

VISION_{pro}TM Software User Guide



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Introduction

This manual explains how to use Thermo Scientific VISION*pro* software. UV-Visible spectrophotometers have been designed for analytical applications in which fast, accurate and reproducible spectrometric measurements are required. The VISION*pro* software supplies PC control of the spectrophotometer in the Windows® 2000 or Windows XP operating system. VISION software is supplied on CD with an instrument and a PC communications cable.

Accessories supported

Calibration Validation Carousel

Smart Sipper

Smart Thermostatted Rotary 7-Cell Changer

Smart Thermostatted Linear 8-Cell Changer

Smart Peltier Thermostatted Single Cell Changer

Smart Linear 16-Cell Changer

Thermostatted Single Cell Holder

Cylindrical Cell Holder

Fiber Optic Sampling Accessory

Long Pathlength Rectangular Cell Holder

Test Tube and Vial Holder

Evolution 300 Mercury Lamp Accessory

Evolution 600 Mercury Lamp Accessory

Standard Rectangular Cell Holder

VN Absolute Specular Reflectance Accessory

DRA-Evolution 600-Diffuse Reflectance Accessory

Solid Sample Holder

Praying Mantis Diffuse Reflectance Accessory

Relative Specular Reflectance Accessory (330° and 45°)

Operation

Insert the software CD into the drive and follow the on-screen instructions.

Starting VISION_{pro}

Follow the steps below to start VISION_{pro} software. For information on other methods of starting applications and more detailed instructions on using Windows features, see your Windows documentation.



Double-click the VISION_{pro} icon on the Windows desktop, or use Start > Programs > Thermo VISION > VISION_{pro}.

Note

To return to Local Control from VISION, select Command > Local Control and then press Home on the spectrophotometer. ▲

Basic Operation

Point and Click

To select any operation from a menu, or to start a process with a toolbar button (icon), first move the mouse so that the cursor POINTS at what you want, then CLICK with the left-hand mouse button.

Drag and Drop

“Drag and Drop” is a fundamental Windows operation, used to move objects (e.g., files, from one window or area to another). It is used within VISION to move data quickly and conveniently.

To drag and drop any object:

1. **Position the mouse so that the cursor is over the object you wish to move.**
2. **Press and hold down the left-hand mouse button.**
3. **With the object you wish to move highlighted, keep the left-hand mouse button held down and move the mouse so that the pointer moves away from the source window.**

The mouse pointer now changes to an arrow.

4. **Move the mouse pointer to the area where you want to place the data.**

When you are in an area where data can be dropped, a batch, sample or cycle symbol will appear as the mouse pointer.

If it is not possible to drop data, a “No Entry” sign will appear.

5. Release the left mouse button when you are ready to drop the data.

Drag and Drop is used in VISION to move data from the Data Store to other windows (e.g., the Graph window or any of the Math windows).

For example, a batch of Scan results can be loaded into the Data Store using File > Open > Batch of Results from the Scan application. The act of opening the file does not put the data into the graph. To see the graph, select the batch, sample or cycle by pointing to it, press and hold the left mouse button, drag the object to the Graph window, and release the mouse button.

Context Menus

Clicking on an object with the right-hand mouse button will open a pop-up menu listing the operations that are available for the object in the current context.

File Association

File Association is a facility of Windows that enables a Windows Application to be opened by double-clicking on a data file obtained from it.

Display the contents of the Library, or any other folder where data has been stored and double-click the name of the file that you wish to use in VISION_{pro}. This will cause VISION_{pro} to start and to open the selected data file.

If data files are stored as icons on the Windows desktop, VISION_{pro} can be started by dragging the data file icon to the VISION_{pro} icon on the desktop, and the selected VISION_{pro} and data file will be opened.

Preferences

The VIEW menu and the TOOLS menu contain facilities which enable the system to be configured to suit the preferences of the user.

- Toolbars can be displayed or turned off.
- Each toolbar can be set up to include only the icons that are required.
- Files load/save behavior can be configured. For example, all instrument and accessory information, report templates, advanced calculation templates and the screen layout can be included in a method file.

- Batch Information can be configured, enabling printed output to contain the information that is required.
- The system can be configured to reload exactly as it was when previously shut down.

Help

To access the Help system:

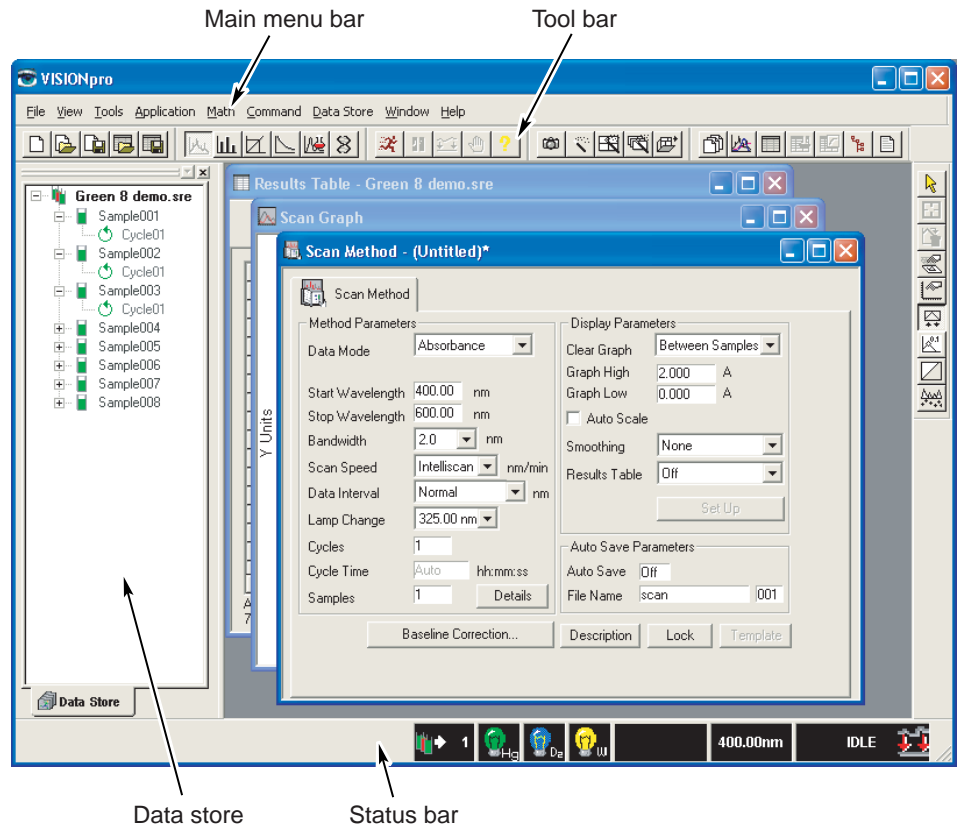


Click the Help icon on the Analysis toolbar, or click Help on the Main Menu bar.

Detailed step-by-step instructions cover all aspects of software and instrument operation. A technical reference section deals with the fundamental principles of UV-Visible spectrophotometry, and contains tables of useful data.

The VISION_{pro} Interface

This section provides a brief introduction to the rich functionality of VISION. For more detailed information refer to the comprehensive on-line Help system or to the following sections of this User Manual.



Work area features

The **Main Menu Bar** provides access to all the operations needed to obtain process, store and retrieve data.

The **Toolbars** give direct access to the most frequently used operations. The composition and positions of the Toolbars are fully user-configurable. The user may set up a tool bar containing only the tools required for the work in hand and elect not to display the default toolbars, or all toolbars may be hidden using the View menu. Thus the workspace may be set up according to individual preferences.

The **Status Bar** enables the user to monitor the state of the instrument and accessories at all times. From left to right the display shows Accessory States (cell changer in this example), Lamp Status, Live Absorbance Display, Wavelength, and Instrument State. If desired the Status Bar may be hidden, using the View Menu. When a baseline is required, the baseline icon is displayed next to the Instrument state. This icon will automatically appear each time a previous baseline expires due to the changes in the application method.

The **Data Store** displays all data currently held in memory, whether obtained from the instrument directly or loaded from disk. The data are organized in a Windows “tree” structure. The Data Store item in the Main Menu Bar gives access to associated commands. The Data Store can be dragged and docked into the position preferred by the user.

The Toolbar Buttons

The following features are provided to identify the tools:

- As the cursor passes over the button, the name of the function appears at the cursor and a brief description is displayed on the left-hand side of the status bar.
- The User can configure which icon groups are displayed and where they appear by using the Tools menu and the Drag and Drop feature.

The toolbars can be configured to the user's preferences, via the View menu.

A summary of the toolbar groups and their functions is given here for reference:

These applications may also be accessed from the Applications menu.

File Operation Group

From left to right

This is the most frequently used set of file operations from the File menu.



Creates a new method

Loads a method from disk

Saves the sample method to disk using its current name

Loads a result file from disk

Saves the selected file to disk using its current name

Application Group

From left to right:



Select the Scan application

Select the Fixed application

Select the Quant application

Select the Rate application – only available with VISION*life*

Select the Multicomponent Analysis application

Select the DNA application – only available with VISION*life*

These applications may also be accessed from the Applications menu.

Analysis Group

From left to right:



Starts a run to measure a batch of samples

Pauses the data collection in the Rate application

Performs a baseline or zero measurement selected in the method

Stops the run currently in progress

Accesses the Help system

These operations may also be accessed from the Command menu.

Window Management Group

From left to right:



Remembers the current window layout

Restores the remembered window layout

Arranges the windows as non-overlapping tiles

Cascades the windows

Loads a window layout from disk (A window layout may be saved or loaded via the File menu)

These operations may also be accessed from the Windows menu.

Active Window Selection Group

From left to right:



- Selects the Method window
- Selects the Graph window
- Selects the Results window
- Selects the Calibration window
- Selects the Kinetics window
- Selects the Data Store
- Select the Report window

The active window may also be selected via the Windows menu.

Graph Group

From left to right:



- Cancels cursor tracking
- Enables cursor tracking (Tracks along each data point, using the arrow keys)
- Clears the graph of all data
- Toggles display of the graph grid
- Sets the graph axis limits
- Toggles the display of the graph legend
- Toggles the display of the peak labels
- Toggles the graph background color between gray and white
- Toggles the graph line type between points and lines

These operations may also be accessed from the Graph menu when the focus is on the Graph window.

The Data Store

The Data Store shows the data currently active in VISION. Newly acquired data will be placed in the data store. Data in the Data Store can be saved, manipulated or deleted using commands in the Data Store menu.

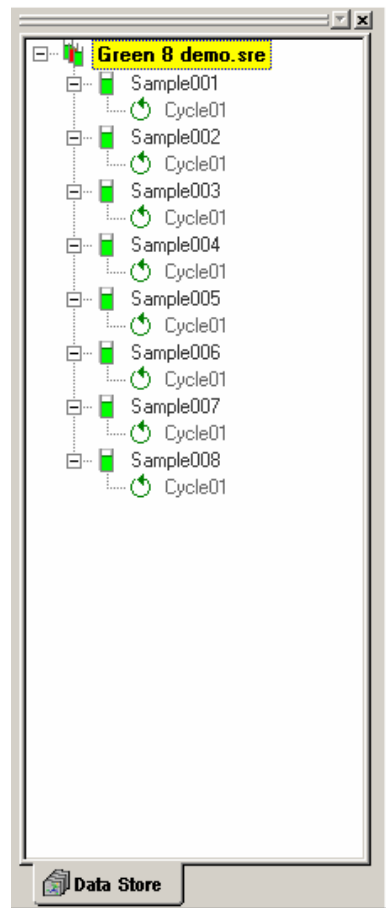
Previously saved data that has been reloaded for analysis is also placed into the Data Store.

The Data Store has a Windows tree structure, and is arranged in a hierarchy of Batch/Sample/Cycle.

- A **Batch** is all of the data collected from one run of a method in the software.
- **Samples** are individual components of the batch. One batch may contain up to 999 samples.
- **Cycles** are the measurements made on the same sample. There can be up to 20 cycles for each sample.

Batches and samples may be collapsed or expanded as required.

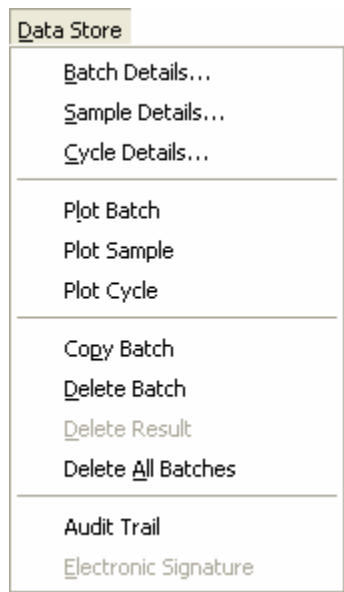
Data can be moved from the Data Store to other elements of the VISION work area (e.g., the Graph window or a Math window) using Drag and Drop.



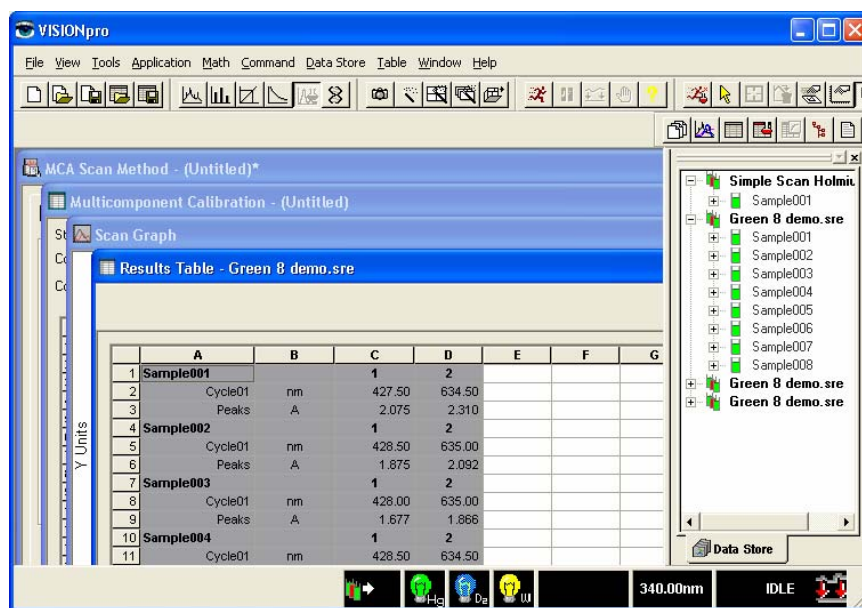
The Data Store menu enables the user to view Batch, Sample or Cycle details by right clicking on the text.

