to seven categories; Properties, Connection Status, Status Bar, Tune Bars, Auxiliary Inputs and File(s).

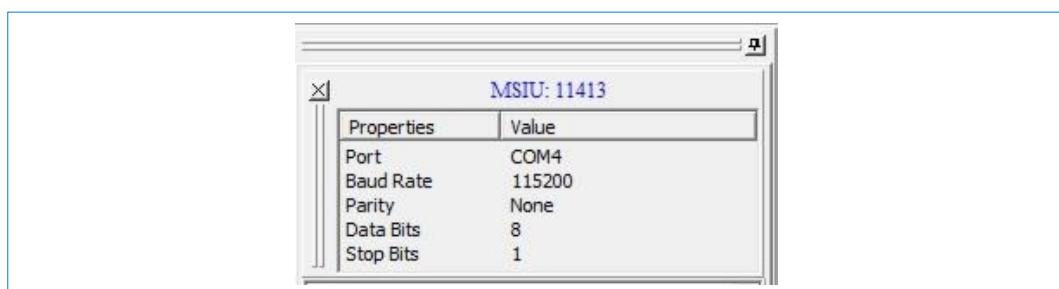
Properties

The Properties node displays the instrument's connection settings. To display the instrument's connection settings double click on the Properties node. This will create a docked Properties Panel for the instrument at the top of the Status Panel.

Serial and USB

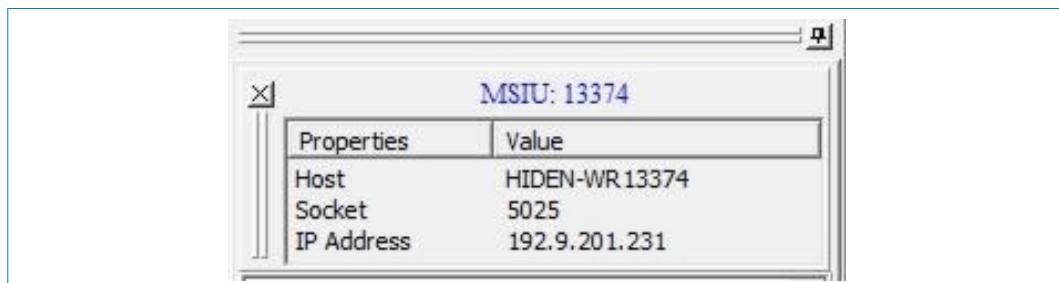
The serial Properties Panel displays the serial connection settings; Port, Baud Rate, Parity, Data Bits and Stop Bits.

USB displays the same settings.



TCPIP

The TCPIP MSIU Properties Panel displays the TCPIP connection settings; Host, Socket and IP Address.



Connection status

The Connection Status node displays the instrument's current connection status.

Connected	A connection has been made to the instrument. The instrument is fully operational, the user is able to create new scans and acquire data.
Disconnected	The instrument has been put in to the “Disconnected” state in the Comms Configuration Utility. MASsoft will not attempt to connect to the instrument. The instrument isn’t available, but the user is able to view existing data and can create new files “off-line”.
Uninterrogated	The control unit couldn’t be contacted to update the configuration settings. The user is unable to acquire data or view existing data.
Connection Failed	MASsoft has attempted to connect to the instrument, but has failed. The instrument isn’t available, but the user is able to view existing data and should be able to create new files “off-line”. When the cause of the failure has been rectified the user may be able to establish communication using the Explore command.
Connection Lost	MASsoft has lost the connection to the instrument while communicating. Any scan in progress will have been aborted. When communication is lost the MSIU will carry on scanning. Filaments will be left on and the multiplier HT voltage may still be applied. Data acquired up to the time of the communication failure will be saved. The instrument is no longer available, but the user is able to view existing data and should be able to create new files “off-line”. When the cause of the failure has been rectified the user may be able to re-establish communication using the Explore command.
Removed	The instrument has been removed in the Comms Configuration Utility. The user is unable to acquire data or view existing data.

Unknown The instrument is in an unknown state. The user is unable to acquire data or view existing data.

Availability status

The Availability Status duplicates the Availability State icon shown on the Status Bar. The availability states are shown below.

Available The instrument is connected and its power supplies are enabled. You may create or open a file and run it.

Protected The instrument is connected and its power supplies are disabled. The power supplies will be enabled when you select any mode, or Shutdown, with a file open or when you run a file.

Tripped The instrument is connected but its power supplies have been disabled due to an external or source pressure trip.

Unavailable The instrument is not connected. See the Connection Status for more information.

Shutdown The instrument is connected and is in Shutdown mode.

Set to current (global) mode The instrument is connected and is in the mode specified as the current (global) mode in scan tree.

Scan starting - waiting for data The instrument has started a scan, but has not yet acquired the first data point. The scan may be paused by an Event Sequence waiting for a start signal, or may be waiting for a gating pulse. In HDR mode the system may be performing the pre-scan.

Scan Running The instrument is scanning and returning data.

Scan Stopping The instrument is waiting for the last cycle to complete.

Degassing filaments The filaments are being degassed.

Running Disconnected (stand-alone) The instrument is scanning, but MASsoft is not collecting data.

On exit MASsoft always leaves the instrument in the “Protected” state.

Stop settings box

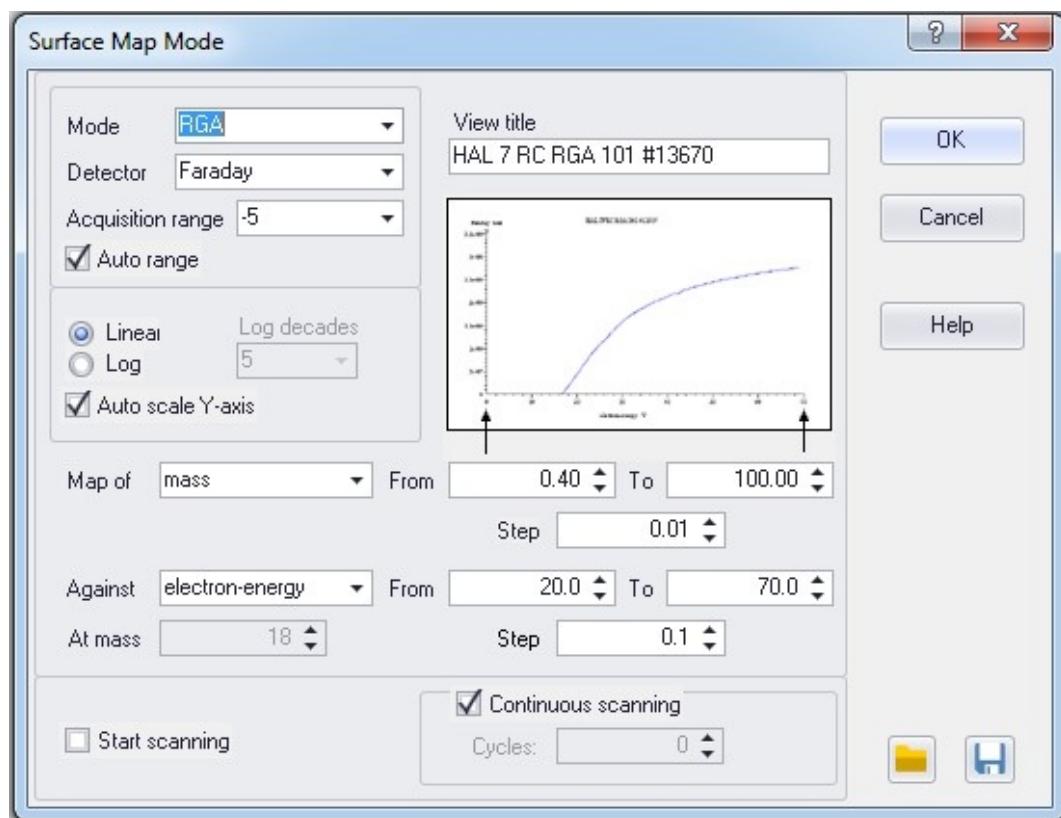
The scan tree's Stop settings holds the settings for the completion of the scan. Double clicking on the Stop settings box will open the Completion Options dialog.

See also:

[Completion options dialog](#)

Surface Map Mode

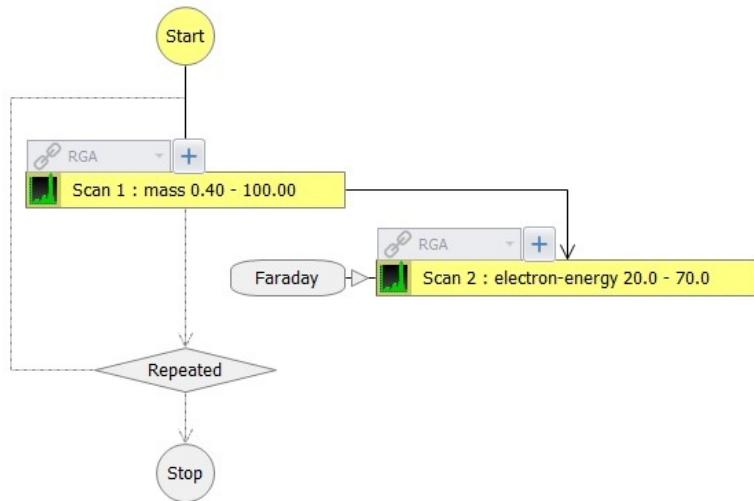
Clicking the **Surface Map Scan** button of the **Easy Scans** tab in the Control Tabs frame opens the **Surface Map Mode** dialog box for a complex scan with a choice of variables to be scanned and mass to be used.



Surface scans are useful for selecting suitable variable operating points, or for setting limits for auto-tune operation.

Map of	Selects the first surface variable. The Map of list box only contains the common surface variables; other variables can be entered by typing the name into the box. A From , a To and a Step control are associated with Map of .
Against	Selects the second surface variable. The variable name may be directly entered into the box. A From , a To and a Step control are associated with Against .
From	Sets the start value for the first or second variable.
To	Sets the stop value for the first or second variable.
Step	Sets the increment for the first or second variable.
At mass	Sets the mass at which the variable is to be mapped. If either the Map of or Against fields have been set to use mass as their variable then this field is disabled. The mass set here will be set into the Global box in the mass spectrometer control window. The other items in the Map Mode dialog are common to other scan mode dialogs.

