

Getting Started with TQ Analyst

This tutorial introduces TQ Analyst, a sophisticated yet easy to use software package for developing analytical methods for spectral applications, including mid-infrared, near-infrared, far-infrared, and raman. This tutorial introduces the basics of ...

- The TQ Analyst window
- The menu bar
- The tool bar
- Method windows
- TQ Analyst methods
- TQ Analyst wizards.

Expert help

With TQ Analyst, you don't have to be an expert analyst to create methods that really perform. Our Help package includes tools for basic training in method development, plus a set of example methods.

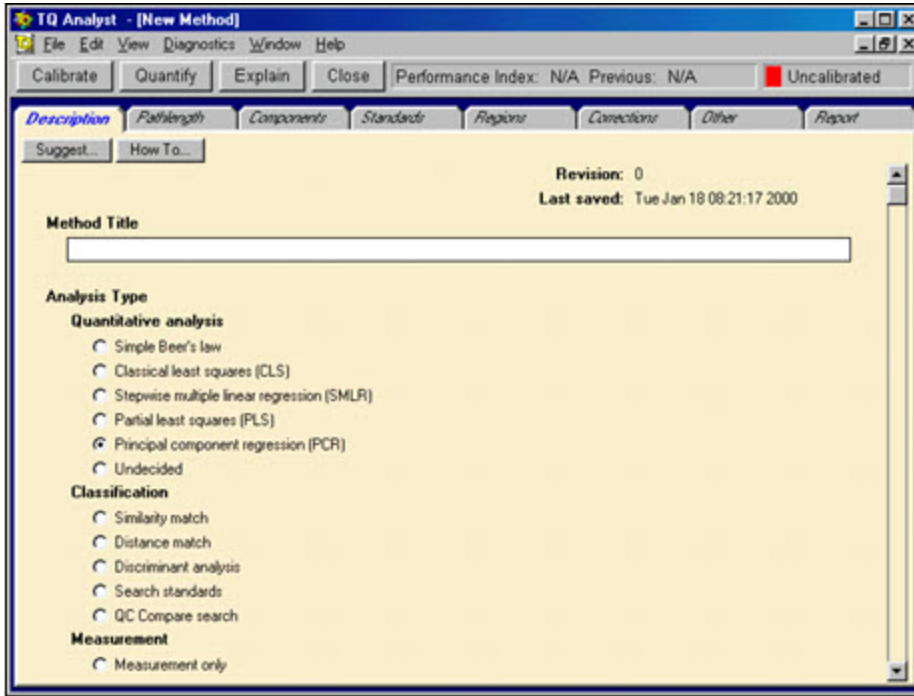
You can also take advantage of TQ Analyst's "suggest" wizards and performance index to get answers to your most important questions (like how to optimize a method to perform best with your samples).

While you are using TQ Analyst, you won't have to waste time searching for bits of information about how a software feature works or when it should be used. TQ Analyst's Explain help window provides truly helpful information instantly on any feature you select.

TQ Analyst window

The TO Analyst window is displayed immediately after you start the TO Analyst application.

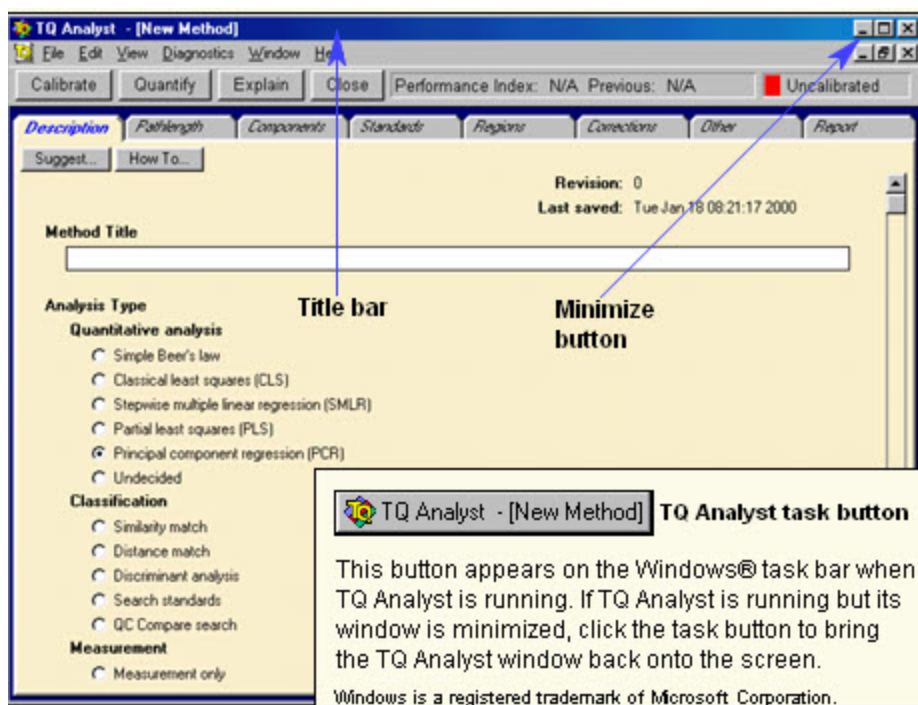
Your TQ Analyst window should look similar to the one shown at the left.