The Plot commands may be used to display the data. Alternatively, you may drag the batch, sample or cycle from the Data Store to the Graph Window.

The Data Store menu contains commands for managing items in the Data Store.



The default position of the data store is at the left of the work area, but it may be docked at the top, bottom or right-hand side if preferred, it also may be undocked and left as a small window floating in the work area, or closed completely.

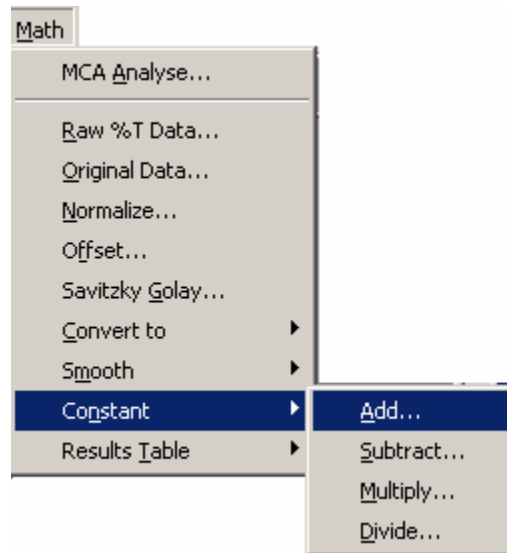


Math Functions

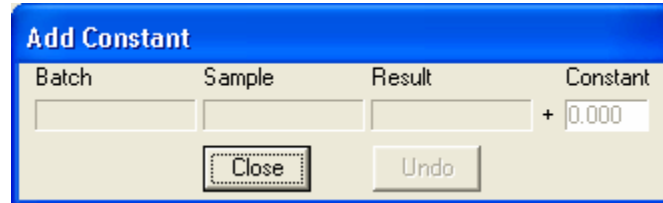
The Math Functions, which are available from the Math pull-down menu, give the user access to a powerful range of manipulations and calculations.

Click the desired operation and drag the required batch, sample or cycle to the Math window, for that operation to open in the work area (see [“Using Math Functions”](#)).

The User may return to the original data at any time. However, since not all data forms can be inter-converted directly, it may be necessary to convert to Raw %T and then back to the original data.



The following is an example of the pop-up window after Add has been selected.

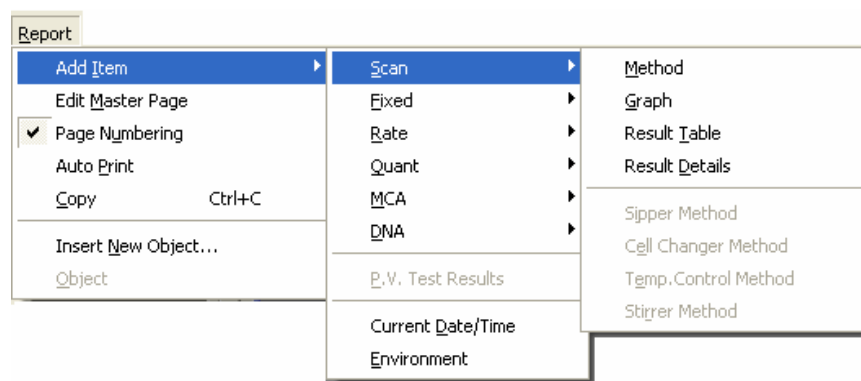


Report Composer

The Report Composer menu is available when the focus is on the Report Composer window.

The Report Composer window appears on the desktop when a new report is initiated by using File > New > Report, or when a report has been loaded from disk, or when the report is selected from the Active window toolbar.

Items to be included in the report are selected from the Report menu and placed in the report by creating and moving individual boxes for the components.



The Report Composer generates a Report Template that displays the current contents of the items. When a report template is saved and attached to a method, a report is automatically produced and updated when the method is run. Objects from other Windows applications, such as a company logo graphic, can be included in reports, creating quality custom documents.

UVcalc Advanced Calculation Facilities

UVcalc is a spreadsheet-like functionality that automates custom calculations using data in the Results Table. Calculations are automatically performed each time the method is executed and may be attached to the method as a Template.

To start UVcalc, click Table > Edit UVcalc Template. Each cell of the spreadsheet can then be accessed by right-clicking anywhere in the Results Table. This opens a context menu appropriate to the cell where you have clicked. The possibilities are:

- Cells within the area occupied by the results (gray background) cannot be edited or moved. Only formatting options are available. Rows and/or columns cannot be inserted into the gray shaded area.

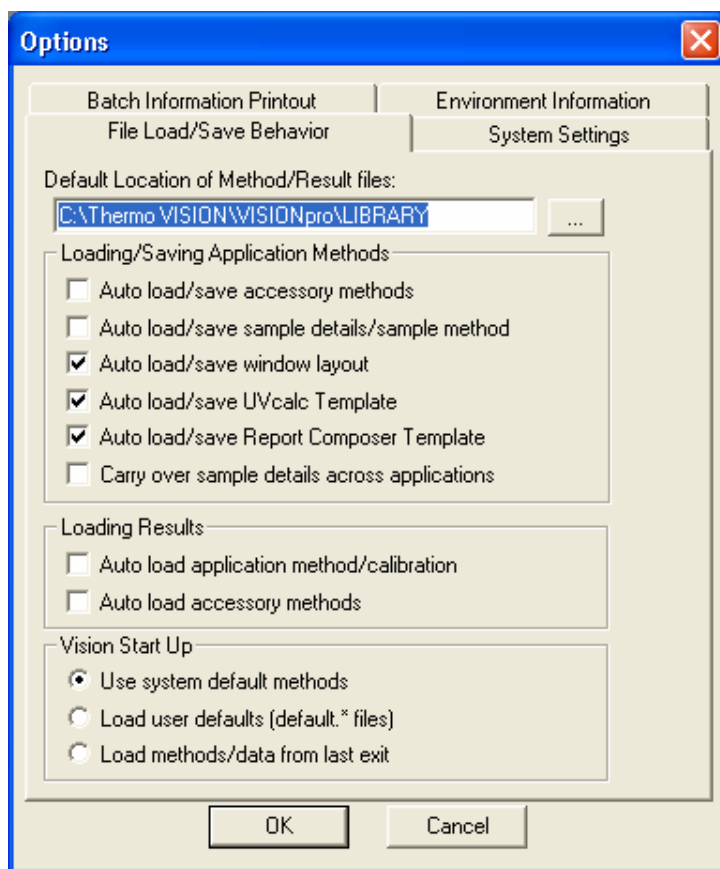
- Cells within the spreadsheet area can be edited and text can be formatted. To edit the contents of a cell either double-click it, or click to highlight it and then click in the editing area at the top of the results window.

A full range of mathematical functions is available from the Function Wizard, which is accessed by clicking on the f_x button located on the bar at the top of the Results window.

Windows Layouts

In VISION, the layout of the windows of an application can be arranged and recalled by the user. A Window layout can be saved with a method so that each time the method is loaded, the program work area is automatically arranged.

To enable this feature, click Tools > Options, then select the File Load/Save Behavior tab. Click in the Auto load/save window layout box, in the “Loading/Saving Application Methods” section, to check this item.



Alternatively, a window layout may be saved or loaded as an independent item via the File menu.

Temperature Control Method

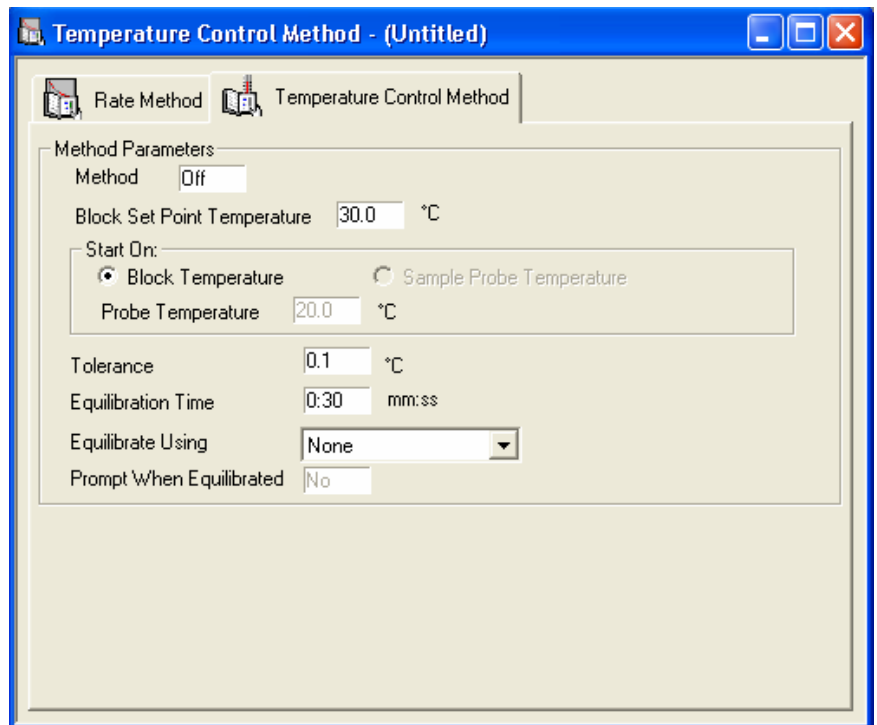
This method can be used in the Scan, Fixed, Rate, Quant and MCA applications.

1. Open the Temperature Control Method.

To open a new Temperature Control Method or to set the currently loaded method to the default values, click File > New > Temperature Method.

To open a previously saved Temperature Control Method, click File > Open > Temperature Method.

The Temperature Control Method page is added to the Method window. Click the tabs to move between the pages.



2. Enter the Block Temperature.

If a Peltier accessory is installed into a system, click in the Block Set Point Temperature field and enter the temperature (in °C) via the numeric entry dialog. The block temperature is only a monitor of the actual temperature of the metal block that holds the cuvette.

Note There will always be a difference between the block temperature and the actual solution temperature. This difference is very small at ambient and slightly above ambient and becomes larger at the extremes of the working range of the system. ▲

Note The block temperature is always higher than the probe temperature when the temperature is above ambient. If you are using a 4mm semi-micro cell, the difference between the block temperature and solution temperature could be as great as 10°C when the block temperature has stabilized to 110°C. ▲

The upper and lower limits available with the temperature control device currently installed will be shown in the dialog box. You must enter a temperature within the permitted range.

3. Choose a Peltier Control Method.

- a. Check the Block Temperature radio button to start the equilibrium process.
- b. For Sample Probe monitoring of the temperature, check the Sample Probe Temperature radio button if you need to start your collection process based on a certain temperature of your sample, not the block temperature.

4. Enter the Probe Temperature.

If a Sample Probe is being used to monitor the sample temperature and the Peltier accessory is not present, click in the Probe Temperature field and enter the temperature (in °C) via the numeric entry dialog.

The upper and lower limits available with the temperature control device currently installed will be shown in the dialog. You must enter a temperature within the permitted range.

5. Enter the Tolerance.

Click in the Tolerance field and enter the tolerance (in °C) via the numeric entry dialog. The range of values available will depend on the capability of the temperature control device currently installed.

The tolerance range is used by the software to establish the equilibration status of the system. The cell, temperature is equilibrated when its temperature has been maintained within the range Target Temperature \pm Tolerance for the duration of the Equilibration Time. If the target temperature is 20°C and the tolerance is 0.1°C, the temperature range will be 19.9 to 20.1°C.

6. Enter the Equilibration Time.

Click in the Equilibration Time field and enter the equilibration time via the numeric entry dialog. The entry format is mmm.ss (0.00 to 100.00).

The equilibration time is the period that elapses between the time when the temperature probe reports the cell has entered the permitted range and the time when it is possible to start a measurement.

7. Select the Equilibration method.

The Equilibrate Using field is used to specify which temperature probe(s) will be used to perform the equilibration.

Click the triangle at the right-hand end of the Equilibrate using field to pull down the menu and click your selection.

Equilibrate Using	Action
None	There will be no equilibration period. You may begin the measurement as soon as the sample enters the permitted temperature range.
Sample Only	<p>The equilibration period will commence when the sample enters the permitted temperature range.</p> <p>If the sample leaves the permitted temperature range the equilibration period will begin again.</p> <p>When the sample has been within the permitted temperature range for the full equilibration period, it will be possible to commence the measurement.</p>

Equilibrate Using	Action
Sample and Reference	<p>The equilibration period will begin when both the sample and the reference have entered the permitted temperature range.</p> <p>If either the sample or the reference leaves the permitted temperature range, the equilibration period will begin again.</p> <p>When both the sample and the reference have been within the permitted temperature range for the full equilibration period, it will be possible to begin the measurement.</p>

8. Prompt when Equilibrated.

Click in the box to toggle between Yes and No.

When Yes is selected, you will be prompted twice in each run. The first prompt will be to present the sample or cell holder. After equilibration has completed, there is a second prompt to allow a user action (e.g., injecting a reagent) to take place after the temperature has been reached but before measurement starts.

When No is selected, measurement begins as soon as equilibration has been completed, without further user intervention.

9. Save the Temperature Method, if required.

Save the Temperature Method if you will want to use it with more than one application method.

To do this, select File > Save as > Temperature Method.

All accessory methods associated with an application method can be attached to that application method and to any results files obtained with it when saved. To enable this behavior, click Tools > Options > File Load/Save Behavior tab. Ensure that the box for Auto load/save accessory methods is checked.

10. Click in the Method field to toggle the Temperature Method On.

The Temperature Method is now ready to use. It can be toggled On and Off as required by clicking in the Method box.

If a temperature controller is installed, it will start going to temperature as soon as the method is turned on.