A two-dimensional scan with the multi-variant scan tree, shown below, will be created.



A 3D graphical view of a surface scan can be obtained after the data has been collected.

Warning: When using the **Surface Map Scan** care must be taken that you are operating in the recommended operating range of the device values you are mapping. It is possible your filaments may be damaged if using the instrument outside the recommended operating region. See Chapter 3 of the RGA Analyser Manual

See also:

[Common dialog items](#) [Easy Scans](#)

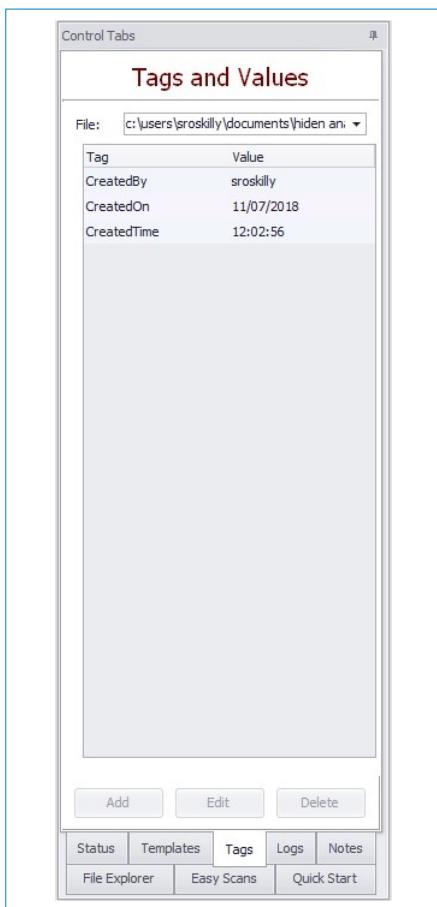
[3D Graphical View](#)

System dashboard

This topic is not described in this version of the manual. Please contact Hiden Analytical for a manual update.

Tags

The **Tags** tab of the Control Tabs frame provides a list of the tags associated with the current experiment file. These tags include who and when the file was created



The **Add**, **Edit** and **Delete** buttons are disabled and not used in this version of MASsoft.

See also:

[Easy Scans](#)

Task Action Step Editor

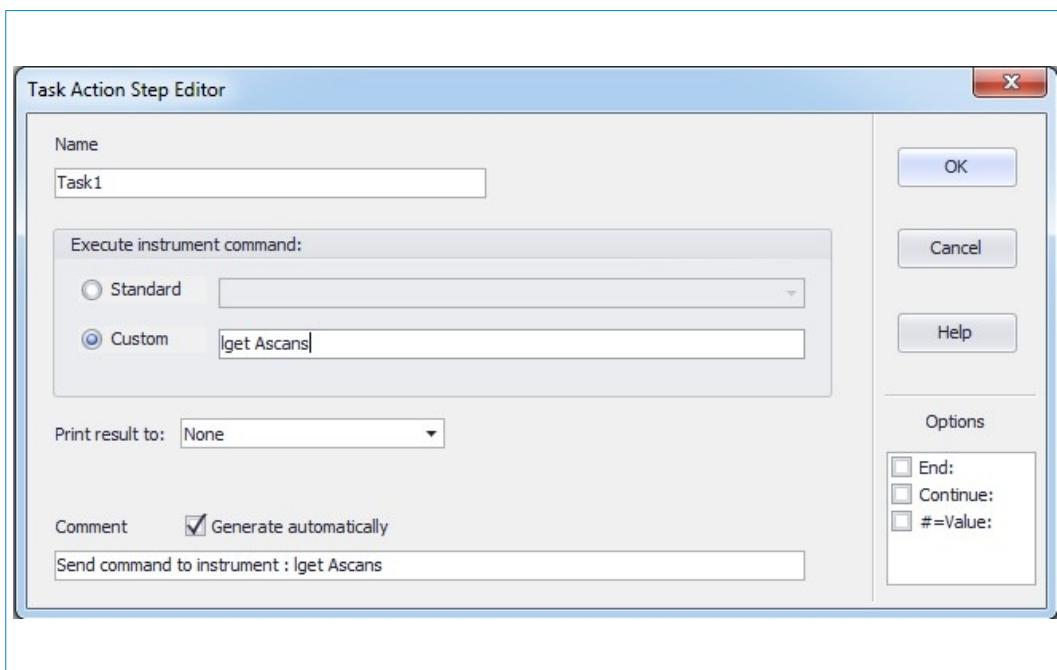
CAUTION

This function should be used under guidance from Hiden Analytical Limited and with great care, as operation of the IU may be compromised by the use of an inappropriate command.

The **Task Action**  function, is similar to a Command action. The specified command is executed as a task by the IU, running in the background.

The **Task Action Step Editor** is displayed when editing a **Task Action**.

An example of a Task Action is shown below.



Fields **Task Action Step Editor** are:

Name	The name assigned to the Task Action.
Execute instrument command	An IU command may be entered into this box; this is executed when the action executes. Standard commands are obtained from the file "msiu commands.txt" in the MASsoft program folder. Custom commands may be any legal MSIU command.
Print result to	If required, any output generated as a result of the command execution can be directed to an output port using this control. Choose from the pulldown list. This field depends on the [STREAMS] entries in the HIDEN.INI file; if this section is missing the field will be blank.
Options	A list of options supported by the firmware version of the instrument is displayed. Double click on an option to select or deselect it. A selected option is ticked.
End:	The message does not continue. The next message will start on a new line. This option is not required if printing results to None

Continue: The message continues. The next message follows on the same line as the output from the command.

#=Value

A # character embedded in the message will be replaced with the event's value, using the value's associated device format. Use a Set event to store the value in the Command event. This option can be used to pass a value as an argument to a command.

For backwards compatibility with old Action Sequences if neither End: nor Continue: are selected then the message continues; the Command event must be followed by a Print Text event which ends the message; failure to end the message will cause MASsoft to crash.

Comment The comment associated with the TaskAction.

If **Generate automatically** is selected, the comment is generated by the selections made within the dialog.

See also:

[Automation page](#)

Templates

Templates provide a quick and easy way of repeating the same experiment.

For example a user may want to carry out the same background vacuum check each day or perform the same mass spectral analysis on a series of samples. Typically, the user will create and run an experiment, modify the experiment until they are happy with it then save it as a Template ready for later use.

Everything associated with the experiment file is saved as the Template except any data.

See also:

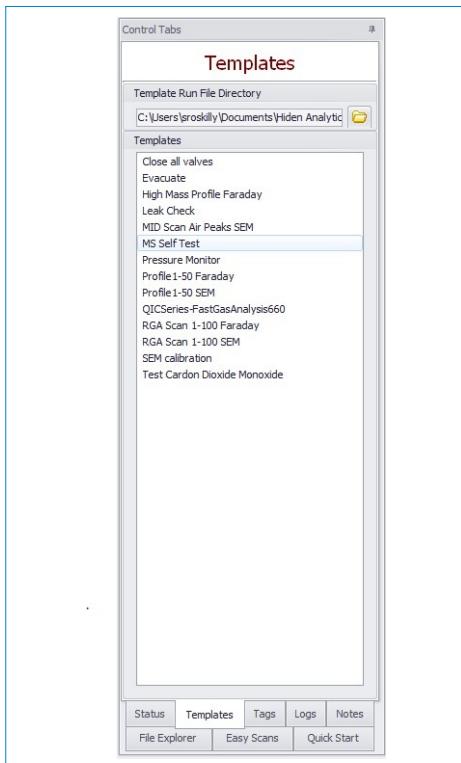
[Save as template](#)

[Templates control tab](#)

Templates control tab

The **Templates** control tab of the Control Tabs frame provides access to MASsoft experiment files that have been saved as templates. The Templates control tab lists the descriptions of each of the Templates stored in the templates folder. When a template is run,

the default data file name associated with it is used as the starting point for generating the name of the new data file.



Right-clicking on an item on the Templates control tab will display a context-sensitive menu containing actions to be taken that are appropriate for that selection.

Items in the popup menu include:

Run

Open and run the selected template file.

A template file can be run by double-clicking it or by pressing **ENTER** whilst it is selected

Edit

Open the selected template file allowing it to be edited.

Rename

Rename the template.

A dialog is displayed allowing the description and default file name to be changed. A template can also be renamed by left-clicking it when it is already selected.

Delete

Delete the template file.

A template can be deleted by pressing **DELETE** whilst it is selected.

Refresh

Refresh the templates list.

Properties

The properties page displayed for a template allows the description and default data file to be viewed, but not edited.

A template file can be run by double-clicking it or by pressing **ENTER** whilst it is selected.