The title bar

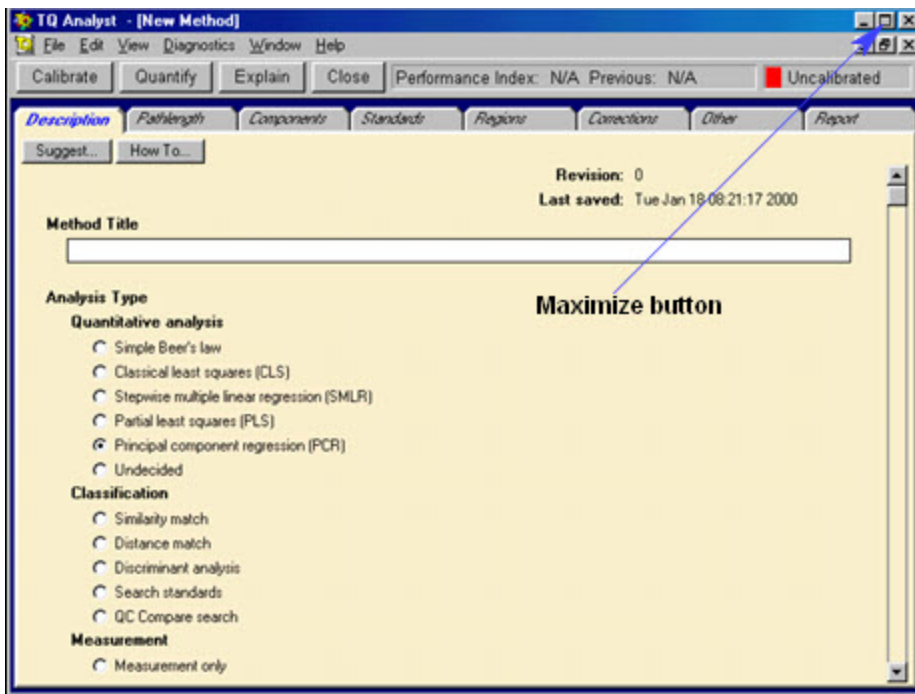
The title bar provides controls for the TQ Analyst window.

Click the Minimize button to run TQ Analyst in the background and leave your display screen free for viewing other programs. Click the TQ Analyst task button to bring TQ Analyst back onto the screen.