Setting up a New Stirrer Method

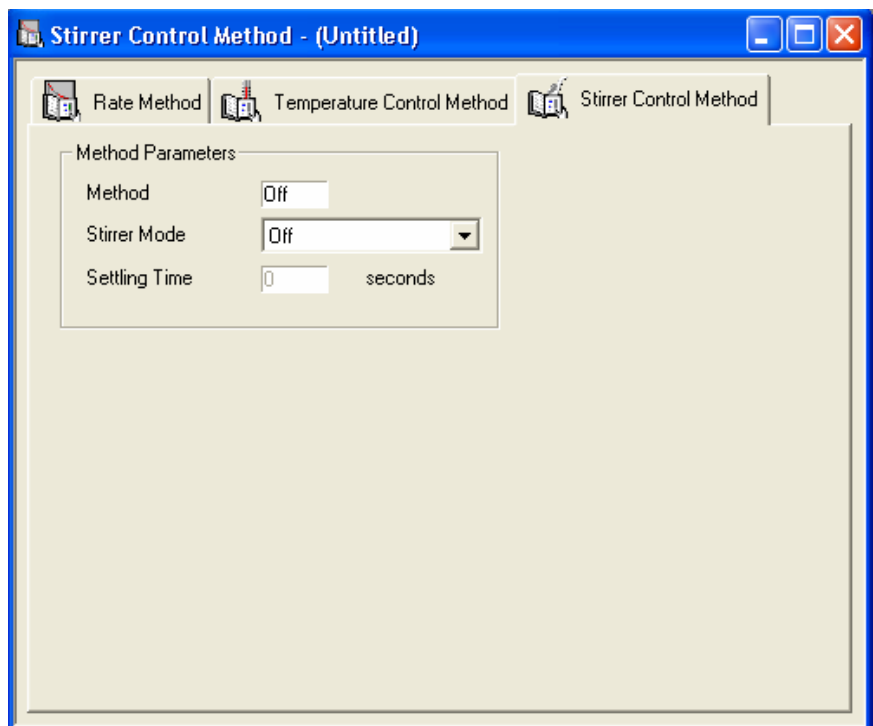
This method can be used in the Scan, Fixed, Rate, Quant and MCA applications.

1. Open the Stirrer Control method.

To open a new Stirrer Control Method or to set the currently loaded method to the default values, click File > New > Stirrer Method.

To open a previously saved Stirrer Control Method, click File > Open > Stirrer Method.

The Stirrer Control Method page is added to the Method window. Click the tabs to move between the pages.



2. Set the Stirrer Mode.

Stirrer Mode	Action
Off	The stirrer is off
Continuous	The cell is stirred continuously
Off Before Measurement	The stirrer is normally on but is switch off prior to and during measurement. A programmable settling time elapses before the measurement is made.

3. Set the setting time, if required.

If the Stirrer Mode has been set to Off Before Measurement, it will be possible to set the Settling Time. This is the number of seconds that will elapse between cessation of stirring and the start of the measurement (0 to 60).

Click in the Settling Time field and enter the required value via the numeric entry dialog.

When 0 is entered, the cell is stirred except during measurement.

4. Lock the Method, if required.

5. Save the Stirrer Control Method, if required.

Save the Stirrer Control Method if you want to use it with more than one application method. To do this, select File > Save as > Stirrer Control Method.

All accessory methods associated with an application method will be attached to that application method and to any results files obtained with it when saved.

6. Click in the Method field to toggle the Stirrer Control Method On.

The Stirrer Control Method is now ready to use. It can be toggled On and Off as required by clicking in the Method box.

There may be an accessory with stirrer control in the sample beam, or the reference beam, or both. In the latter case, both stirrers are switched together. It is not possible to switch off the stirrer on one beam while running the stirrer in the other beam.

Using Scan

Running samples

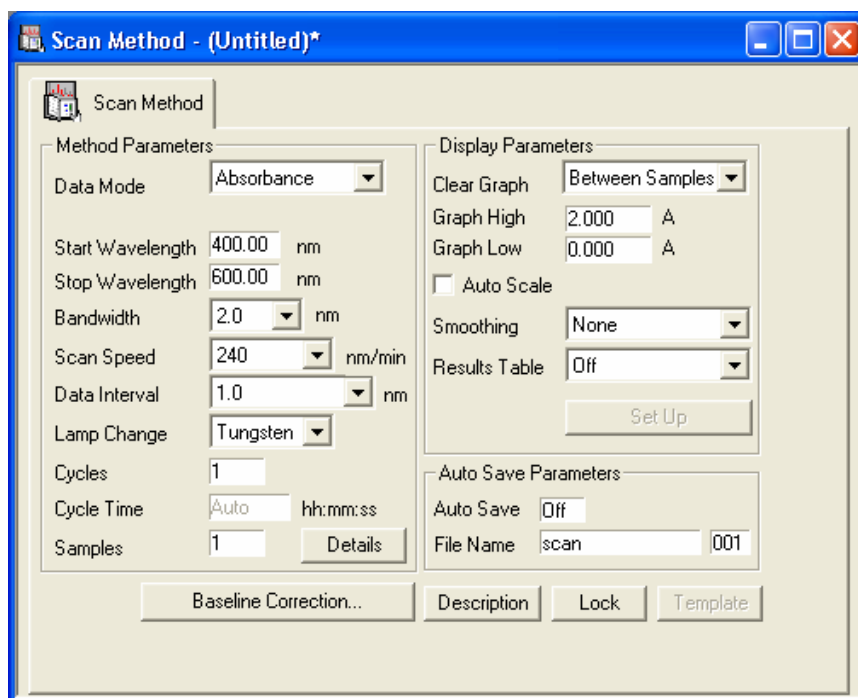
1. Launch VISION.



2. Start the Scan Application by clicking on the Scan icon.

Alternatively, you can click Applications on the menu bar and then click Scan.

3. Set up the Scan Method.



- Select the Data Mode from the available options in the pull-down menu.
- Click in the numeric field for Start Wavelength. This will open the numeric entry dialog. The wavelength may be entered either by

clicking with the mouse on the keys of the virtual keypad or by using the computer keyboard. Similarly, enter the stop wavelength.

- c. Select the bandwidth, scan speed and data interval (also the Lamp Change wavelength if applicable).
- d. Enter the number of Samples.

If desired, the sample name(s) and details may be entered as part of the method by clicking on the Details button. Double-click the sample name to edit it if required.

- e. Set Cycles and Cycle Time.

This sets the number of times each sample is measured (permitted range is 1 to 999). Collecting several cycles of data is a convenient way to monitor reaction kinetics using a scan rather than fixed wavelength measurements. The reproducibility of the cycle timing will allow some kinetic parameters to be extracted.

The Cycle Time is the time between the start of one cycle and the start of the next.

- f. Select the required display properties. Smoothing and Results Table operations may be performed at the time of data collection or later using the functions in the Math menu.
- g. Set Auto Scale.

The Auto Scale button in the scan method (any application method with a graph will have this feature) automatically changes the scale of the graph to show all of the data collected as soon as the data acquisition is complete. If this item is left unchecked, the values for the maximum and minimum of the absorbance axis specified above this selection box will remain after the data acquisition is complete.

- h. Set Smoothing.

Smoothing may also be performed at run time if enabled in the application method.

The smoothing algorithm used in VISION is based on a Savitzky-Golay algorithm modified to reduce high frequency breakthrough;

i.e., to reduce the amount of noise present on the spectrum. The Savitsky-Golay algorithm is based on performing a least squares linear regression fit of a polynomial of order k over at least $k+1$ data points around each point in the spectrum to smooth the data.

To smooth the data, select the degree of smoothing required from the Scan Method.

The different degrees of smoothing correspond to the number of data points used by the algorithm when performing the polynomial fit.

Degree of smoothing	Points
Low	9
Medium	17
High	33
Very high	67

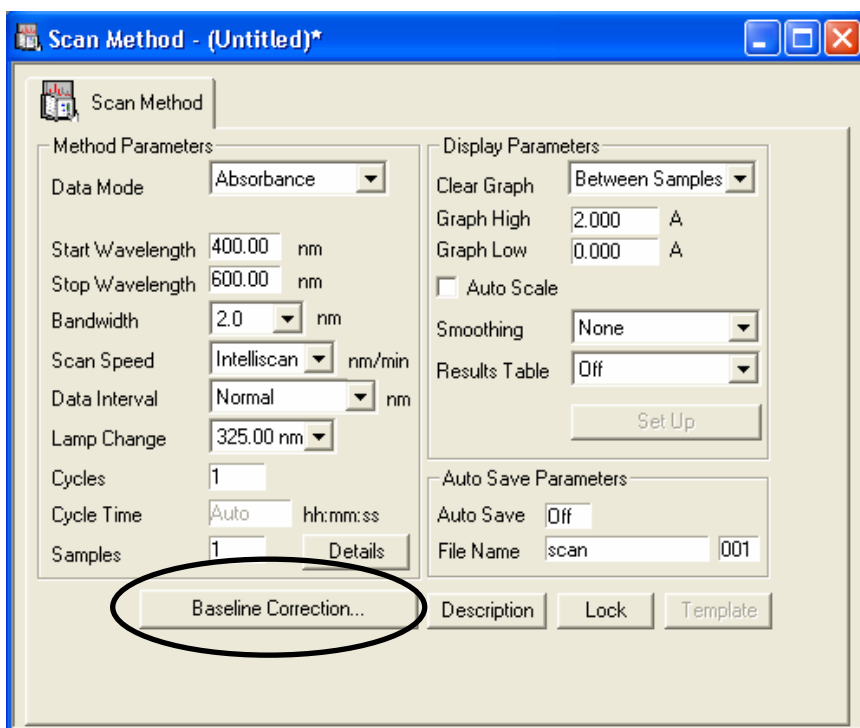
Note A higher degree of smoothing will produce a greater signal-to-noise ratio but this is achieved at the expense of spectral resolution. ▲

- i. To use AutoSave, click in the On/Off box to turn AutoSave on and enter the seed file name and number.
- j. The method may be locked by clicking on the **Lock** button. You will be prompted to enter a password.

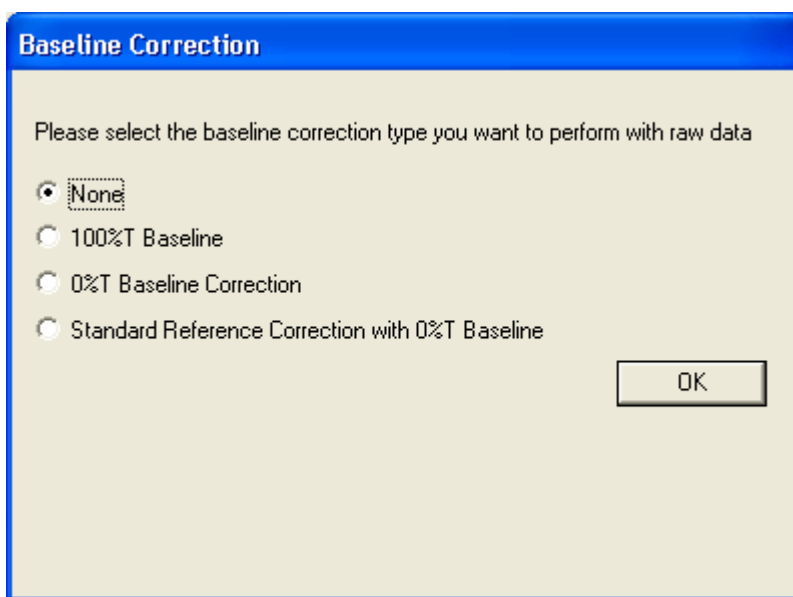
Note You will need to re-enter your password in order to unlock the method. ▲

Note The default contents of some fields will depend on which instrument is connected. ▲

4. Refer to [“Setting up a Cell Changer Method”](#) if a cell changer is to be used.
5. To set up the type of baseline correction applied to the data, click the **Baseline Correction** button





The following window will open:




6. Select the appropriate Baseline Correction you wish to perform.

The standard user baseline correction selection will be the 100%T Baseline. If you have a Diffuse Reflectance Accessory (DRA) attached to your spectrophotometer, then the other two options, 0%T Baseline

Correction and Standard Reference Correction with 0%T Baseline, can be applied.

Parameter	Function
None	When this baseline correction is performed, the sample signal is subtracted from the default baseline currently stored in the instrument.
100%T Baseline	<p>When this baseline correction is performed, the calculation in transmission performed in the instrument is simply:</p> $\frac{S}{100\%T}$ <p> Note: Clicking on the baseline icon will always collect a 100%T Baseline.</p>
0%T Baseline Correction	<p>This baseline correction is used after performing a 100%T Baseline scan to correct for any inherent variations in the electronic zero line of the instrument. This can be more of a factor at lower light energy levels present in a DRA type accessory and when working at high absorbance levels.</p> <p>For more information, you can also refer to ASTM method E903. the calculation performed in transmission performed in the instrument is simply:</p> $\frac{S - 0\%T}{100\%T - 0\%T}$ <p>You must have a 100%T Baseline recorded in the Data Store before a 0%T baseline can be applied to the data. Collect a 100%T Baseline before selecting 0%T Baseline from the Command menu.</p> <p> Note: The 0%T Baseline can only be collected by selecting 0%T baseline from the Command menu. Clicking on the baseline icon will always collect a 100%T Baseline.</p>

Parameter	Function
Standard Reference Correction with 0%T Baseline	<p>This baseline correction is used to apply a 100%T Baseline correction and a zero line correction (0%T Baseline) to a sample (S) measured with a reflectance accessory which is not absolute (e.g., a Diffuse Reflectance Accessory). The VISION software then multiplies the scan result by the appropriate value in the Baseline Standard Reference (Std. Ref.) file, which are the transmission values associated with the Standard Reference material. The calculation in transmission performed in the instrument is simply:</p> $\frac{S - 0\%T}{100\%T - 0\%T} \times \text{Std. Ref.}$ <p>Note: the Standard Reference file must be created outside of VISION in another program such as Notepad or MS Word, saved as a plain text (*.txt) and stored as X delimiter Y pairs.</p> <p>Example with delimiters of "." And "" (blank):</p> <pre>190:0.81 240:0.85 300:0.89 350:0.90 400:0.91 420:0.92 440:0.93 460:0.94 480:0.95 500:0.96 600:0.97 700:0.98 800:0.99 900:0.99</pre> <p>You must have a 100%T baseline recorded in the Data Store before a 0%T Baseline with Reference Correction can be applied to the data. Collect a 100%T baseline before selecting 0%T baseline from the Command menu.</p> <div style="display: flex; align-items: flex-start;">  <p>Note: The 0%T Baseline can only be collected by selecting 0%T baseline from the Command menu. Clicking on the baseline icon will always collect a 100%T Baseline.</p> </div>



7. Click the Zero-Base icon.

- When the Present Reference(s) dialog box appears, place the requested reference in the sample beam or in the correct sample position for the accessory, close the lid of the sample compartment and click the **Proceed** button.