See also:

[Templates](#)

[Easy Scan](#)

Timer Action Editor

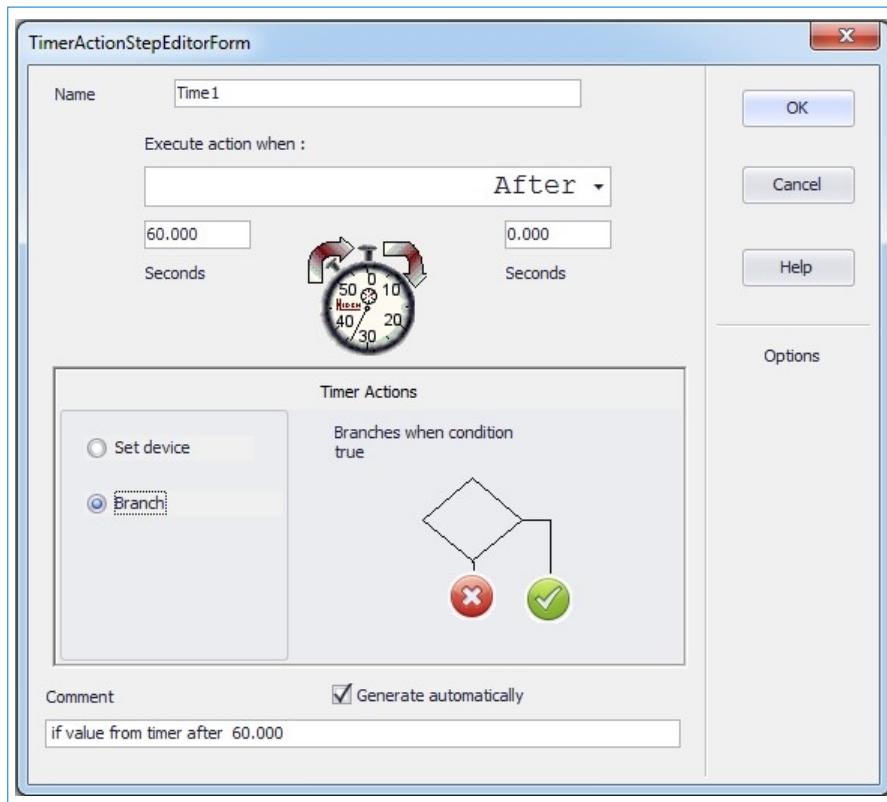


The **Timer Action** , can be used as a simple timer or used to take periodic actions.

The **Timer Action Step Editor** is displayed when editing a **Timer Action**.

A Timer Action's value is set to zero when the Action Sequence is run and its value returns the time in seconds since it was first run (with the format of the device *timer*). A timer can be reset by using a Set Action with the Timer Action as its destination. A Timer Action can be paused by setting its **enable** property to 0 using a Command Action.

An example of Timer Action is shown below where a branch is created After.



Fields **Timer Action Step Editor** are:

Name The name assigned to the Timer Action.

Execute action when: This control gives a list of the comparison functions available and these are associated with the values entered into the Left hand **Seconds** and Right hand **Seconds** fields.

The left hand **Seconds** value (Before) sets the earlier timer set point in seconds. It also sets the frequency in seconds for **Every**.

The right hand **Seconds** value(After) sets the later timer set point in seconds. It also sets the **Every Until** value.

The following comparison functions are available.

After True after the number of seconds entered in the **Seconds** field on the left?

Before True before the number of seconds entered in the **Seconds** field on the right?

Every True every the number of seconds entered in the **Seconds** field on the left and right.

Every Until	True every the number of seconds entered in the Seconds field on the left, until the time on the right.
Before or After	
Between and	True when a value is between the Seconds field on the left and right.
	When and When
	True when a value is the Seconds field on the left, and then on right.
	Enter the values for comparison in the two Seconds fields.
Timer Actions	The timer actions can be used to set a device value or to create a branch in the Action Sequence.
Set device	Choose the Device to set from the list of available output devices, and the Value set when the condition is false and when it is true. The values in the Condition false and Condition true fields are set into the output device selected in the combination box when the trip switches between active and inactive modes.
Branch	A branch is added to the Action Sequence. One path of the branch occurs when the condition is false, and other when the condition is true.
Comment	The comment associated with the Timer Action. If Generate automatically is selected, the comment is generated by the selections made within the dialog.

Title bar

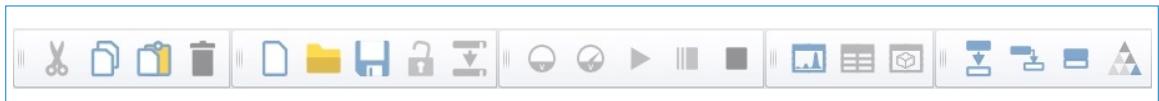


The Title bar appears at the top of the MASsoft window and contains the application title, MASsoft, and the normal Windows maximize, minimize, close and restore buttons.

Tool bars

There are a series of Tool bars that are initially displayed in one line, displayed under the Menu bar. The Tool bars contain buttons to provide quick access to common commands. Which Tool bars are displayed and which buttons are active, depends on what window is currently active in MASsoft and the state of the instrument MASsoft is connected to. An

example is shown below of the tool bar which is displayed when the Home window is selected.



Hover the mouse point over the button to display a brief description of the button's function.

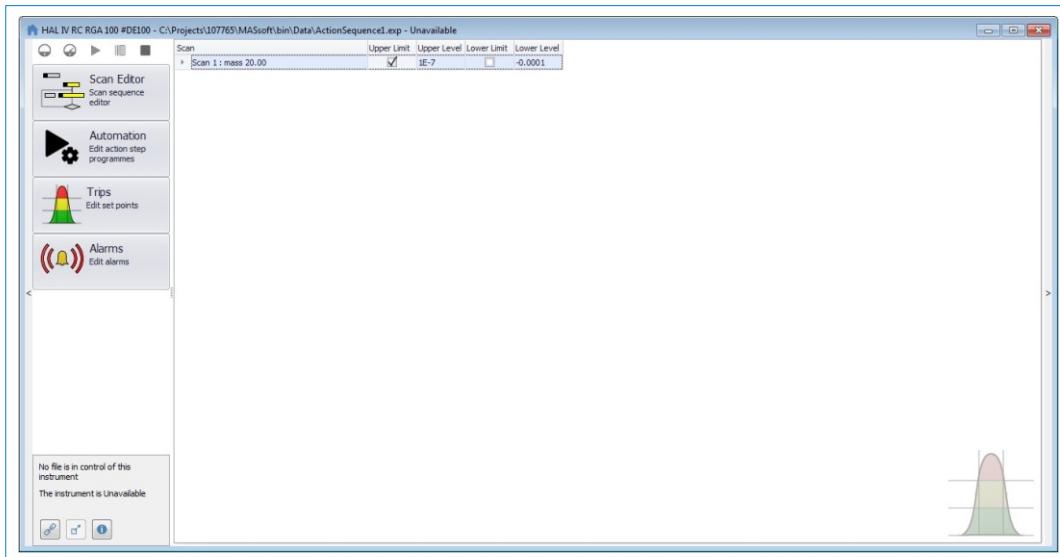
Tool bars can be dragged to a different position in the MASsoft menu bar.

The size of the buttons (Small, Medium or Large) is determined by the Tool Bar Icon Size in the **Interface** tab of the **Preferences**.

See also: [Preferences](#)

Trips Page

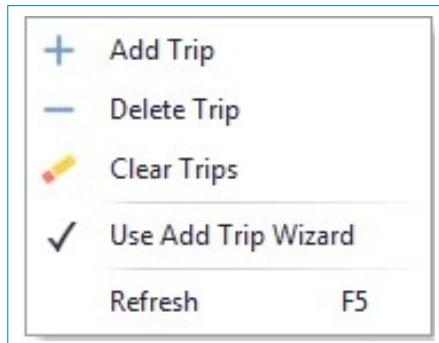
A new trip and action structure may be created by inserting trip or event objects on an individual basis on the Automation page, alternatively, trips can be created on the **Trips** page of the Home Window of a MASsoft experiment file. The Trips page is displayed when the **Trips** button is pressed. Initially this is page is displayed empty. Otherwise if a trip has previously been created then it is displayed as a row in the trips table on the page. An example where a trip has been created is shown below.



A new trip can be added to the **Trips** page using a popup menu or the Tool bar shown below



Right-clicking on the Trips page brings up the Trips popup menu.

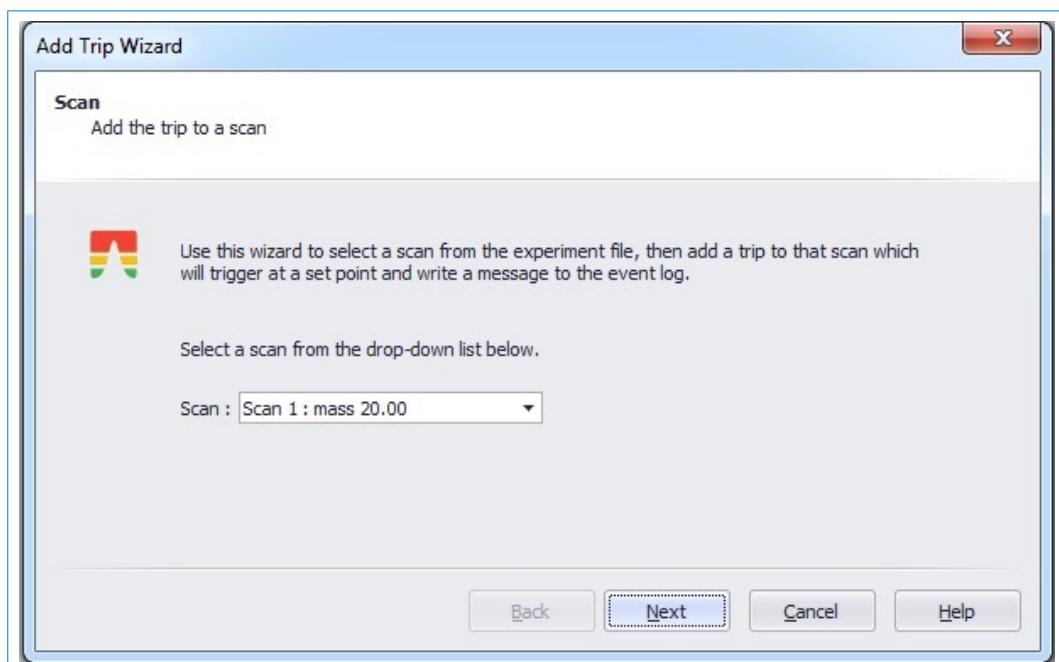


Add Trip

If the option to use it is enabled, then this opens the **Add Trip Wizard**.

Otherwise a row is added to the table displayed on the Trips page. The values entered in the table can be edited.

The first page of the **Add Trip Wizard** is shown below.