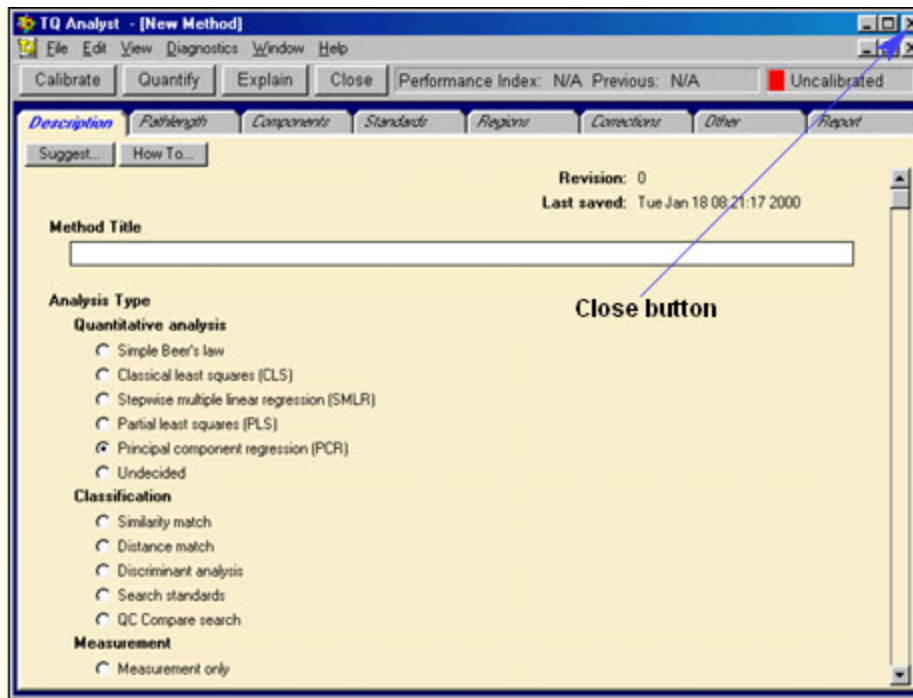
Maximize button

Use the Maximize button to change the size of the TO Analyst window. Click the Maximize button to toggle between the Full Size and Custom Size settings. Full Size expands the window to fill the screen. Custom Size allows you to drag the window's right, left and bottom borders to achieve the desired size.



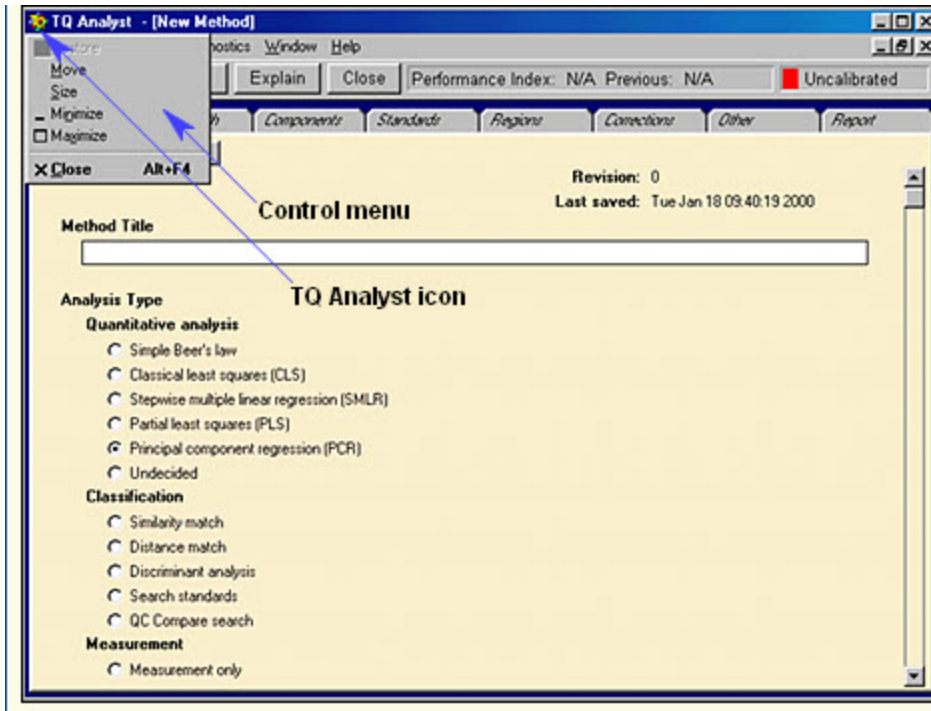
Close button

The Close button closes the window and exits the TQ Analyst application.