8. Click the Run icon.

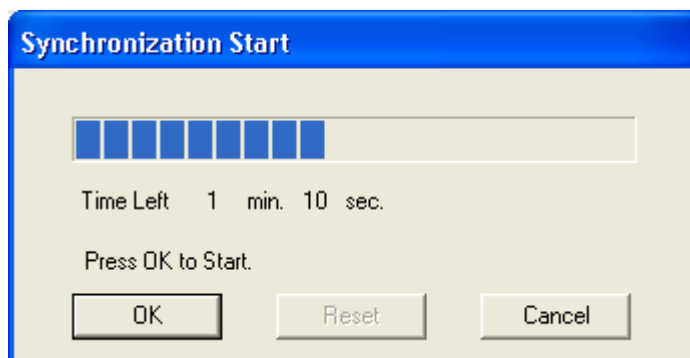
- The Present Sample dialog box opens. If the sample name and description have not been entered via the method window (see above), it can be entered now.
- Place the sample in the sample beam or in the correct sample position for the accessory and close the lid of the sample compartment.

9. Click the Proceed button.

10. A Synchronization Start option is available to help with the timing of kinetics experiments. This option can be enabled from Tools > Options > System Settings > tab.

Synchronization Start sets the instrument up so that data will be collected immediately after the OK button is pressed or after the countdown timer expires.

The following is an example of the Synchronization Start countdown dialog box in progress:



Note You can press any key on the keyboard to start the run when the Synchronization Start dialog box is visible. ▲

11. Initiate the reaction in the first cell by adding reagents, if necessary; close the lid of the sample compartment and click the Proceed button.

If the Synchronization Start option is disabled, the run will start after the Proceed button is pressed.

12. The first sample will be measured and the Cell Changer will bring the next sample into the beam.

You will then be prompted to start the reaction in the next sample.

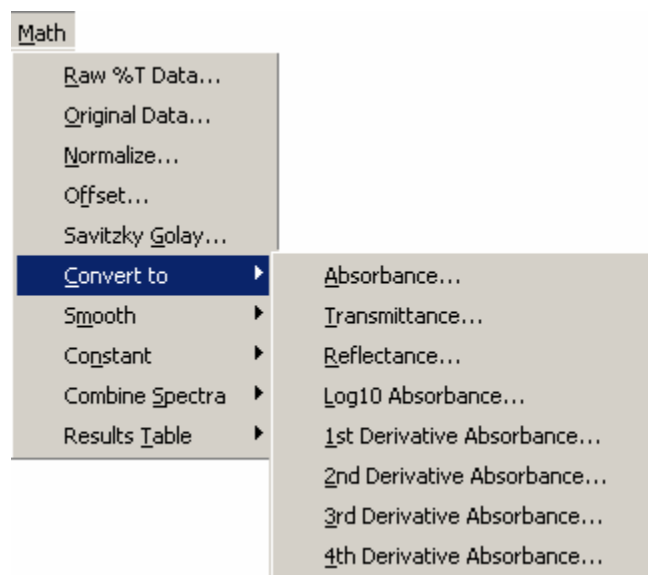
- 13. The data collection can be paused at any time by pressing the Pause icon or selecting Pause from the Command menu.**

The instrument will continue to perform the experiment (i.e., the time from the duration will elapse); however, the data will not be displayed until the Pause icon is pressed again (or selected from the Command menu). Data collection will resume according to the method parameters.

- 14. Continue in this way until all the samples have been measured.**

Manipulating scan data

The Math Menu enables you to access a comprehensive suite of data analysis functions.

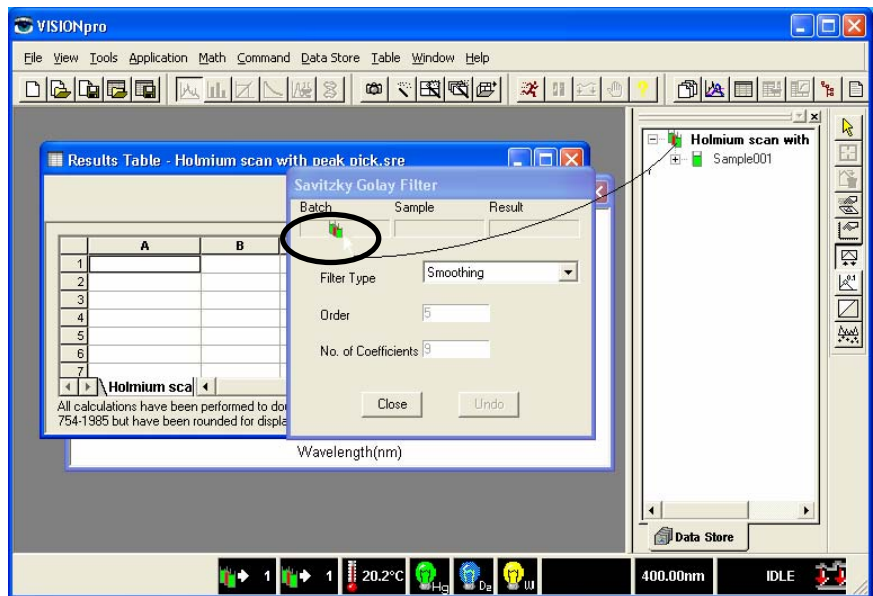


- 1. Click Math on the menu bar and select the Math operation from the menu or sub-menu.**

A window for the operation opens in the work area.

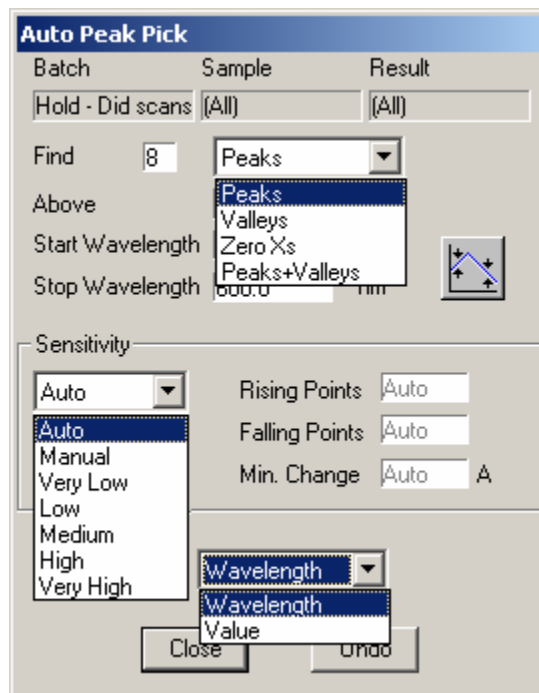
2. In the Data Store, point to the batch, sample or result that you wish to manipulate. Press and hold the LEFT mouse button, drag the data onto the Batch, Sample or Result area of the Math window.

As you drag the data, its “ghost” follows the cursor over the Data Store and the cursor arrow changes to a black circle with a bar across it. When you reach an area where the data may be dropped, the cursor arrow returns and a batch, sample or result symbol represents the data. Release the mouse button to drop the data.

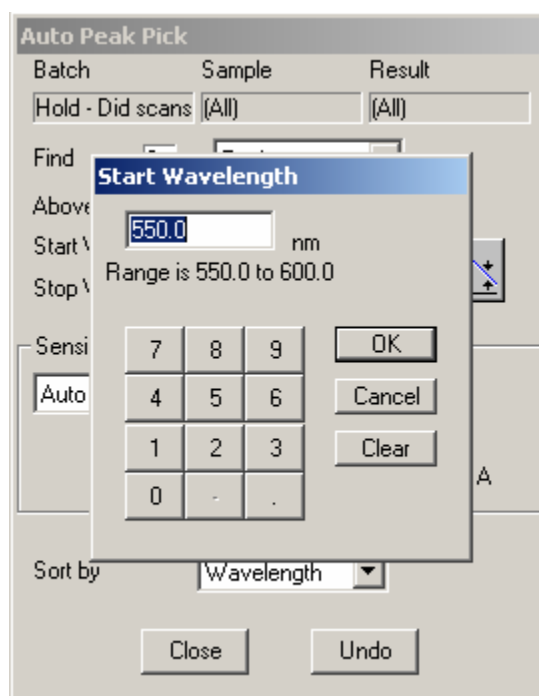


3. If required, set the parameters in the Math window.

For example, in the case of Peak Pick, there are three pull-down menus within the Peak Pick window:

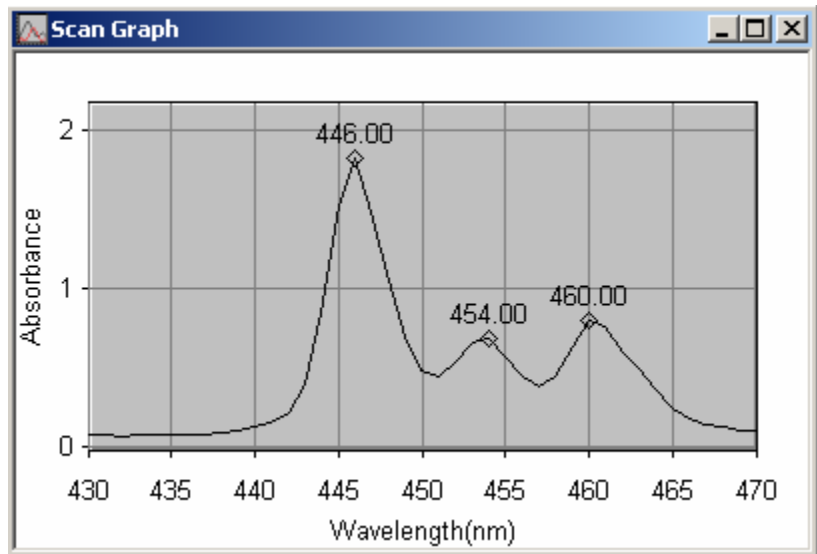


You can edit the numeric fields by clicking on them to open the Numeric Entry keypad.



The three Sensitivity parameters become editable when **Manual** is selected in the Sensitivity pull-down menu.

4. The calculations or modified spectra data may be viewed on the Scan graph.



- a. Drag the batch, sample or cycle from the Data Store onto the Scan Graph window.
 - b. Click a cycle to view the Peak Pick data for that cycle.
 - c. Select Peak Labels from the Graph menu and select the form of labeling that you require. Toggle the labeling on and off with the Toggle Labels button on the Graph Toolbar.
5. Depending on the function, results may also be viewed in the Results Table.

You may choose whether to display the results in order of wavelength or of absorbance using the pull-down menu in the Math window.

The Results Table window displays a table of results for the 2nm MCA Demo Results.sre file. The table has six columns labeled A, B, C, D, E, and F. The data is organized into rows, with the first row showing Sample001, Cycle01, ComponentA, ComponentB, G.O.F., and Conc. Error. The table is scrollable, and the bottom of the window shows the file name and a note about calculations.

	A	B	C	D	E	F
1	Sample001		Conc.	Error		
2	Cycle01	ComponentA	1.932	0.229		
3		ComponentB	5.992	0.186		
4		G.O.F.	0.000			
5						
6						

1.5 nm MCA Demo Results.sre 2nm MCA Demo Results.sre

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

Working in the Fixed Application



1. Start the Fixed application by clicking on the icon.

Alternatively, you can click Applications on the menu bar and then click Fixed.

2. Set the parameters in the Fixed Method window.

Fixed Method - (Untitled)*

Fixed Method

Wavelengths

1	500.00	3	OFF	5	OFF	7	OFF	9	OFF
2	550.00	4	OFF	6	OFF	8	OFF	10	OFF

Method Parameters

Data Mode: Absorbance

Fixed Mode: Normal

Integ. Time: 0:00:01 hh:mm:ss

Lamp Change: 345.00 nm

Bandwidth: 2.0 nm

Cycles: 1

Cycle Time: Auto hh:mm:ss

Samples: 1 Details

Reference Wavelength Correction: ☒

Ref. Wavelength: 320.00

Auto Save Parameters

Auto Save: Off

File Name: fixed 001

Description Lock Template

- a. Depending on the Fixed Mode selected, up to 10 **wavelengths** can be measured. Click in the box and enter the value(s) using the on-screen keypad or your PC keyboard. Wavelengths may be entered in any order.
- b. Set the **Data Mode**. Choose between Absorbance and %T.

- c. Select the **Fixed Mode**. Choose between Normal, Arithmetic Combination of 2 wavelengths, and Peak Height. In Peak Height mode enter the peak value and one wavelength on each side of the peak.

Method Parameters

Data Mode: Absorbance

Fixed Mode: Normal (dropdown menu open showing: Normal, Wavelength1 + Wavelength2, Wavelength1 - Wavelength2, Wavelength1 * Wavelength2, Wavelength1 / Wavelength2, Peak Height)

Integ. Time: []

Lamp Change: []

Bandwidth: []

Cycles: 1

Cycle Time: Auto hh:mm:ss

Samples: 1 [Details]

Reference Wavelength Correction: ☐

Ref. Wavelength: OFF

Mode	Description
Normal	A measurement will be made at each of up to 10 wavelengths and the results, in A or %T depending on the Data Mode selected, will be displayed in the Results Table.
Wavelength1 + Wavelength 2	The values of the data in the selected mode at λ_1 and λ_2 will be added together and the result displayed in the Results Table.
Wavelength1 - Wavelength 2	The values of the data in the selected mode at λ_2 will be subtracted from the value at λ_1 and the result displayed in the Results Table.
Wavelength1 * Wavelength 2	The values of the data in the selected mode at λ_1 and λ_2 will be multiplied together and the result displayed in the Results Table.
Wavelength1 / Wavelength 2	The values of the data in the selected mode at λ_1 will be divided by the value at λ_2 and the result displayed in the Results Table.
Peak Height	Enter three wavelengths. The peak height is calculated on the assumption that the lowest wavelength value represents the start of the peak, the middle value is the wavelength at the peak and the highest value is the end of the peak.

Note Each wavelength can also be corrected using a reference wavelength. This feature is enabled by selecting the checkbox for Reference Wavelength Correction. When the reference wavelength correction feature is enabled, the wavelength entry field for entry of the wavelength is active. ▲

d. Set the remaining method parameters.

e. Set the **number of samples**.

If desired, the sample name(s) and details may be entered as part of the method by clicking on the Details button. Double-click the sample name to edit it if required.

f. Set the Auto Scale

The Auto Scale button in the scan method (any application method with a graph will have this feature) automatically changes the scale of the graph to show all of the data collected as soon as the data acquisition is complete. If this item is left unchecked, the values for the maximum and minimum of the absorbance axis specified above this selection box will remain after the data acquisition is complete

g. If you are using **AutoSave**, click the On/Off box to turn AutoSave on and enter the seed file name and number.

h. The method may be locked by clicking the **Lock** button. You will be prompted to enter a password, **which you will need to re-enter in order to unlock the method**.