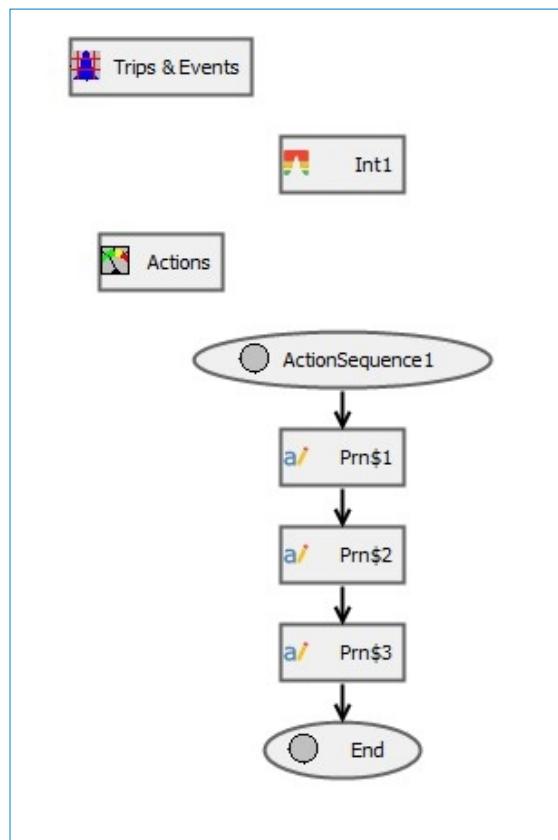


The following controls are found on the pages of the wizard

Scan

The scan to be monitored is selected from this list box.

Upper Limit	If the Trip when signal rises above Upper Limit is enabled then the Upper Limit for the trip can be selected from, or typed in, the associated combination box. The units are those of the input device of the selected Scan .
Lower Limit	If the Trip when signal falls below Lower Limit is enabled then the Lower Limit for the trip can be selected from, or typed in, the associated combination box. The units are those of the input device of the selected Scan .
	A Upper and/or Lower Limit must be set.
Message	A trip message, dependent on whether Upper limit or Lower limit , or both, is selected, is automatically generated in this box; alternatively, the user can enter a message of up to 30 ASCII characters. The message is sent to the event log file. However it can be changed to another instrument via the Print text editor dialog box.
Text Colour	Selects the colour for the message displayed in the event log.
Text Size	Selects the font size for the message displayed in the event log.
Beep when message is written to event log	If Windows sound is enabled, an audible “beep” is made when a trip message is generated.
Do not display the wizard again	When enabled the Add Trip Wizard is not displayed the next time Add Trip is selected. When the Finish button is selected a row is added to the list of trips displayed on the Trips page. A trip added to the Trips page automatically creates the corresponding action sequence on the Automation page. For example the following entry on the Automation page is created when a trip is added.



If required, the intensity trip, and print text function, can be edited, from the Automation Page by double clicking on the object boxes.

Delete Trip

Delete the highlighted trip in the list of trips on the Trips page. This will automatically delete all elements associated with that trip from the Automation page.

Clear Trips

Clear all trips in the Trips page. A warning message is displayed asking if you wish to carry this action.

Use Add Trip Wizard

Ticks on or off, whether the **Add Trip Wizard** will be used when **Add Trip** is selected, or if trips are added directly to the trips table.

Refresh

Refresh the trips list.

See also:

[Automation page](#)

[Home Window](#)

[Intensity Trip Editor](#)

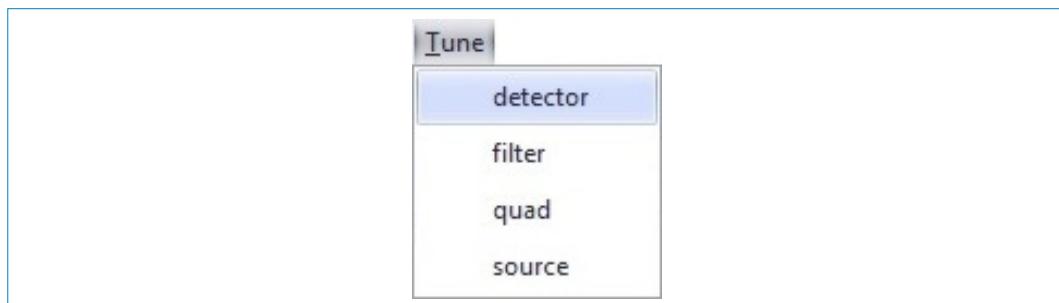
Tune files

This topic is not described in this version of the manual. Please contact Hiden Analytical for a manual update.

Tune menu

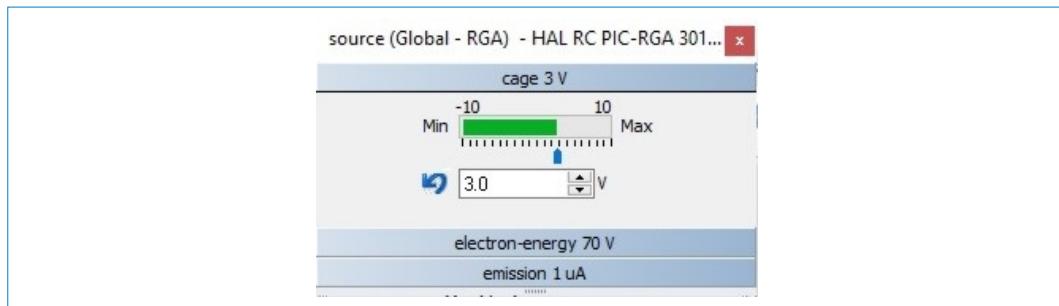
The **Tune** menu contains commands to tune (adjust while scanning) mass spectrometer variables in function groups. Each group allows a function of the mass spectrometer to be tuned. Refer to the Hardware Manual supplied with the instrument for full details of tuning.

The **Tune** menu shows the available function groups for the currently selected mass spectrometer; these depend on the capabilities of the mass spectrometer. A typical **Tune** menu is shown below.



The **Tune** menu may be applied to the file settings by selecting (i.e. clicking on) the scan tree **Global** box or, if it has one, a scan's local environment by selecting the scan before selecting the **Tune** command.

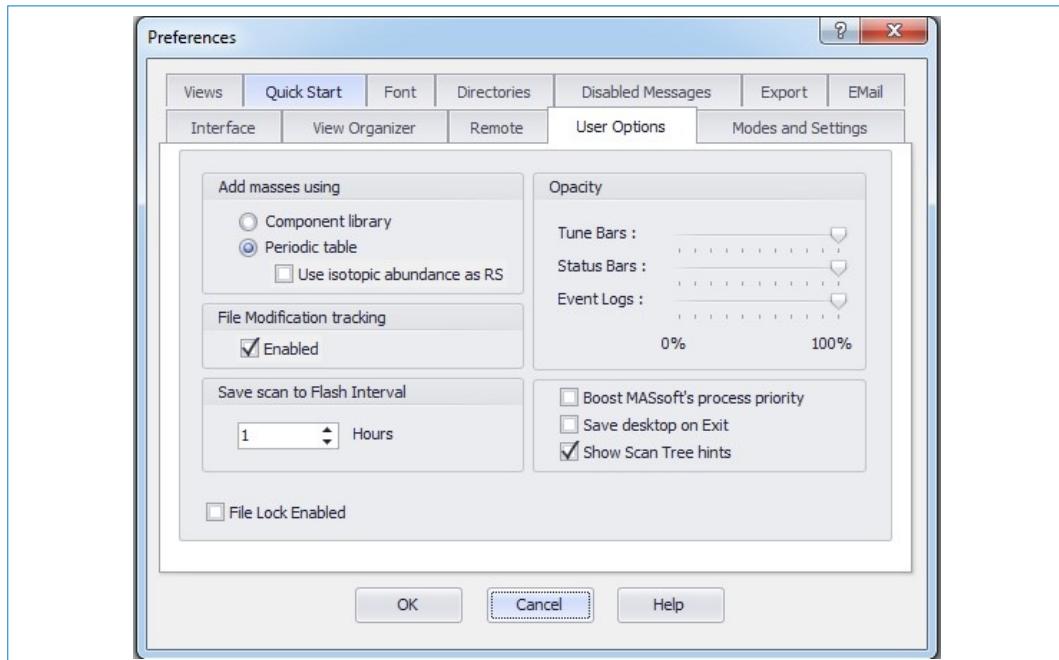
Clicking on one of the items in the Tune menu will open a tune bar dialog which contains tuning controls for devices in the selected group. A typical tune bar dialog for the source group is shown in the figure below.



A tune bar dialog can also be opened from the Status tab by right-clicking and selecting Tune from the pop-up menu.

 Click on the  button to return the device's value to that at the time the tune bar dialog was opened.

User options



To view the User Options select **Preferences** on the **Edit** menu then select the **User Options** tab.

Add masses using	There are a number of dialogs in MASsoft that allow a mass to be selected from a library of components. There are two ways of doing this; either by selecting a mass belonging to one of the components in the MASsoft internal library or by choosing an isotope belonging to one of the elements in the periodic table. Click on the appropriate radio button to select a preferred method.
Opacity	This feature allows the transparency of floating Tune bar, Status bar and Event logs to be adjusted so that the windows and in particular the data in the windows below are still visible. This can prove useful when there are many windows open and little space available to position a toolbar.
File Modification tracking	If this option is enabled when a new file is created, or a file is saved, tag values are saved which are associated with the experiment. They track who created the file and when it was created. When an experiment with file modification tracking enabled is opened the information is displayed in the Tags Control Tabs frame.
	See also: Tags
Save scan to Flash Interval	Sets the interval period for the saving of state variables, on the control unit, into flash memory. This is only available on HAL 7 control units.

The control unit retains the following settings when switched off:

- Scan and event sequences
- Instrument environment settings
- Parameters
- Multiplier usage count

Older control units automatically store these settings in battery backed memory.

With HAL 7 units they must be written to flash memory periodically, or after important changes have been made.

Boost MASsoft's process priority	When checked MASsoft's process priority will be raised to "Above Normal" which can substantially decrease the time taken to remotely open and close files. This should be enabled when using Script Interpreter.
Save desktop on Exit	If selected, when starting MASsoft the window size and position will be restored to when last used. If not selected the default size and position will be used.
Show Scan Tree hints	If selected a hints box will be displayed when the mouse pointer is hovered over a item in the scan tree.