Control menu

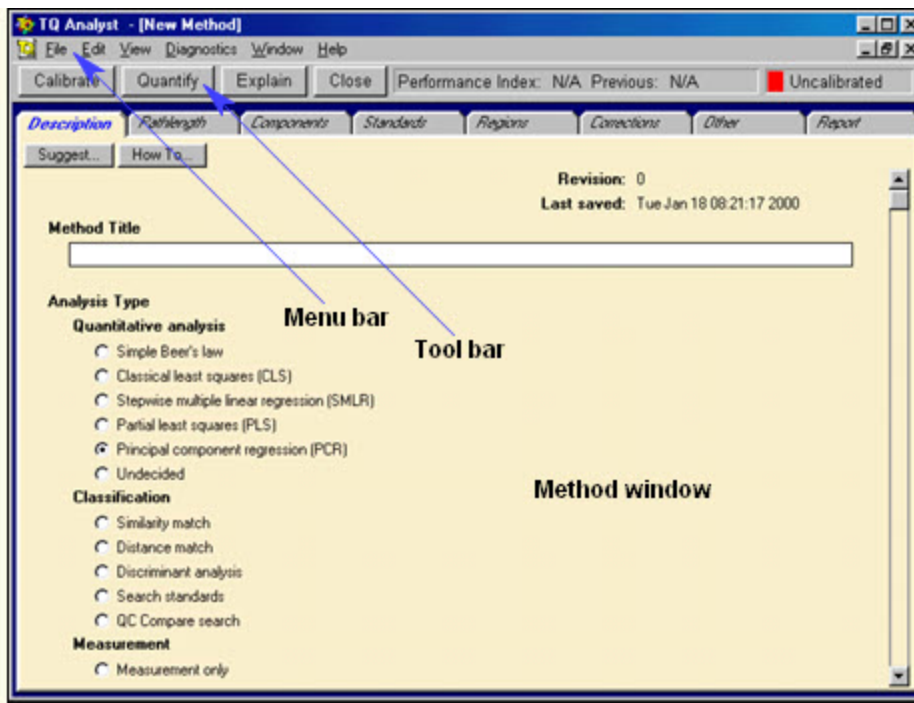
Click the TQ Analyze icon to display the TQ Analyst control menu. These commands affect the TQ Analyst window.



Main components

The TQ Analyst window is divided into three parts:

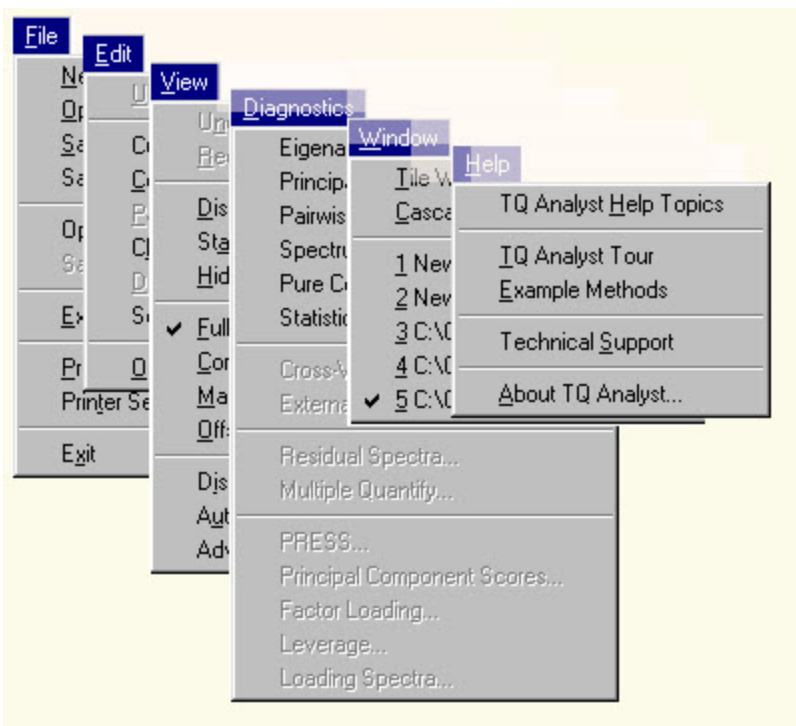
- The menu bar
- The tool bar, and
- The method window



Menu bar

The menu bar contains menus of useful commands for working with TO Analyst method files and spectral data. You will also find a menu of diagnostic commands which can be used to evaluate your method as you develop it.

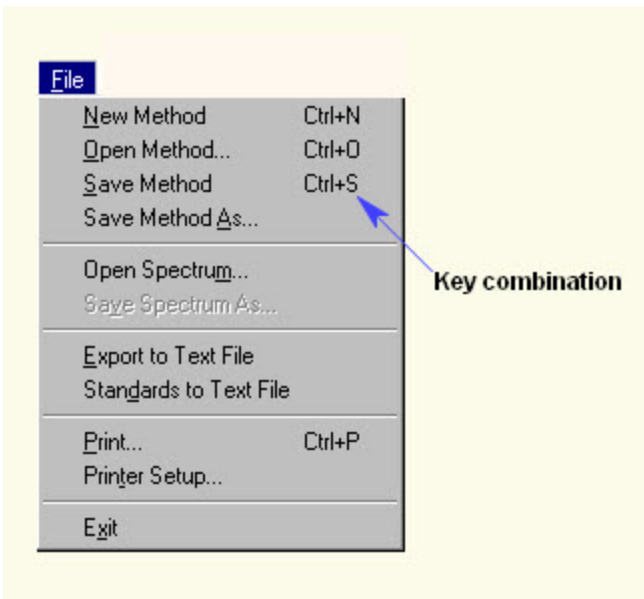
The Help menu allows you to access TQ Analyst's extensive online help system any time you need information.