Note The default contents of some fields will depend on which instrument has been connected. ▲

3. **When using a cell changer, refer to “[Setting up a Cell Changer Method](#)”.**



4. **Click the Zero-Base icon.**

- When the Present Reference(s) dialog box appears, place the requested reference in the sample beam or in the correct sample position for the accessory, close the lid of the sample compartment and click the **Proceed** button.



5. Click the Run icon.

- The Present Sample dialog box opens. If the sample name and description have not been entered via the method window (see above), it can be entered now.
- Place the sample in the sample beam or in the correct sample position for the accessory and close the lid of the sample compartment.

6. Click the Proceed button.

Performing a Quant Calibration

Calibrating

Before the concentration of samples can be measured, a calibration using solutions of known concentration must be performed.



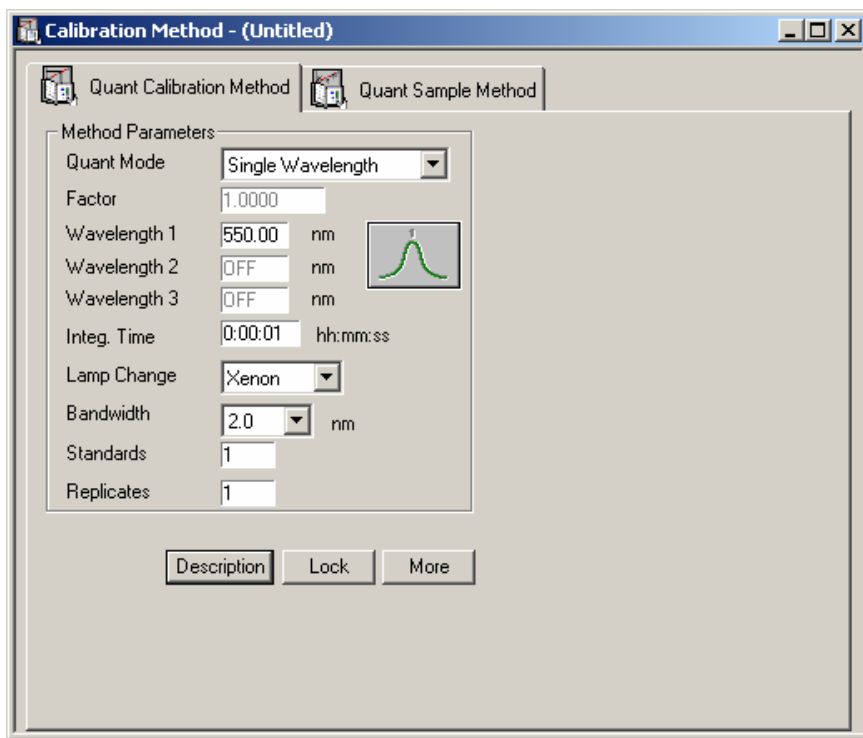
1. Start the Quant application by clicking on the Quant icon in the Applications toolbar.

Alternatively, you can click Applications on the menu bar and then click Quant.






2. In the Quant Method window, click the tab for the Calibration Method

You will not be able to make any sample measurements until a valid calibration is present. A calibration may be loaded from disk or performed following the procedure described in this section.

3. Enter the required values for the parameters on the Calibration Method page.



4. Select the required Quant mode from the pull-down menu.

	Single wavelength	The absorbance is measured at a single wavelength.
	Reference wavelength	The absorbance at λ_2 (the Reference Wave-length) is subtracted from the absorbance at λ_1 .
	Dual wavelength	The absorbances at two wavelengths are used in the calibration.
	Peak height	The height of the peak is calculated from the absorbances at the peak and at the wavelengths at each side of the peak. The software assumes that the middle wavelength is the peak.
	Factor	A previously measured factor is entered to produce a linear calibration.

5. Enter the required Wavelengths(s), and the Factor, if required.

6. Set up Auto Scale

The Auto Scale button in the scan method (any application method with a graph will have this feature) automatically changes the scale of the graph to show all of the data collected as soon as the data acquisition is complete. If this item is left unchecked, the values for the maximum and minimum of the absorbance axis specified above this selection box will remain after the data acquisition is complete.

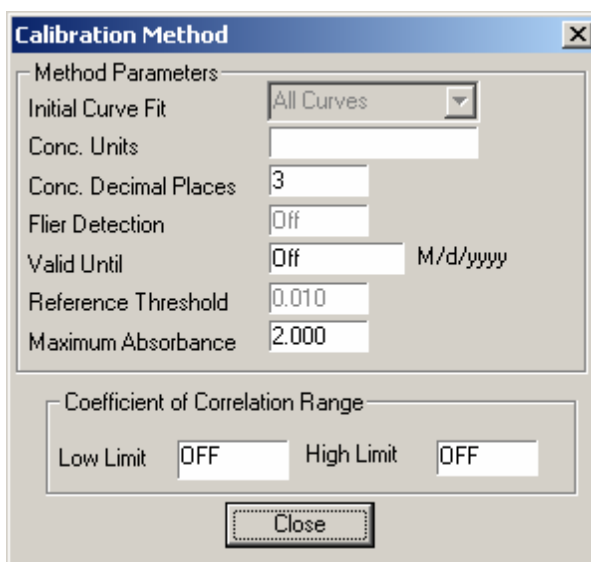
7. Set up the remaining method parameters.

8. Enter the Number of Standards to be used (1 to 50) and the number of replicates per standard (1 to 3).

Note The VISION software treats a replicate as an independently prepared solution of the same concentration. If you are taking multiple measurements of the same sample solution for averaging purposes, simply present the sample solution when the replicate is requested by the software. ▲

9. Click the More button.

A secondary method parameters window opens.

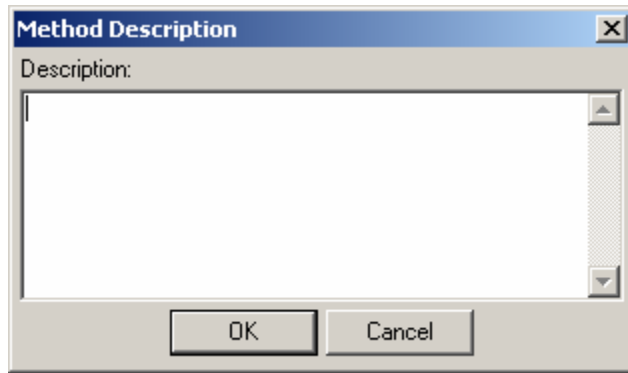


The screenshot shows a dialog box titled "Calibration Method" with a close button (X) in the top right corner. The dialog is divided into two main sections. The first section, "Method Parameters", contains the following fields: "Initial Curve Fit" with a dropdown menu showing "All Curves", "Conc. Units" with an empty text box, "Conc. Decimal Places" with a text box containing "3", "Flier Detection" with a dropdown menu showing "Off", "Valid Until" with a dropdown menu showing "Off" and a date format "M/d/yyyy" to its right, "Reference Threshold" with a text box containing "0.010", and "Maximum Absorbance" with a text box containing "2.000". The second section, "Coefficient of Correlation Range", contains two dropdown menus: "Low Limit" showing "OFF" and "High Limit" showing "OFF". At the bottom center of the dialog is a "Close" button.

In this window you may select the Initial Curve Fit, enter the Concentration Units, select the number of decimal places to be displayed, and enter an expiration date (if desired) for the calibration in the Valid Until field. Flier Detection may be toggled On/Off. The Reference Threshold and Maximum Absorbance may be set when applicable. You can also set low and high limit of correlation coefficient.

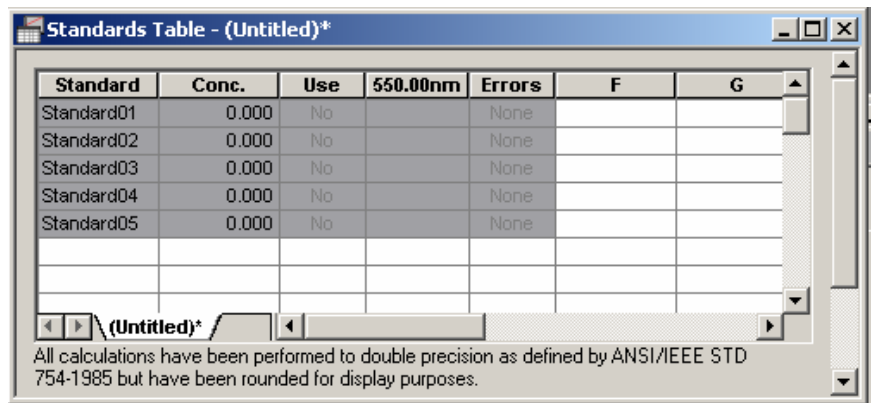
Note If you select the All Curves option for the initial curve fit, you must select a specific curve fit in the Quant menu or by using the graph toolbar before unknown samples can be measured. ▲

- 10. Return to the Calibration Method window by clicking the Close button.**
- 11. Click the Description button to enter a description of the calibration method.**



The method may be locked by clicking on the **Lock** button. You will be prompted to enter a password, which you will need to re-enter in order to unlock the method.

12. Enter the concentrations of the standards in the Standards Table.



- The active area of the Standards Table is shaded in gray, corresponding to the number of standards that you entered in Step 7. The size of the active area can only be changed by editing the number of standards in the Quant Calibration Method.
- Click cells in the Standards column to enter the **names of each standard**.

Note Standard names cannot be altered after calibration. ▲

- Click in the cells in the Conc column to enter the **concentrations of each standard**.

13. If a cell changer is to be used to perform the calibration, guidance for setting it up may be found in [“Setting up a Cell Changer Method”](#).
14. If a sipper is to be used to perform the calibration, guidance for setting it up may be found in [“Setting up a Sipper Method”](#).

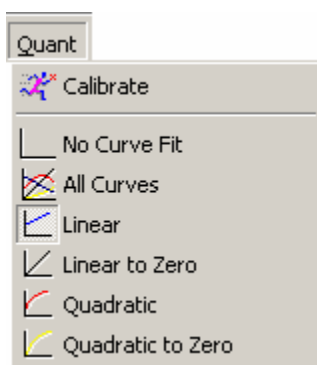


15. Click the Zero-Base icon.

When the Present Reference(s) dialog box appears, place the blank or reference solution in the sample beam, close the lid of the sample compartment and click the Proceed button

16. Click Quant in the Main Menu Bar and then click Calibrate to initiate calibration.

Alternatively, click the Calibrate Run button in the Graph Toolbar.



No curve fit will be indicated at this stage.

If required, the curve fit can be changed after the standards are measured.

Follow the on-screen instructions.

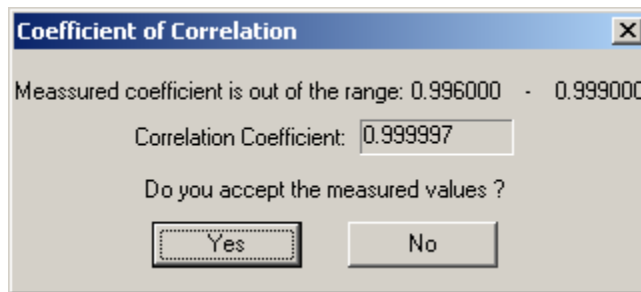
Note If a manual calibration is being performed, you will be prompted to present each standard and/or replicate. ▲

Note If a Cell Changer is being used, you will be prompted to present the first cell holder. Calibration will then proceed until completed or until all cells have been measured, when you will be prompted to re-load the cell basket. ▲

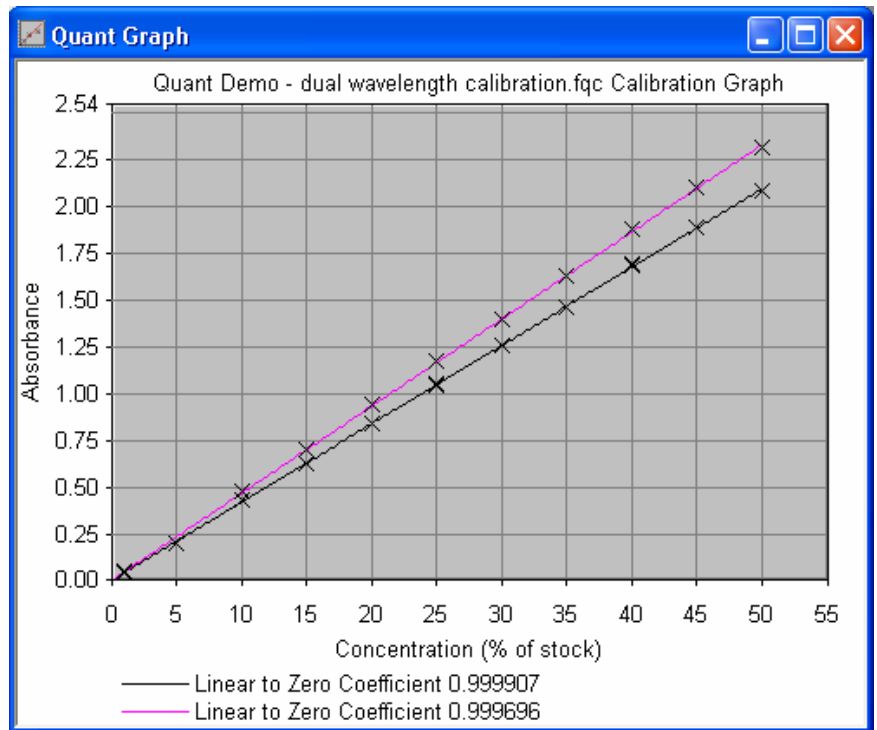
In either case, after each standard has been measured, the absorbance will be reported and the point will be displayed on the Quant Graph. You will have the option to accept the value or repeat the measurement.

If the measured value of Coefficient Correlation is out of the range of the prompt, the following dialog box will appear.

If you do not accept the value, your Quant Calibration Method will not be valid.