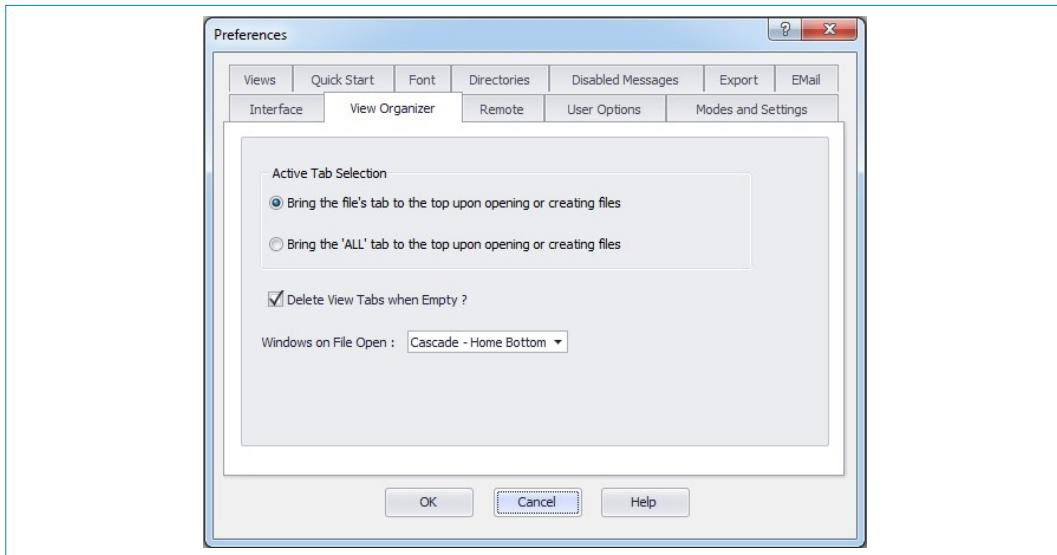
File Lock
Enabled option

File Lock is switched on by default. Files are locked in order to make sure that the data in the file matches the parameters which created that data. During scanning, only device values which can be tuned during the scanning can be changed, any other parameters are automatically locked. Once scanning is stopped, all parameters are locked and the file contains the data that has been collected during the scan. In order to change a parameter the file must first be unlocked. This will return the message that the data is invalidated, and that if you save the file to the same name it will contain no data. The data in the current file is only actually lost or replaced when the file is saved overwritten with the same name. Hence, if the **File | Save As** option is used to save the file with a new name, the data in the original file is preserved.

When **File Lock Enabled** is first disabled a warning message informs of the potential consequences. When File Lock is disabled it is possible that until the file is saved, some of the scan parameters associated with the file may not be the same as those which generated the data. **File Lock Enabled** should only be disabled if you are an experienced user and understand the consequences of using MASsoft with file lock not enabled.

When file lock is disabled parameters in scan dialogs may be changed without pressing an unlock button. When changing parameters have a direct effect on the graphical and tabular views, for instance the scan ranges, scan structure or input device, the views are cleared of data, and a warning message displayed. Other parameters which do not directly affect the views can be changed, without returning a message. However if an attempt to save to the file to the same name as the existing file name made, a warning message appears. These messages warn that saving the file with the same name will result in any data associated with the file being lost.

View organiser



To view the Views Organiser select **Preferences..** on the **Edit** menu then select the **View Organiser** tab.

Bring the file's tab to the top upon opening or creating files.

If selected when a file is opened or a new file created a new tab is created with just that file's window. This new tab is made the current "top" tab.

The default setting is to have this option selected.

Bring the All tab to the top upon opening or creating files

If selected when a file is opened or created the "ALL" tab is made the current "top" tab.

The default setting is to have this option deselected.

When files are created automatically as they are in End Point Detector systems they are shown in a new tab which will obscure the Event Log window which persists from run to run and is not present in the new tab. In such systems it is usual to have only one file open at a time, so having the ALL tab on top enables both the file window and the event log window to be seen.

The **Windows on File Open** option determines how views are displayed after opening an experiment file. Four choices are given as to how the windows / views are displayed when an existing file is opened.

Cascade – Home in front

The Home window is displayed in front of the Views.

Cascade – Home behind

The Home window is behind the Views.

Tile – Vertical

The Home window and Views are tiled vertically.

Tile - Horizontal

The Home window and Views are tiled horizontally.

Views

A view is a window that contains a display of data from one or more scans. The data may be displayed in the form of a graph (graphical view) or a table (tabular view). Data may be viewed during acquisition, or existing data, held in experiment files, may be viewed.

The presentation of the data in a view may be customised; multiple views of the same scan allow the data to be presented in different formats simultaneously.



In the top left of each view is the Home icon which when clicked will bring the Home window associated with the current experiment to the front of the views. Each view also has a bar on the right and left hand side which when clicked will bring the next and previous view, respectively, associated with the current experiment to the front.

One of these views, including the Home window will be the current active view. The active view changes when a new window is selected by clicking on the views window. Depending on which view is active, the Views menu options will change to display only the options relevant to the currently selected view. These options allow graphical and tabular views to be created, destroyed and customised. Right-clicking over the active view displays a popup menu with most of the same options as displayed in the main menu.

See also:

[Home window](#)

[Views menu](#)

Views menu

Most of the options displayed in the Views menu change depending on which window is currently the selected active view.

Options which are common to all views are.

Control Tabs	Allows the Control Tabs to be visible or hidden. MASsoft saves the visible or hidden state information and restores the selected state on re-starting.
Destroy All Views	Clears all views associated with the experiment Home window.
Destroy Selected View	This closes the view to which it applies. This option is not given on the Home window.

The other options depend on which type of view is selected.

See also:

[Bar/Profile plot view](#)

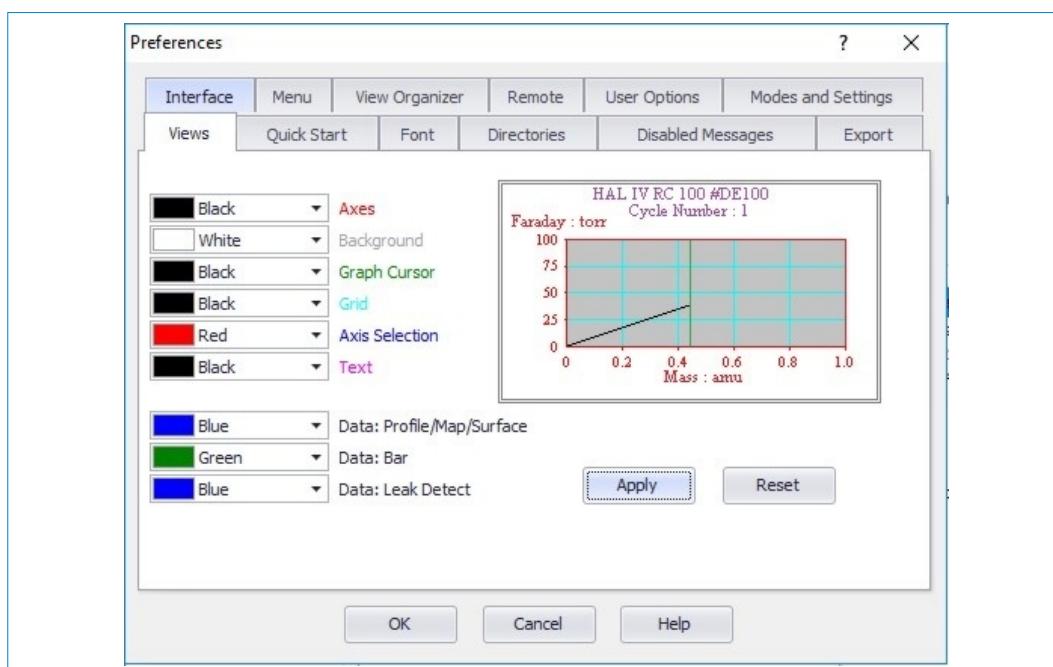
[Control tabs](#)

[Home window views menu](#)

[MID graphical view](#)

[MID tabular view](#)

Views preferences



To view the Views preferences select **Preferences..** on the **Edit** menu then select the **Views** tab.

The user may change the colours used in Views to display data using the controls in the Views tab. The controls relate to various aspects of the graphical view with the graphic within the View tab providing a guide. The colour is selected from the drop-down list displayed by clicking on the down arrow button to the right of the control.

Clicking the **Apply** button causes changes to be applied immediately to any visible Views.

Clicking the **Reset** button returns the colours to the default settings.

Clicking **Cancel** will close the **Preference** dialog box with no changes being implemented.

The View colours are not stored with the data. The current colours defined on the Views tab will be applied to any new views and to any historical views.

View tabs

View tabs provide the means to organise the experiment files and views into a user specified group. Each group is represented by a view tab. These tabs are displayed in a bar under the region where the views are displayed.

By default the Home window and all Views associated with an experiment are organised on the same tab. If multiple experiments are open at the same time, each one will have its own Home window and associated views organised onto different tabs.

Selecting the view tab results in all visible views/windows being hidden and all views associated with the selected view tab being displayed. Each view tab will retain the size and position and layout of each view stored within it. Whenever a data file is opened or newly created a new view tab is created for that data file automatically. The view tab control can also automatically delete the view tab when the data file, or the last view, is closed.

The **New**, **All** and **Dashboard** tabs are permanently displayed. Additional tabs are added to the right of these.

The **New** tab allows a tab to be manually created. A dialog appears in which you must enter the name of the new tab.

The **All** view tab provides the means to display every view/experiment file, except the Dashboard, that is currently open at once.

The **Dashboard** tab displays the System Dashboard.

Right-clicking over a tab displays a pop-up menu with the following options:

Organise...	Opens the Organise Views dialog.
New...	Creates a new tab.
Rename...	Renames the existing tab. A dialog appears in which you can edit the name of the tab. This option is not available for the permanent tabs.
Delete	Deletes the tab. A message queries if you wish really want to delete the tab. This option is not available for the permanent tabs.