CHOOSING MENU COMMANDS

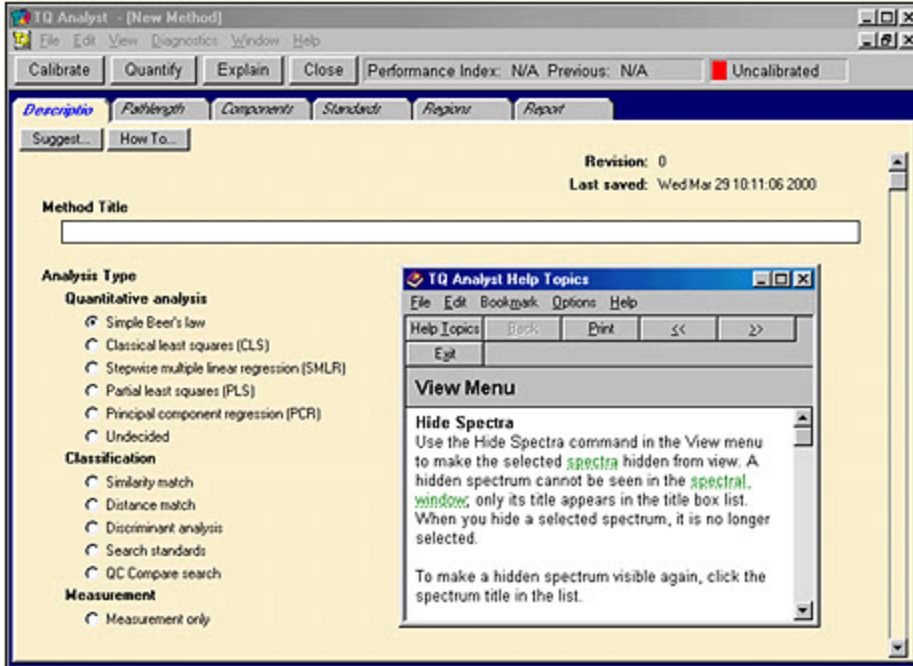
You can choose commands in TO Analyst menus just as in other Windows applications: by using the mouse or by typing key combinations on the keyboard.

The key combinations are shown in the menus.



GETTING HELP INFORMATION FOR A MENU COMMAND

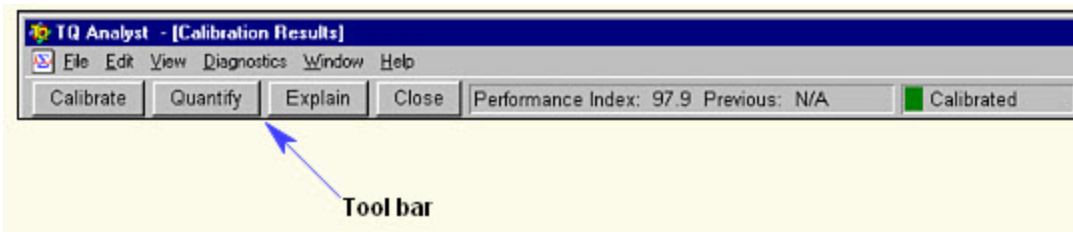
Use the F1 key on your keyboard to display help information about any menu command. To display the help screen for a menu command, click the menu and use the down arrow key on your keyboard to highlight the command in the menu. Then press F1.



Tool bar

The tool bar contains buttons for calibrating a method, quantifying a sample spectrum, opening the Explain help window, and closing the active window.