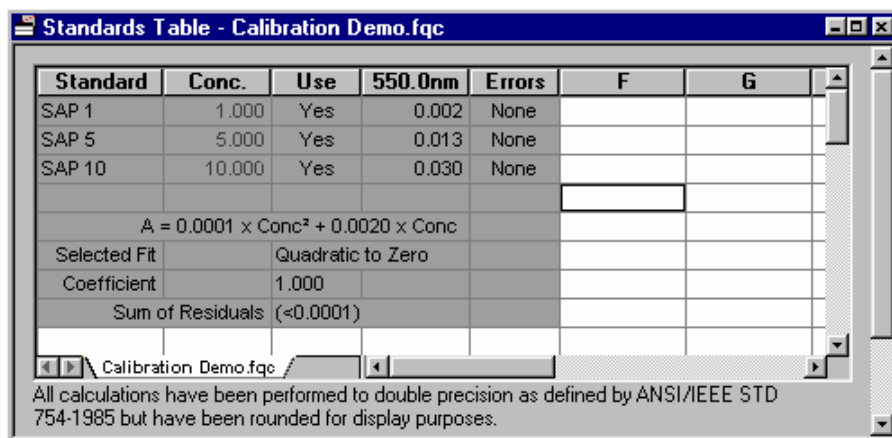
17. **After the calibration is complete, the measured standards will be plotted in the Quant Graph Window with the selected Initial Fit applied.**



The Quant Graph toolbar is now visible.

Icon	Description
	Select Linear through zero fit
	Select Linear fit
	Select Quadratic fit through zero
	Select Quadratic fit
	Select all curve fit
	Select no curve fit

18. The Standards Table will show the measured absorbances, the equation for the selected curve fit, the correlation coefficient and the sum of residuals.



Standard	Conc.	Use	550.0nm	Errors	F	G
SAP 1	1.000	Yes	0.002	None		
SAP 5	5.000	Yes	0.013	None		
SAP 10	10.000	Yes	0.030	None		
A = 0.0001 x Conc ² + 0.0020 x Conc						
Selected Fit		Quadratic to Zero				
Coefficient		1.000				
Sum of Residuals		<0.0001				

Calibration Demo.fqc

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

19. The Curve Fit may be altered if required from the Quant menu on the Main Menu Bar, or by using the Curve icons on the Graph toolbar.

In general, the curve fit should be chosen to minimize the Sum of Residuals and/or give an optimal value for the Correlation Coefficient.

Note The quadratic fit may mathematically be a better fit for linear data due to the addition of the second fitting parameter. Therefore, only a significant improvement in the quality of the fit should be observed. Care should be exercised when selecting the most appropriate fit for the data. ▲

20. Save the completed calibration by clicking on File > Save > Calibration or right-click the calibration method and select Save or Save As from the context menu. Save via a normal windows dialog.

Measure samples



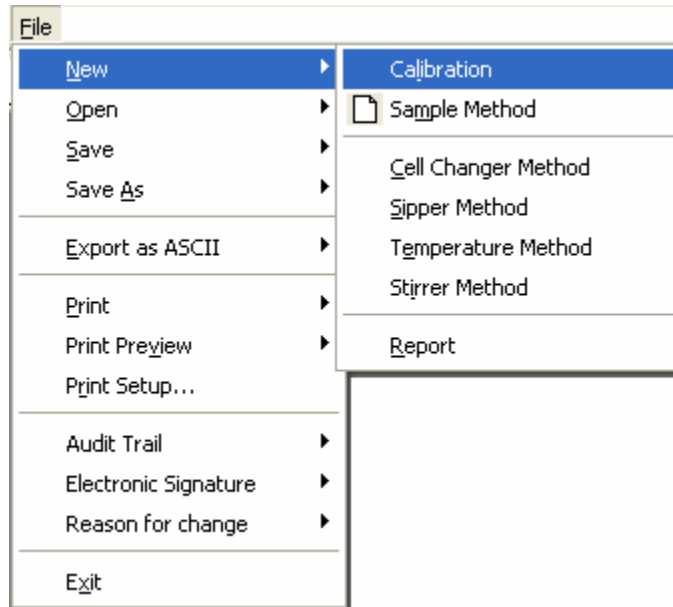
1. Start the Quant application by clicking on the icon in the Applications toolbar.

Alternatively, you can click Applications on the menu bar and then click Quant.

2. The method is set in the Quant Method window. This window contains pages for the Sample Method and the Calibration Method.

3. A valid calibration must be present before measurements can be made.

- If a **new calibration** needs to be made, refer to “[Performing a Quant Calibration](#)”.
- To **load a calibration** select Open > Calibration from the File Menu.



4. To set up a new Sample Method, click the Quant Sample Method tab in the Method window.

Sample Method - (Untitled)*

Quant Calibration Method Quant Sample Method

Method Parameters

Samples: 5 Details

Replicates: 3

Zero every: NONE sample(s)

High Limit: OFF Conc

Low Limit: OFF Conc

Auto Save Parameters

Auto Save: Off

File Name: quant 001

Weight/Volume Correction

☒ Correction

Method Weight: 5.000 mg

Method Volume: 10.000 mL

Sample Name	Actual Weight / mg	Actual Volume / mL
Sample001	1.0000	1.0000
Sample002	1.0000	1.0000
Sample003	1.0000	1.0000
Sample004	1.0000	1.0000
Sample005	1.0000	1.0000

Description Lock Template

- Click in each of the method boxes to enter the **number of samples** (1 to 999), **number of replicates** per sample (1 to 3), frequency of **zero** setting (None or 1 to 10), high and low **limits** (0.0001 to 9999.9999), and **Auto Save** parameters.

Note The VISION software treats a replicate as an independently prepared solution of the same concentration. If you are taking multiple measurements of the same solution for averaging purposes, simply present the sample solution when the replicate is requested by the software. ▲

- Click the **Details** to enter the sample details (names and descriptions). From this dialog, individual sample names can be entered, or a single sample name can be entered and incremented using the checkbox.
- Click the **Description** button to enter the method description.

- Weight/Volume Correction is a convenient feature to automatically calculate the concentration of the solutions prepared either by weighing a specific amount of material and/or by adding a particular volume of solution. If you know the weight and/or volume of material used to prepare each sample, you can use the weight/volume correction feature to calculate the actual concentration of your sample. This feature helps to avoid time-consuming calculations that are often necessary after measuring samples against the standard curve.

Click the Correction checkbox if you want to incorporate Method Weight and Method Volume correction in your calculations.

- If Method Weight is known, enter the sample weight specified in your analytical method.
- If Method Volume is known, enter the sample volume specified in your analytical method.
- If the Actual Weight for a sample is known, enter the individual weights of each sample. If the weight of one or more samples is not known, enter the Method Weight for the Actual Weight(s); this will determine the concentration solely from the calibration curve.
- If the Actual Volume for a sample is known, enter the individual volumes of each sample. If the volume of one or more samples is not known, enter the Method Volume for the Actual Volume(s); this will determine the concentration solely from the calibration curve.

Note For more detailed information about calculations performed using these corrections, refer to the Online Help system. ▲

- The method may be locked by clicking on the **Lock** button. A password must be supplied, which will be required in order to unlock the method.

- The **Template** button will be enabled if an *UVcalc* advanced calculation template is present. Refer to “[Getting Started with Advanced Result Calculations](#)” for details.

To **Save** the Sample Method, click File or right-click the sample Method. Select Save > Sample Method from resulting menu and save via a normal Windows dialog.

5. To load a stored method click File or right-click the Sample Method.

Select Open > Sample Method from the resulting Menu.

6. Load or set up Cell Changer and Sipper Methods or temperature or stirrer if these are required.

See “[Setting up a Cell Changer Method](#)” and “[Setting up a Sipper Method](#)”.



7. To perform a blank or zero measurement click the Zero-Baseline icon.

8. When the prompt box appears, place the reference solution in the sample beam, and close the lid of the sample compartment and click the Proceed button.

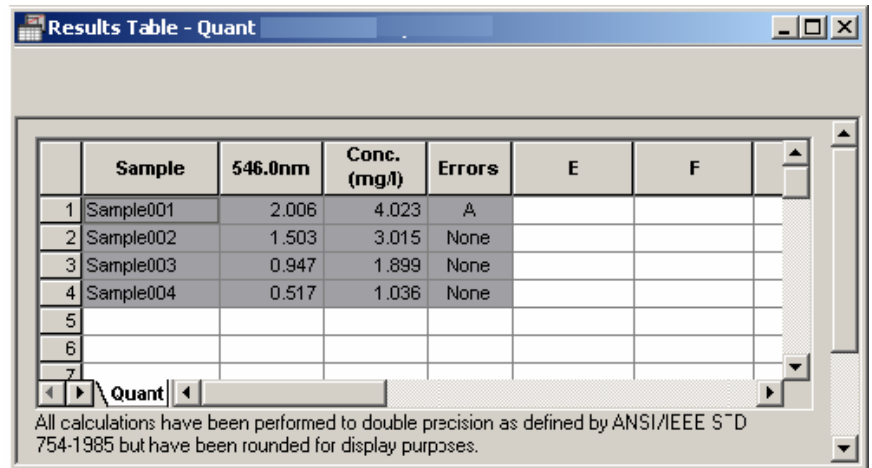


9. To run samples, start by clicking on the Run icon.

- The **Present Sample** window opens. If the sample name and description have not been entered via the method window (see above), they can be put in at this point. If a cell changer method is being used you will be prompted to present the first basket.
- Place the sample in the cell holder in the sample beam, or insert the loaded cell holder, and close the lid of the sample compartment.
- Click the Proceed button.

10. When the method has been run, the results will be in the Results Window and the data will be in the Data Store.

If necessary, scroll the results window to the top to see all the data.



	Sample	546.0nm	Conc. (mg/l)	Errors	E	F
1	Sample001	2.006	4.023	A		
2	Sample002	1.503	3.015	None		
3	Sample003	0.947	1.899	None		
4	Sample004	0.517	1.036	None		
5						
6						
7						

All calculations have been performed to double precision as defined by ANSI/IEEE S'D 754-1985 but have been rounded for display purposes.

- Each batch of results will be put onto a separate sheet in the Results Window.
11. To save a batch of results, click File or right-click the batch in the Data Store, and select Save or Save As > Batch of results from the resulting menu.
 12. If further calculations are required, refer to [“Getting Started with Advanced Results Calculations”](#).
 13. A report may be produced. Refer to [“Producing Printed Output”](#).

Working with Multicomponent Analysis

Calibrating

1. Set up the MCA scan method. The method parameters set at this stage will determine the parameters for the entire analysis. Refer to [“Using Scan”](#) for details.
2. Prepare the standards.

There must be at least as many standards as there are components in the analysis. Standards may be single components or mixtures. If mixed standards are used, they must be linearly independent. Please refer to the Help for a detailed explanation of linear independence.

Only one single component solution can be used for each component present as by definition all other single component solutions would be linearly dependent on that single component solution.

Note It is strongly recommended that you calibrate the MCA application using mixtures of all of the components at known concentrations. You should ideally use at least three times the number of components as standards. The standards for the component mixtures should span the entire concentration range you intend to measure. Additionally, the standards should include a mixture containing the highest concentration of each of the components and the lowest concentrations of each of the components. The practice of using single component calibrations standards is highly discouraged when a high degree of precision is required. ▲



3. Click the Run icon to scan the standards.

If scans that have been measured previously are to be used, load the files into the Data Store.

4. If a previous calibration is present, clear the MCA Standards table by clicking on File > New > Calibration.

5. Enter the following into their respective fields in the Multicomponent Calibration window:

- The number of standards.
- The number of components.

Note The number of components must not be greater than the number of standards. ▲

- The following may be altered or left as their defaults: Conc. Units, Conc. Decimal Places and Valid Until date.
- Set the Auto Scale. The Auto Scale button in the scan method (any application method with a graph will have this feature) automatically changes the scale of the graph to show all of the data collected as soon as the data acquisition is complete. If this item is left unchecked, the values for the maximum and minimum of the absorbance axis specified above this selection box will remain after the data acquisition is complete.

6. Transfer the spectra of the standards to the MCA calibration.

- Drag each sample onto a new line of the calibration table. The spectral data for the sample will be transferred to the calibration and associated with that line in the table.
- An entire batch may be used as the calibration set by dragging the name of the batch from the Data Store to the Standards Table.

7. When the First standard or batch is put into the calibration, you may choose to replace the current Scan method with the one that was used to scan the standard.

This provides a quick way to set up the measurement parameters for the analysis. The software will check that the methods for the second and subsequent standards are compatible with the current scan method.

8. The entry in the Present column changes from “No” to “Yes” when a standard has been successfully transferred to the calibration.

If the methods are incompatible the status changes to “Invalid”. The Present column must read “Yes” for all standards before the calibration can be used. An invalid standard must be replaced, or the Scan method parameters must be altered to accommodate it (e.g., by changing the wavelength range). Please refer to the Help system for a detailed explanation of the criteria for method compatibility.

9. **To replace a standard in the calibration, drag the new standard from the Data Store and drop it on top of the standard you wish to replace.**
10. **Enter Standards Information. Left-click the name of each standard to open its Standards Information window and edit as required.**
11. **Enter the concentrations of each component in each standard into the relevant cells of the Multicomponent Calibration window.**
12. **Double-click the Component column headers to open the Component Information window, and edit the name of each component as desired.**
13. **Click File > Save As > Calibration and save the completed calibration.**

Analyzing samples






A valid calibration needs to be present in the MCA Calibration window before you can analyze a sample.

Multicomponent Analysis in Real Time

1. **If you require normal scan results (e.g., Peak Pick) at run time in addition to the Multicomponent Analysis (MCA), set up the Results Table section of the Scan method as required.**
2. **Ensure that a valid calibration is present. Load the calibration from disk or perform the calibration (see “[Working with Multicomponent Analysis](#)”).**
3. **Set up or load the required accessory methods if a cell changer or a sipper is being used.**
4. **Click the Run samples icon in the tool bar to scan the unknown samples using the current calibration. If scans that have been measured previously are to be used, load the files into the Data Store.**



- When the prompt appears, place the first unknown sample in the cell holder or load the cell changer as appropriate. Enter the sample name and description if required, and then click Proceed.
- MCA differs from Scan in that each cycle is treated as a separate replicate solution. If a sample contains more than one cycle, you will be prompted to present a new sample after each cycle.
- While the unknown sample is being scanned, the sample spectrum and/or the concentration trends graphs for the components can be viewed in the graph window. The display of the MCA graphs can be toggled from the Graph toolbar or the Graph menu.

Icon	Title	Description
	Standards Spectra	Displays the scans for the standard(s)
	Sample Spectrum	Displays the scan for the sample(s)
	Trends Graphs	Displays the concentration trends
	Synthetic Spectrum	Displays the spectrum calculated by MCA for the sample
	Residuals	Displays the residuals of the spectrum fit to the sample spectrum

5. When the scans on the unknown samples have been completed:

- The Results Table will contain estimates of the concentrations of each component, plus indications of the likely error. If Results Table operations were included in the MCA Scan method, the Results Table will also contain these results.
- The Synthetic and Difference Spectra are computed. Use the buttons on the Graph toolbar to display them as required.