See also:

[Home window](#)

[System dashboard](#)

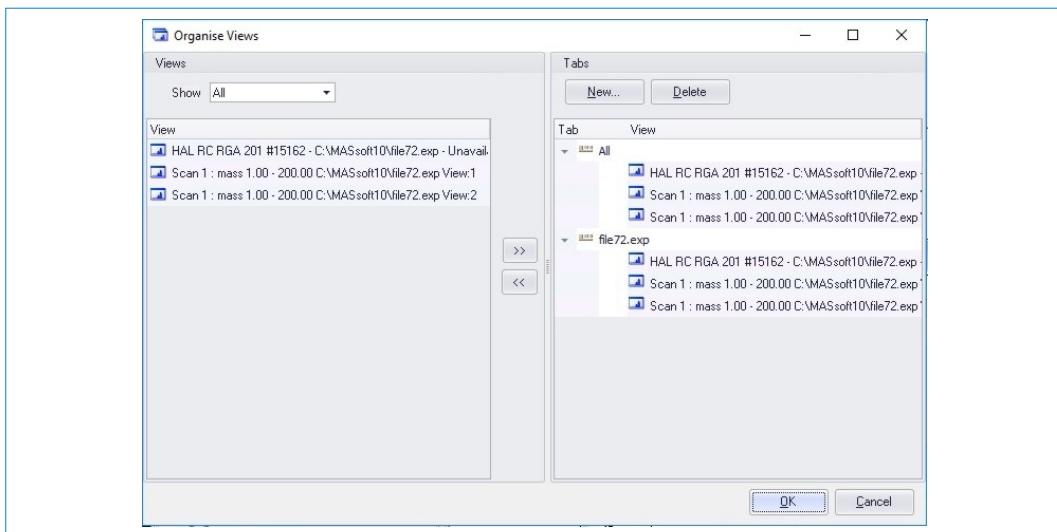
[Views](#)

[View tabs organise views](#)

View tabs organise views

The **Organise Views** dialog allows deleting and configuring of which views are displayed on which View tabs.

To open the **Organise Views** dialog right-click on any views tab and select **Organise...** from the pop-up menu.



On the right of the dialog is the **Tabs** panel, which lists the available tabs and which views are currently associated with these tabs. The **New** button adds a new tab and **Delete** button deletes the selected tab.

On the left of the dialog is the **Views** panel. This lists all the available views.

A view can be added to a tab, by selecting a view in the **Views** list, then clicking a tab in the **Tabs** list and pressing the > button.

Alternatively views can be removed from a tab by clicking on the view in the **Tabs** list and pressing the < button.

Note that a view can be added to multiple tabs, but only one instance of a particular view can be added to the same tab. If all views are removed from a tab, a message is displayed asking if you wish to delete the tab.

See also:

[View tabs](#)

Window menu

Items on the Window menu are described below.

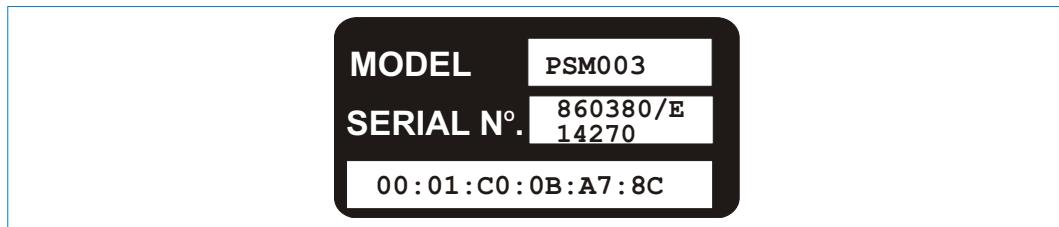
Tile Vertical	Tiles the non-iconised windows to fit the MASsoft window, orientating them vertically.
Tile Horizontal	Tiles the non-iconised windows to fit the MASsoft window, orientating them horizontally.
Cascade	Arranges the non-iconised windows in a cascade from the top left corner of the MASsoft window, with the current window at the front.
Arrange Icons	Arranges the iconised views in rows at the bottom left of the MASsoft window.
Tile Views Vertical	Tiles the non-iconised views to fit the MASsoft window, in a vertical orientation. Control windows are automatically iconised.
Tile Views Horizontal	Tiles the non-iconised views to fit the MASsoft window, in a horizontal orientation. Control windows are automatically iconised.

Works reference number

MASsoft uses the Works Reference number (WR number) to identify each instrument.

The WR number is a unique five digit number given to each Hiden mass spectrometer control unit. No two control units will have the same WR number.

The WR number is displayed on the serial number label attached to the rear panel of the control unit. A typical serial number label is shown in the figure below.



In the example the WR number is: 14270

It is worth making a note of this number before installing the control unit if the rear panel will be inaccessible.

The unit's WR number can be obtained by using the TTY test program and typing the command:

pget ID

the WR number will be returned.

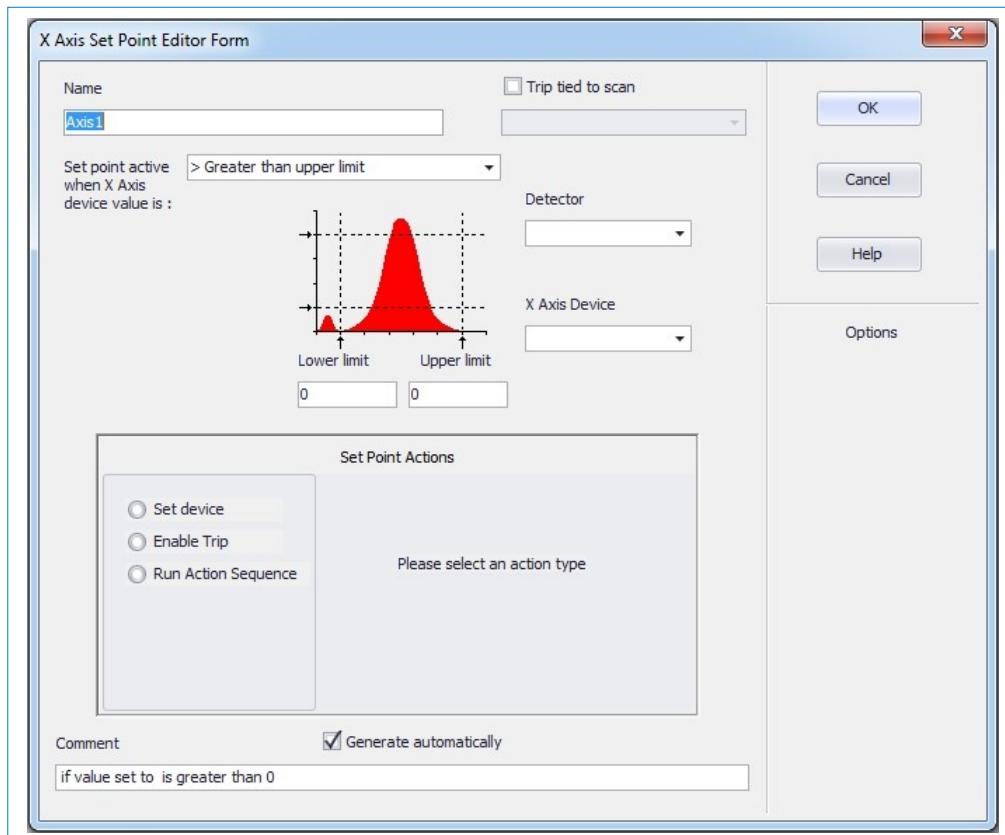
The TTY test program is described the TTY Serial test section of the Hiden Software Suite Installation Guide.

X Axis SetPoint Editor

X-Axis Set Points , perform comparisons of output device values against set limit values, and perform output actions as a result of these comparisons. The output device monitored can be attached to one particular scan, or to any scan using that device.

X-axis set points can be used to enable other trips or to signal to external equipment when an output device is in a certain state.

The **X Axis Set Point Editor** dialog is opened when a **New X-axis set point event** is selected from the **Automation** popup menu, or when an **X-Axis Set Point** is edited.



Fields in **X Axis Set Point Editor** are:

Name	The name assigned to the X-Axis Set Point.
Trip tied to scan	When this is checked, the associated combination box contains a list of the current scans in the tree, and the trip may be tied to one of these. If this option is not checked, the trip applies to any scan which acquires data over the defined X-axis region and with the defined X-axis device.
Set point active when X Axis device value is:	This control gives a list of the comparison functions available; these are associated with the values entered into the Upper limit and Lower limit text fields.
Detector	Selects the detector (input device). If the trip is tied to a scan, this control is grayed out (not active) and the detector selected in the tied scan is displayed, but if the trip is global, i.e. not tied to a scan, an input device MUST be selected.
X Axis Device	This combination box contains a list of available output devices. One must be selected if the trip is global. If the trip is tied to a scan, this control is grayed out (not active) and the scanned device selected in the tied scan is displayed.
Apply Point Actions	When checked, the From and To text fields are enabled to allow the output device range to be set. If this is not set, the trip operates over the full range of the output.
Lower limit	Sets the lower boundary of the output device range.
Upper limit	Sets the upper boundary of the output device range.
Set Point Actions	This frame contains controls which allow the output action to be programmed. Choosing one of the Set device , Enable Trip or Run Action Sequence options configures the frame contents and the controls to suit the output action selected.
Set device	When this option is selected, the values in the Value set when: Trip Active and Value set when: Trip Inactive fields are set for the output device selected in the pulldown box when the trip switches between active and inactive modes.
Enable Trip	The pulldown box contains a list of the trips and actions which can be enabled. When the trip goes active, the selected trip or action is enabled, and vice-versa.

Run Action Sequence

When this option is selected you can set an **Action Sequence to run when:** **Trip Active** and **Trip Inactive**. Choose a previously created action sequence from the pulldown box. The type of actions listed can be filtered using the **Show sequences**, **Show all actions** and **Sort** options.