6. The MCA Result window (*but NOT the Calibration window*) may also contain a UVcalc advanced calculation template.

MCA post-run

An MCA analysis can be carried out post-run on any Scan data file that is compatible with the MCA calibration.

1. **Ensure that a valid calibration is present in the calibration table. Load the calibration from disk or perform the calibration (see [“Working in Multicomponent Analysis”](#)).**
2. **Load the results that you wish to analyze into the Data Store.**
3. **Click Math in the Main Menu Bar and select MCA Analyze from the pull-down menu.**
 - The Analyze dialog opens.
 - Drag the Batch, Sample or Result into the appropriate field in this dialog.
 - The data are analyzed and the estimated concentrations are entered into the Results Table.

	A	B	C	D	E	F
1	Sample001		1	2		
2	Cycle01	nm	427.50	634.50		
3	Peaks	A	2.075	2.310		
4	Sample002		1	2		
5	Cycle01	nm	428.50	635.00		
6	Peaks	A	1.875	2.092		
7	Sample003		1	2		

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

4. **Drag the data to the Graph window in order to view the Sample, Standards, Trends, Synthetic and Difference spectra.**

Setting up a Cell Changer Method



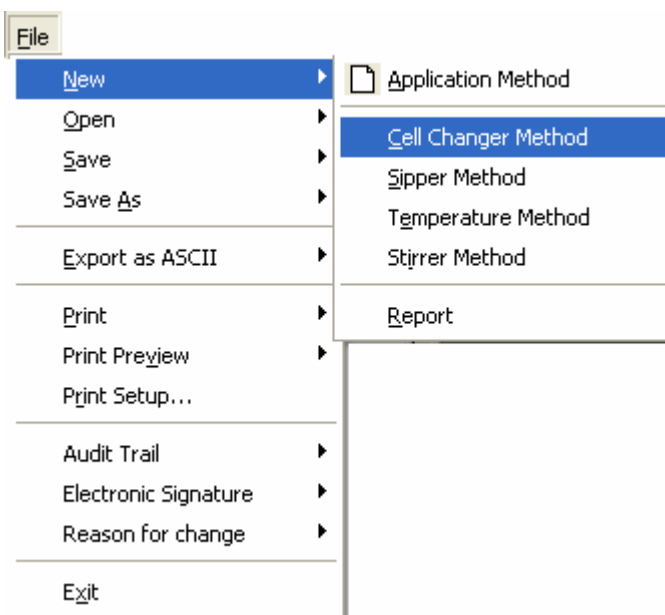
When a cell changer is installed, its icon appears on the status bar.



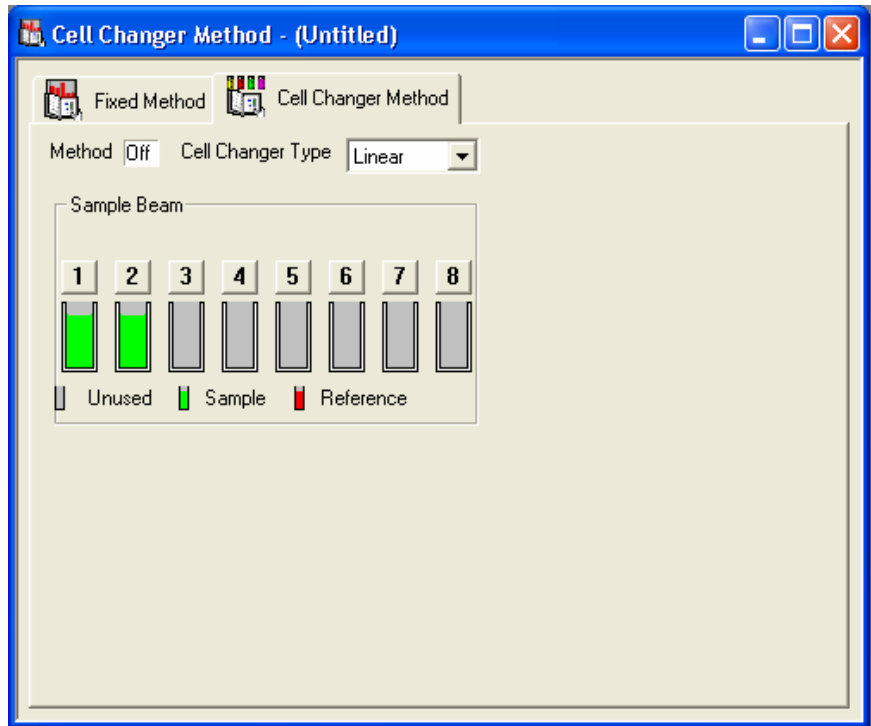
If two cell changers are installed (7-Cell Changers can be installed in the sample and reference positions), two cell changer icons will appear in the status bar.

The number shows the cell that is currently in the beam.

1. From the File menu select New then Cell Changer Method.

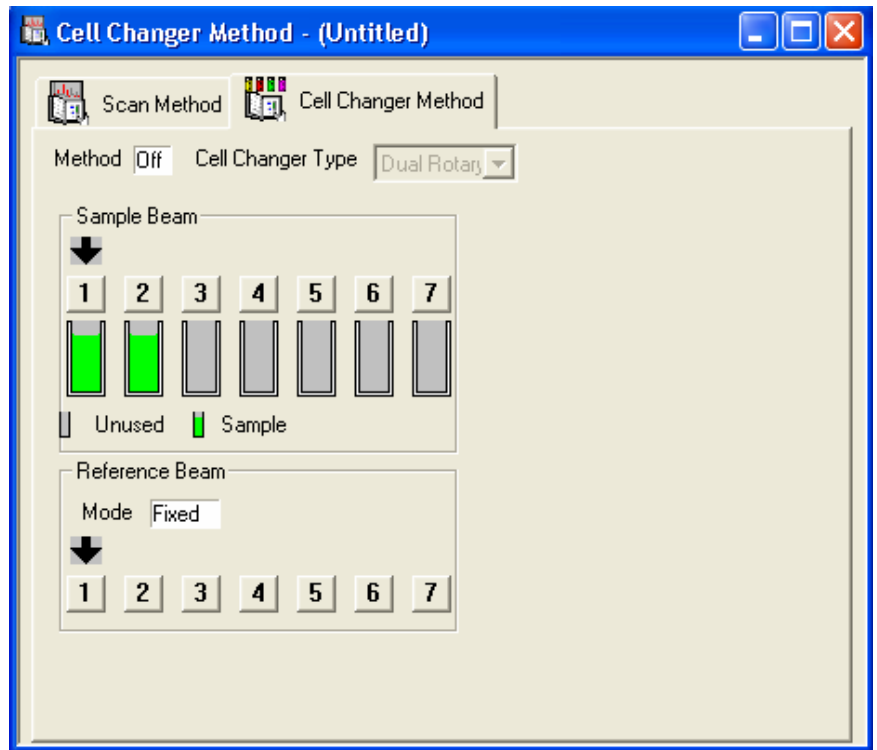


2. The Cell Changer Method opens as an additional tab in the application method window.



- The **Cell Changer Type** box will show the type of cell changer that is currently installed.
 - Set up the **Sample Beam** cells. The available functions are Unused, Sample and reference. Clicking on a cell steps through these options.
 - Set up the **Reference Beam** cell changer if used.
3. **Save the Cell Changer method for future use if required.**
 4. **Click in the Method field to turn the method on.**
 5. **Move to the application method by clicking on its tab in the method window and set the number of samples.**
 - If the number of samples is greater than the number of positions in the cell changer, the software will pause and prompt for the next cell holder to be presented.

- If two cell changers are present, the changer in the reference beam has two options. The first is auto which moves the reference cell changer as the sample cell changer moves. The second is fixed where a single cell from the cell changer is used as a reference for all the cells in the sample beam.



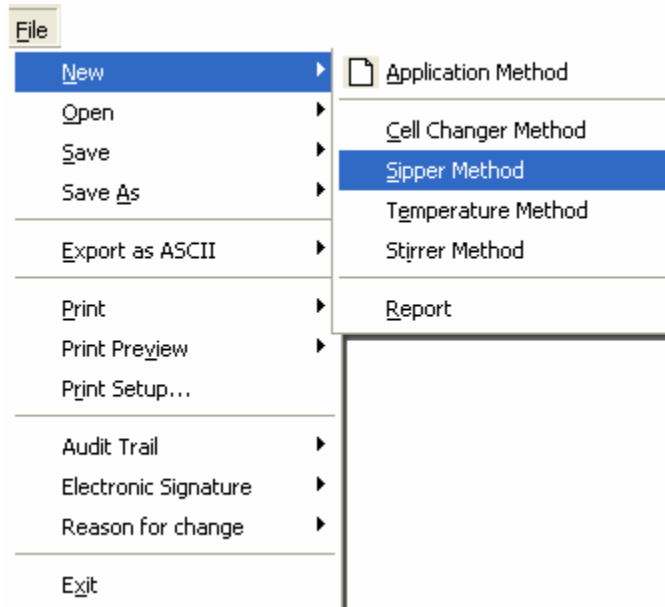
6. If you wish to remove an accessory method page from the Method window, right-click it to open the context menu, and click Delete.

Setting up a Sipper Method

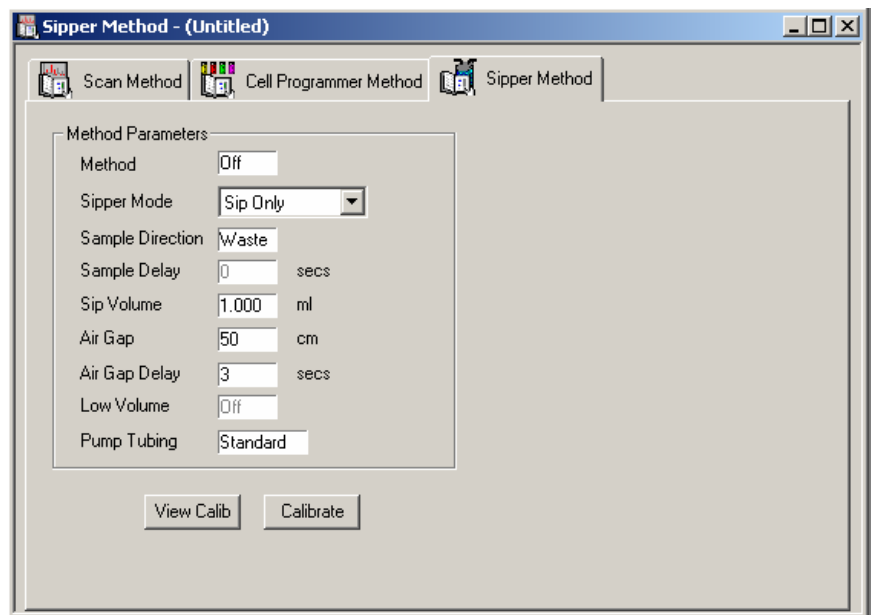


When a sipper is connected, its icon is present on the status bar.

1. To set up a new sipper method, select **New > Sipper Method** from the File menu.
 - If you wish to use an existing sipper method, select **Open > Sipper Method** from the File menu.



2. The Sipper Method opens as an additional tab in the application method window.



- Click in the box beside **Method** to turn the method **ON**.
- Select the **Sipper Mode** from the pull-down menu. Choose between:

Sip Only

Press the sipper switch to make the sip, and then click Run to make the measurement.

Sip and Run	Click Run to start the sipper method. The measurement follows automatically.
Continuous	After the switch has been pressed, the sipper pumps continuously until the switch is pressed again. This mode is used to flush out the system.

- Click in the box beside **Sample Direction** to toggle between:

Waste	The sample is pumped to waste after measurement.
Return	The sample is returned after measurement.

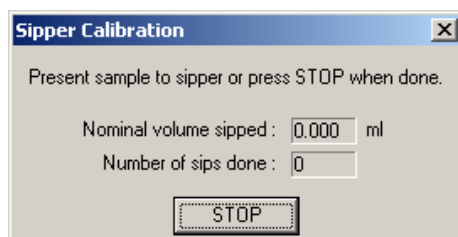
- Click in the boxes to edit the values of:

Sample Delay	Time between sipping and start of measurement (0 to 99 s)
Sip Volume	Volume of sample to be sipped (0.2 to 10ml).
Air Gap	Length of air gap (0 to 500cm).
Air Gap Delay	Delay between sipping sample and pumping air gap (1 to 20 s)

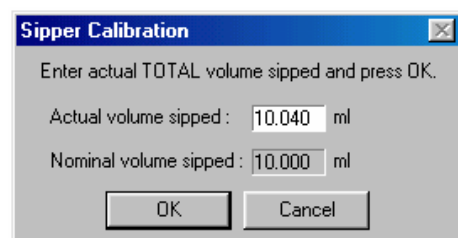
- Leave **Low Volume** set to **OFF** unless narrow diameter (0.8mm) uptake tube is being used.

3. Calibrate the sipper as follows:

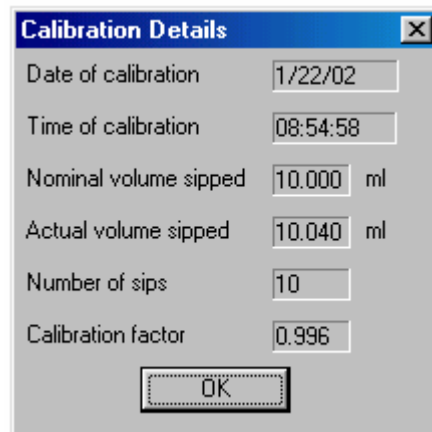
- Click the **Calibrate** button on the sipper method page. This opens the Sipper Calibration window.



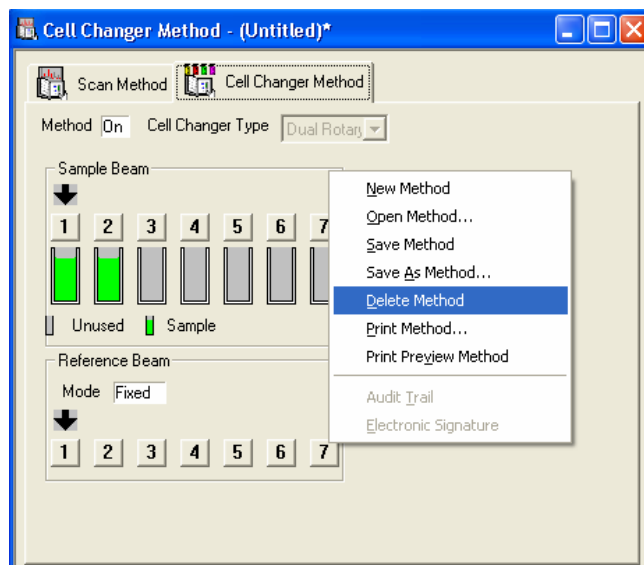
- Put some water into a suitable graduated container (e.g., a graduated cylinder) and record the volume. Present the container to the sipper and press the sipper switch. Follow the on-screen instructions. The sipper will sip the volume and air gap set in the method. The Volume and Number of Sips Done will be updated. Press the switch again. Continue until a suitable number of sips have been done (e.g., 10). Click the **STOP** button.



- Measure the volume of water remaining and hence calculate the total volume that has been sipped. Enter this value into the Actual Volume Sipped field and click OK.
- The software will calculate the Calibration Factor. This factor will be used until the sipper is calibrated again.



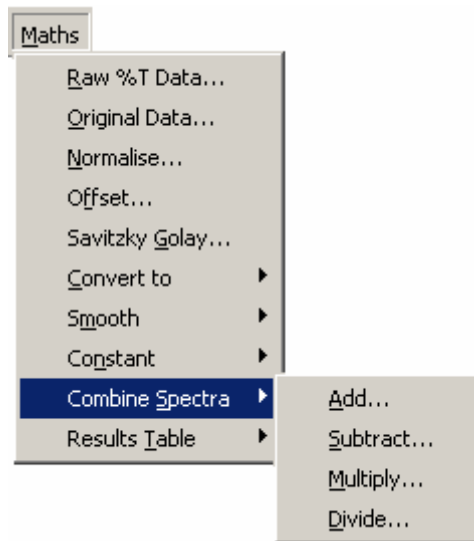
4. The current sipper calibration may be viewed by clicking on the View Calib button on the Sipper Method page.
5. The sipper must be recalibrated when the tubing is changed. Recalibration is periodically advisable to compensate for aging in the pump element tubing.
6. If you wish to remove an accessory method page from the Method window, right-click it to open the context menu, and click Delete.



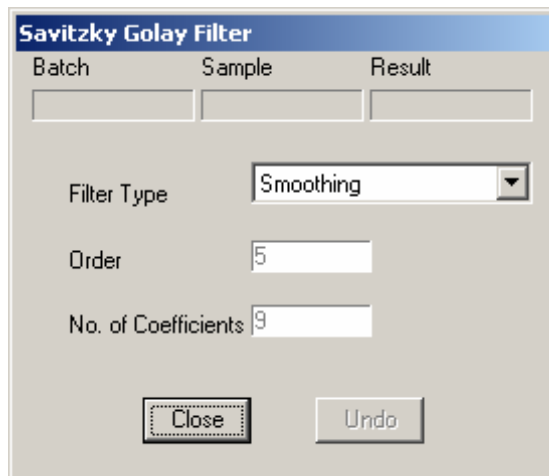
Using Math Functions

A full range of calculations and manipulations is available for post-run analysis in the Math menu. The options available options will depend on the application being used.

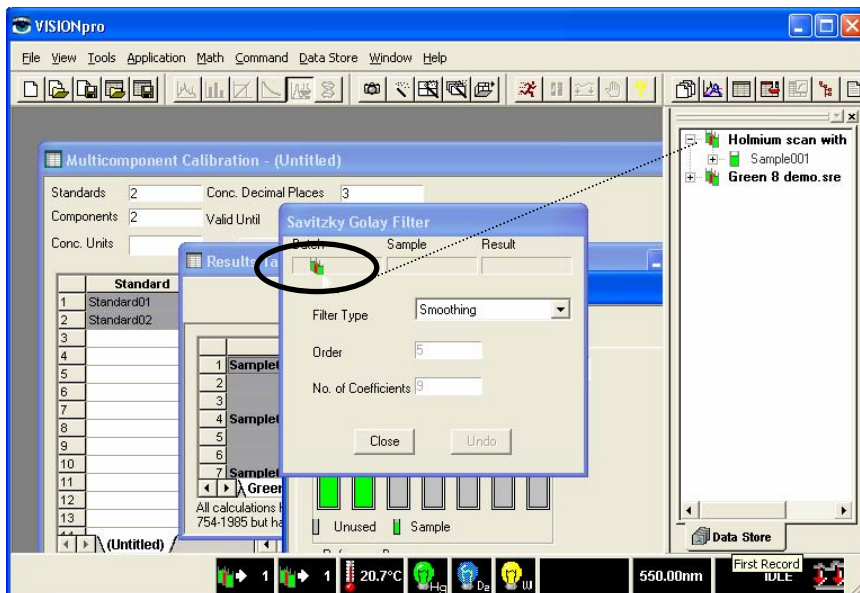
1. **Click Math in the Main Menu Bar and select the desired calculation or manipulation from the main Math menu or from one of its sub-menus.**



2. **When you click the required function, a Math manipulation window will open.**

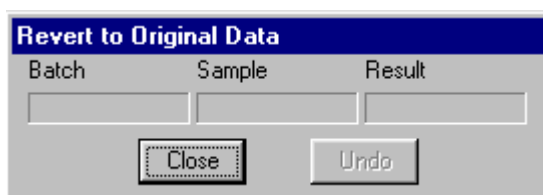


3. Drag the batch, sample or cycle from the Data Store to its space in the manipulation window.



4. The calculation or manipulation will be carried out. The effect of the manipulation will be shown in the Graph window or Data Store, as applicable.
5. You now have the following options:
 - Click Close to accept the result of the calculations or manipulation and close the window.
 - Click Undo to undo the current calculation or manipulation.
 - Convert another batch, sample or cycle. You will not then be able to undo the calculation or manipulation you just performed.
6. The original data have not been lost and may be retrieved at any time by selecting Original Data from the Math menu.

Convert the data by dragging it to the Math window as above.



7. If you need to keep a copy of your original data in the Data Store at the same time as the results of manipulations, create a copy of the batch using the Copy Batch command in the Data Store menu. Perform the Math operations on the copy.

Getting Started with Advanced Results Calculations in *UVcalc*

The Results Table has spreadsheet-like functionality called *UVcalc* that allows customized calculations may be performed on the data.

Calculations and formatting instructions can be **attached** to the method as a template and **saved with the method**. The spreadsheet operations will then be carried out automatically each time the method is run.

Click the Template button on the application Method page to see the template.

1. **When Results are present, they will appear in the Results Table. Results may be generated at run time or post-run via the Math menu.**

	A	B	C	D	E	F	G	H
1	Sample001		1	2	3	4	5	
2	Cycle01	nm	361.00	419.00	446.00	453.00	460.00	
3	Peaks	A	0.641	0.200	1.797	0.686	0.803	
4								

Results Table - Holmium scan with peak pick.sre

Attach Sample001 A1

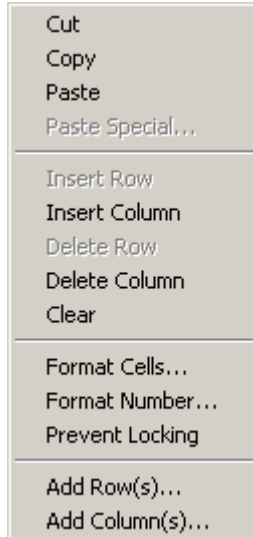
Holmium scan with peak pick.sre

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

2. Cells containing results have a gray background. The contents of these cells and their column headings cannot be used for calculations; however, they can be formatted.
3. Text, numeric values and formulae can be entered into the areas to the right of, and below, the gray shaded area in the Results Table.
4. Start *UVcalc* by clicking on Table > Edit *UVcalc* template.

5. Right-click in the Results Table to open the spreadsheet menu.

Operations that are not available in the current context will be grayed out.

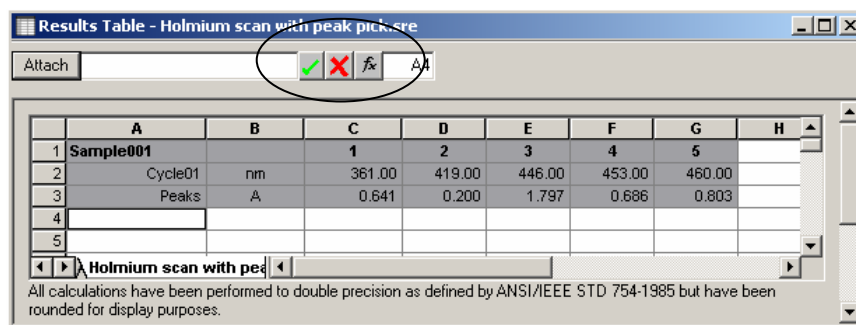


The operations are:

Item	Function
Editing	Cut, Copy, Paste and Paste Special are supported. The copy command can be used to transfer data to the other Windows applications via the clipboard.
Insert and Delete	Rows and columns may be inserted or deleted, or the contents of the selected area may be cleared. New row(s) will be inserted above the selected row(s). New column(s) will be inserted to the left of the highlighted column. Note: New cells may not be inserted into the gray shaded Results Area and the contents of the cells in this area may not be cleared.
Cell Formatting commands	Click Format Cells to open a tabbed dialog from which the font, colors, borders and alignment may be formatted.
Number Formatting	Clicking on Format Number will open a dialog from which it is possible to choose the number of decimal places to be displayed, and to specify whether the number will be displayed in floating point, scientific or compact notation (trailing zeros suppressed). Max of 15 decimal places.

Item	Function
Prevent Locking	The selected area will not be locked when the method is locked, and can be edited
Add Rows or Columns	The specified number of rows is added to the bottom of the spreadsheet, and columns to the right of the spreadsheet. Use this command if the default spreadsheet is not big enough.

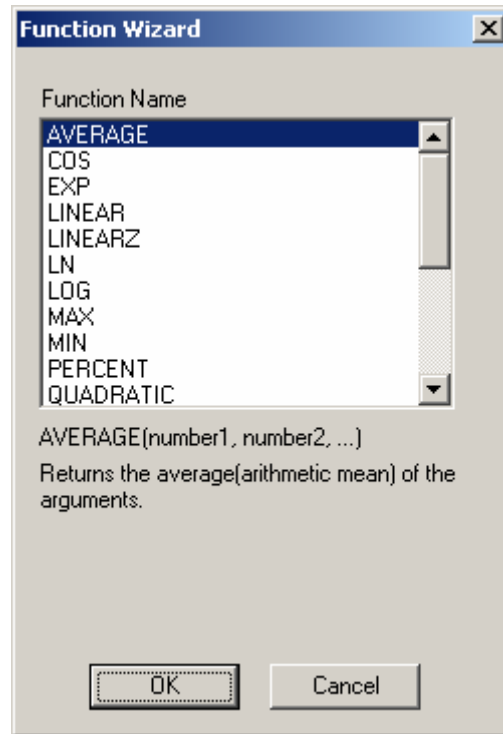
To **enter numbers, text or formula** into the spreadsheet, double-click in the required cell. Three new buttons appear as shown and the cursor is moved into the editing field.



Button	Function
	Enter the formula from the Edit field into the spreadsheet.
	Clear the current formula
	Open the Function Wizard

The box at the right-hand end of the group shows the address of the currently selected cell.

The **Function Wizard** enables you build up a sequence of functions into a formula.



- The available functions are listed in the scrollable window.
- The **name** of the selected function, its **syntax** and a description of its **operation** are displayed in the area below the scrollable window.
- Enter a function by selecting it in the Wizard and clicking on the OK button. The function will appear in the Edit Window with the cursor in the right position to enter the arguments. The arguments may be numbers or references to cells containing numeric values. Cell addresses (Column Row) and numbers must be entered explicitly from the PC keyboard.

The following guidelines apply when building up a formula in the Editing Area:

- First type an equals sign (=) into the edit field. Without the equal sign, the contents of the edit field will be treated as text.
- Simple arithmetic operators (+ - * /) are entered directly from the keyboard.
- You can refer to cells in the following ways:

- Specify the address of a single cell (e.g., B7).
- Specify a range of cells, e.g. A1:A5 refers to cells A1, A2, A3, A4 and A5.
- Specify a set of non-contiguous cells (e.g., C3, C7, C9 refers to cells C3, C7 and C9).
- All cells in a range of cells must be in the same row or column. Blocks of cells covering multiple rows or columns will generate an error message.
- Functions may be linked with arithmetic operators.
- Brackets (parentheses) are supported.

Producing Printed Output

VISION provides you with two methods of producing printed output: the **Print command** and the **Report Composer**.

Print

Individual items, such as the application method or the results, may be selected and printed via the **Print** command in the File menu or by right-clicking on a printable object and selecting Print or Print Preview from the context menu.

- Items which are not available for printing in the current context will be grayed out.
- **Print Preview** may be used to see the appearance of the page before it is printed.
- Use **Print Setup** to choose the paper size and orientation and to set printer options.

Report Composer

The Report Composer automates the process of producing quality, customized reports.

1. To start a new report, select New > Report from the File menu.

- A blank Report Composer window will open and a Report item will be added to the Main Menu Bar.

2. To add components to the template go to the Report menu and select Add Item. Click your choice in the menu or sub-menu.

- You will be returned to the Report Composer window. The cursor will have changed to crosshairs. Place the crosshairs where you want the top left-hand corner of the item to be, then **click and drag a rectangle to contain the item.**
- The rectangle can be re-sized by dragging its handles, and can be dragged to change its position in the report. If the rectangle is too small, not all of the chosen item will be displayed. You can either re-size the rectangle until all of the contents are displayed or use the arrow keys to scroll the text through the rectangle so that the required part is in view. Graphs will be re-sized to fit the designated area when printed.
- The Edit Master Page item enables you to insert items that will appear on every page of your report (e.g., headers and footers or a company logo).
- **Page numbering** can be toggled on and off with the Page Numbering item.
- When **Auto Print** is enabled a report will be printed automatically after each batch of samples has been run.
- To delete an item from the template select it and press the Delete key on the PC keyboard.

3. The Insert New Object command enables objects from other Windows applications to be linked to or embedded in the report.

- This facility can be used to insert a company logo, formatted text or a table from a spreadsheet into the report.

4. **When the content and layout of the report are as required it may be printed via the Print > Report command in the File menu.**

The Report Template may be **saved** using Save As > Report Template in the File menu. When it is re-opened the layout will be preserved and the contents of the included items will be those current in VISION at the time that the template is re-opened.