Comment

The comment associated with the X Axis Set Point action.
If **Generate automatically** is selected, the comment is generated by the selections made within the dialog.

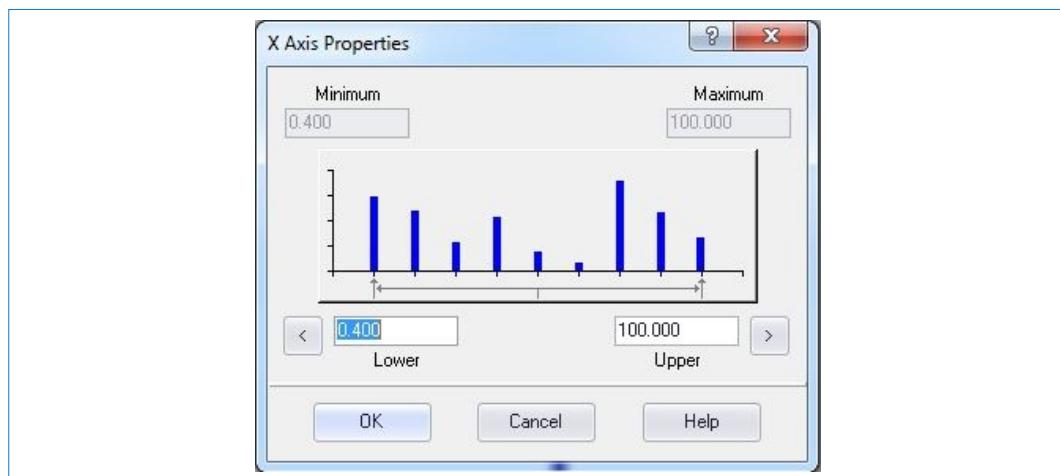
See also:

[Automation page](#)

X Axis properties dialog

The display and scaling of the X-axis can be altered either by double-clicking on any of the number annotations displayed under the X-axis, or by selecting **Configure X Axis** option of the View menu for a graphical view.

The **X Axis Properties** dialog provides control of the X-axis. Options differ between MID and Bar/Profile plot views. The dialog box for a **Bar/Profile Plot** view is shown below.



Common to both view types are these options.

X minimum

Shown for reference only, this displays the minimum value of available X-axis data.

X maximum

Shown for reference only, this displays the maximum value of available X-axis data.

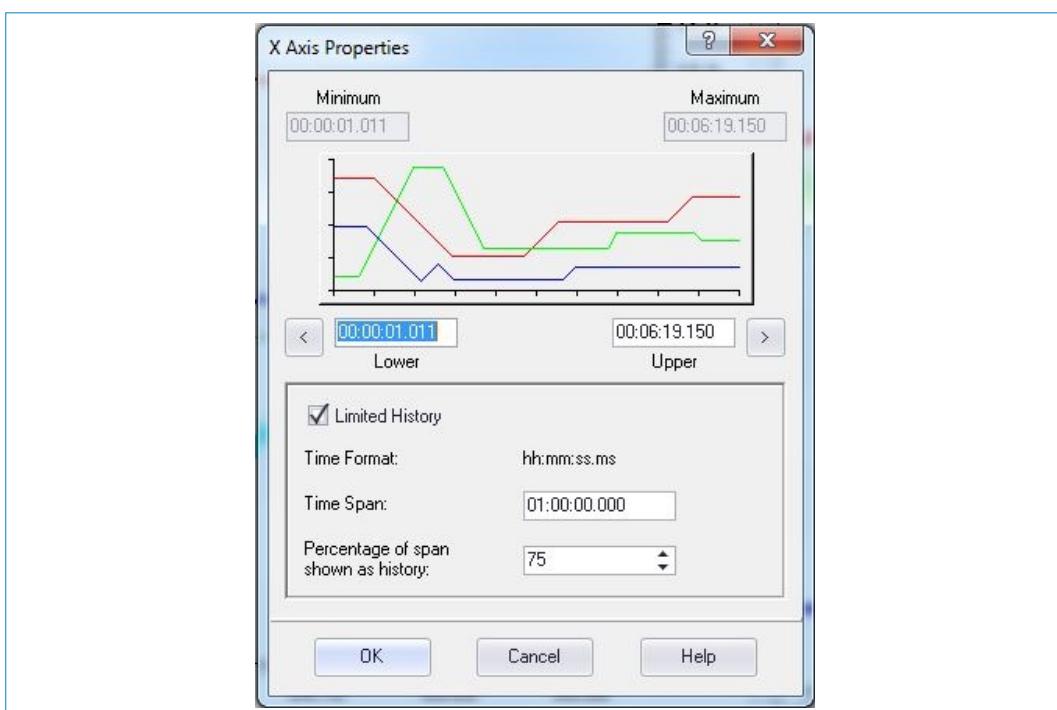
Lower

The X-axis lower limit can be entered directly in the box. The < button sets this value to the X minimum as displayed above.

Upper

The X-axis upper limit can be entered directly in the box. The > button sets this value to the X maximum as displayed above. Changing the **Lower** or **Upper** will alter the plot to display data in the X range between the two values.

For MID plot views, the dialog has additional options available.

**Limited History**

When selected, the amount of data on the screen is limited to the time range shown in the **Time span** box. If this box is not checked and the display is zoomed out, the display extends from the start of the acquisition to the present time; for long acquisitions this may lead to a loss of display resolution.

Time Span

The time range can be entered in this text box when the **Limited history box** is checked.

Percentage of span shown as history

When the data reaches the right-hand edge of the display, the display has to be redrawn to make room for more data. This field defines the amount of data that is retained and shifted to the left of the display.

Note:

If **Limited history** is not selected, MASsoft will eventually run slowly in long acquisitions due to the large amount of data that has to be redrawn. This can be avoided by selecting **Limited history**, in conjunction with a short **Time span**, or by using a tabular view rather than a graphical view.

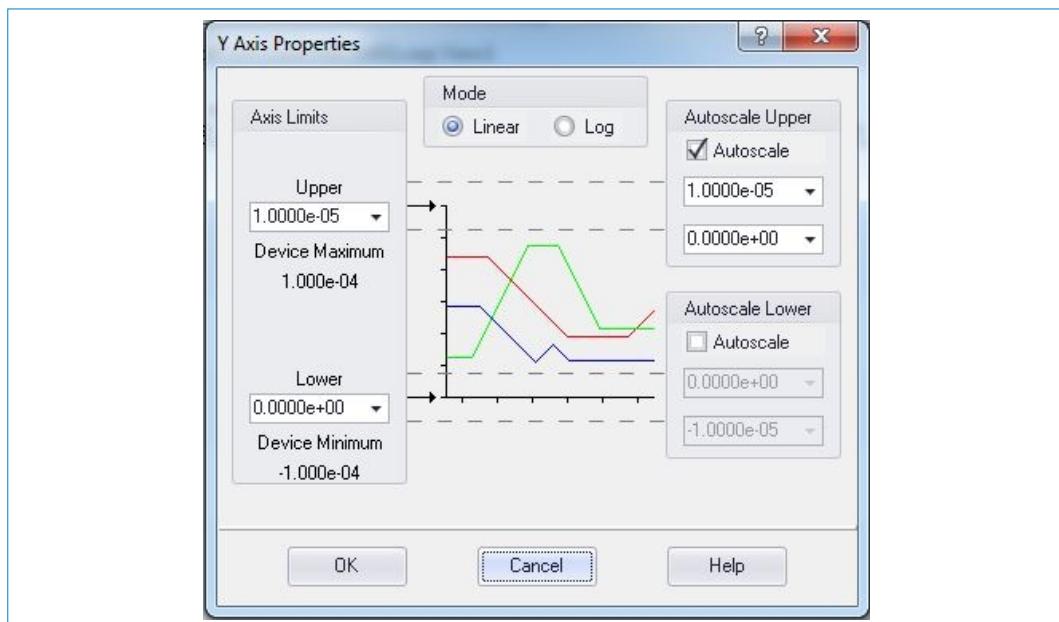
See also:

[Views menu](#)

Y Axis properties dialog

The display and scaling of the Y-axis can be altered either by double-clicking on any of the number annotations displayed on the currently selected Y-axis, or by selecting **Configure Y Axis** option of the View menu for a graphical view.

Options differ between MID and Bar/Profile plot views. The dialog box for a **MID Graphical** view is shown below.



For **MID Graphical** views, which can have two or more axes, the dialog allows you to change the Y axis scale of the selected axis. For multi-axes plots, the axis is selected by clicking on any of the number annotations which mark the values of on that axis. The selected axis is displayed in red.

Common to both view types are these options.

The **Axis Limits** frame contains the following controls:

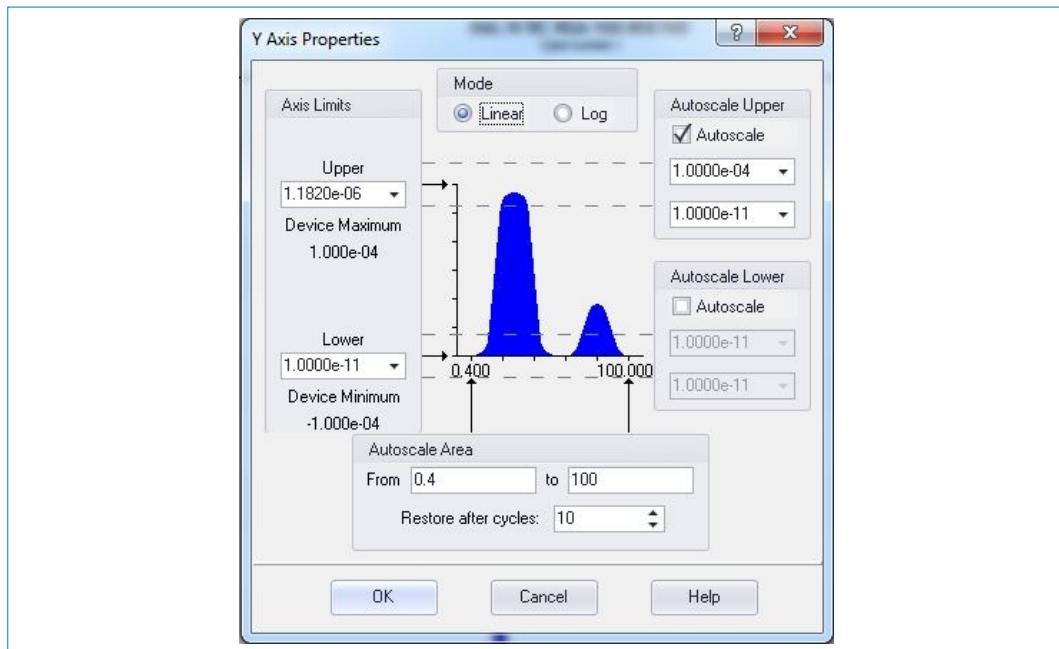
Upper	This combination box sets the Y-axis upper limit. The value may also be entered directly into the box. This value defaults to the maximum value on the start range of the scan's input device or 1000 counts per second for pulse counting systems.
Lower	This combination box sets the Y-axis lower limit; the value may also be entered directly into the box; this value defaults to 0.0 .

Note:

*Positive or negative values can be entered in the **Upper** and **Lower** combination boxes.*

Mode Linear	When selected, the selected Y-axis is linear.
Mode Log	When selected, the selected Y-axis is logarithmic (log 10).
Autoscale Upper	Checking this option turns on the Y-axis upper limit autoscaling. The option is accompanied by two combination boxes which specify the upper and lower values between which the autoscale algorithm may set the Y-axis upper limit. The limits may also be entered directly into the boxes.
Autoscale Lower	Checking this option turns on the Y-axis lower limit autoscaling. The option is accompanied by two combination boxes which specify the upper and lower values between which the autoscale algorithm may set the Y-axis lower limit. The limits may also be entered directly into the boxes.

For Bar/Profile plot views as shown below, additional options are available which effect auto scaling of the Y axis while data is being acquired.



Autoscale Area From To

These text boxes specify the X-axis boundaries between which the Y-axis autoscaling data is taken; this can be used to prevent a large peak swamping lower-level data by setting the boundaries such that data from the large peak is excluded.

Restore after cycles

This value indicates the number of cycles displayed before the system checks for under-range on the Y-axis (e.g. if the intensity of the displayed data drops for a number of cycles before rising again, the Y-axis upper limit is not immediately adjusted to a lower value over this number of cycles).

When manually zooming into an area of the plot, autoscaling controlled by the parameters entered here is temporarily switched off while the plot is in a zoomed state. Once the plot exits a zoomed state, either by double clicking, or by setting the X or Y axis limits then auto scaling is reinstated if it was switched on originally.

See also:

[Views menu](#)

[Zooming](#)

Zooming

There are three types of possible zooming available for graphical plots.



When the **Vertical/Horizontal** zoom type, , is selected then left clicking and dragging with the mouse within the plots data area a box is displayed, which when the left button is lifted is zoomed into. The plot is redisplayed with the new x and y axis ranges now set to those of the previous zoomed area.



When the **Horizontal** zoom type,  is selected left clicking and dragging with the mouse zooms into an area where the Y axis values are fixed at their current limits, but X range is changed.



When the **Vertical** zoom type, , is selected left clicking and dragging with the mouse zooms into an area where the X axis values are fixed at their current limits but Y range is changed.

Multiple zoom operations can be performed in succession, zooming further into the graphs data.

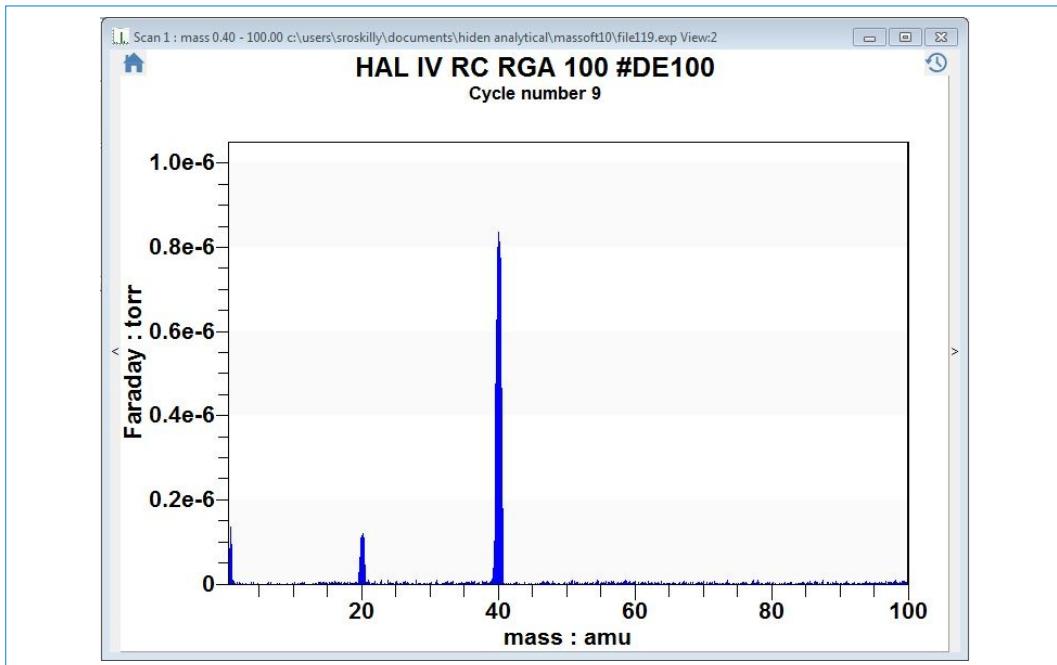
When in a zoomed state, double-clicking on the plot, returns to the pre-zoomed state. This is the case even after multiple zooms have occurred.

With the Bar / Profile View whether the plot is in a zoomed state or not is indicated by a zoom box displayed in the top right-hand corner of the plot. When this is visible, it indicates that the display is in a zoomed state.

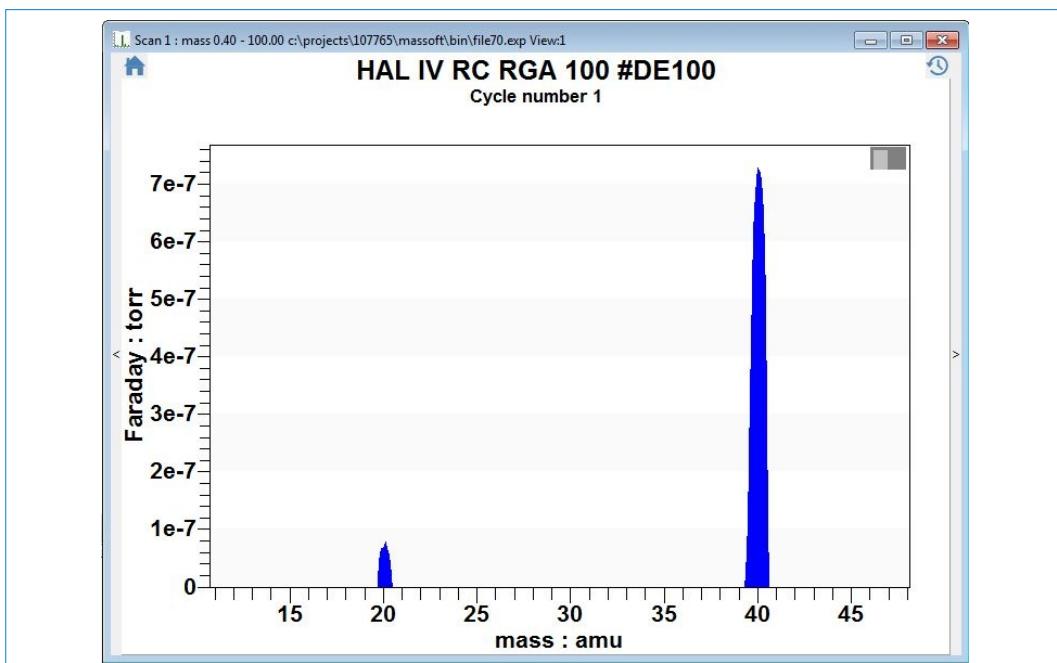
The zoomed state is reset after the **Configure X Axis** or **Configure Y Axis** dialogs have been used to adjust the axis limits. Therefore, double clicking does not always return to the full range of the x and y axes.

To help illustrate an example is given here, where the data have been collected over the data

range 0.4 to 100 amu, and has a mass 40 peak at approximately $7\text{e-}7$ in height, and smaller peak at $1\text{e-}7$. The default plot is shown below.



Using the **Vertical / Horizontal** zoom type we zoom into a region surrounding the mass 20 and mass 40 peaks, and a zoom box is displayed in the box left. As shown below.



Note that this displays a zoom box in the top right-hand corner. If we double-clicked on this plot it would return to the pre-zoomed state, which in this case is the full x range, as shown earlier.

If instead we open the **Configure X Axis** dialog, which is displayed with the **Lower** and **Upper** X axis bounds set at the zoomed values, then we press **OK**, the view is still displayed with the same x and y axis as before we entered the dialog. However, we are now no longer in a zoomed state, and the zoom box is not displayed. Double-clicking has no effect.

To restore the full x range, and return to the default state, we can press the **Set Axes Limits**

to Full Scale,



button.

Panning in Horizontal zoom

A feature available, while in Horizontal zoom mode, is to pan the plot to the left or the right. If the zoom box is dragged to the far left or far right, then the zoom expands beyond the current visible extent of the plot to display the data to the X range minimum (when panning to the left) or data X range maximum (when panning to the right). The Y limits are not changed.

*Care should be taken with this feature for MID Graphical Views, because when panning to X axis minimum all the data collected so far will be reloaded and a large amount of data may have to be redrawn. This will occur even when collecting data with **Limited history** enabled.*

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