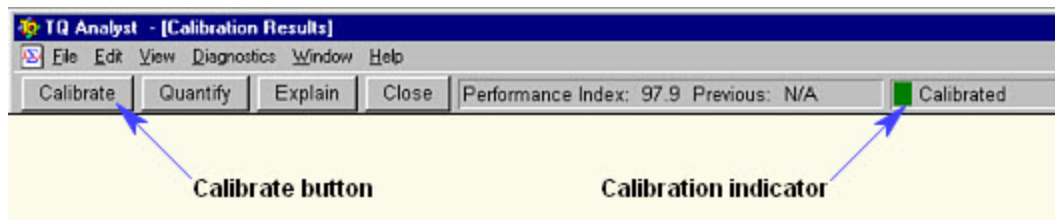
To use a feature on the tool bar, click the appropriate button.



CALIBRATE BUTTON

The Calibrate button calibrates the active method. Calibration may take 1 second or several hours, depending on the method type and the number of standards. When calibration is

complete, the calibration indicator on the tool bar changes from red to green and the "Uncalibrated" message changes to "Calibrated."

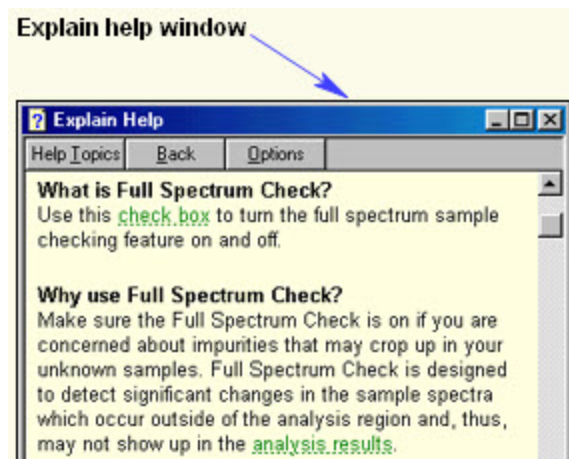


QUANTIFY BUTTON

Use the Quantify button to quickly analyze a single spectrum using the active method.

EXPLAIN BUTTON

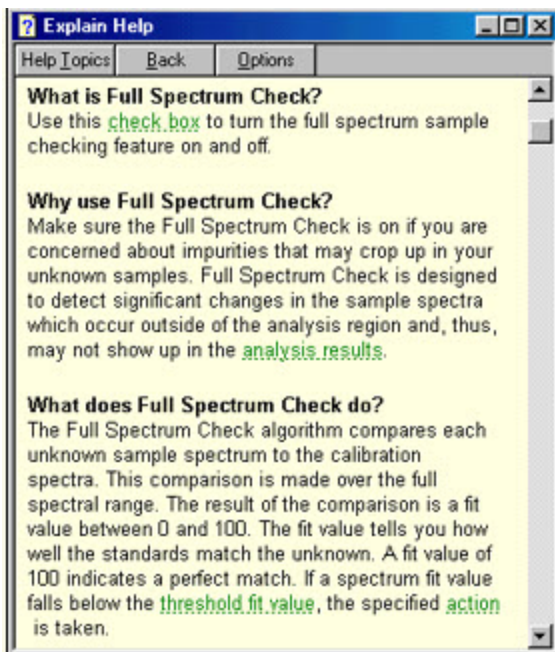
The Explain button opens and closes the Explain help window, which provides in-depth information about TQ Analyst software features. To display information about an item in the TQ Analyst window, open the Explain help window and then use the mouse to select the item.



EXPLAIN HELP WINDOW

Three characteristics of the selected item are typically provided in the Explain help window: a definition of the item, a description of how it works, and tips on when the item should be used.

To display help information for another item in the TO Analyst window, use the mouse to click the item. The information provided in the Explain help window is updated automatically each time a new software item is selected.

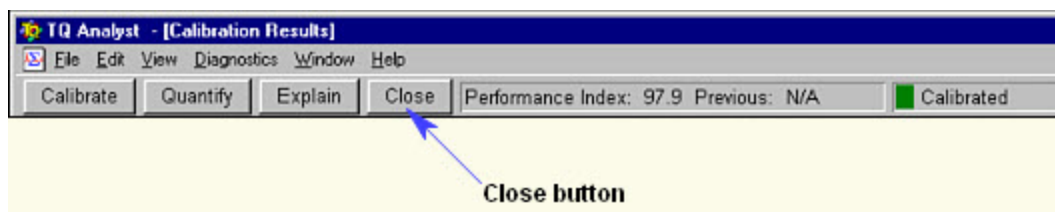


If you want to read about an item such as an action button without activating it, use the right mouse button to click the item. The Explain window will be updated but the status of the feature you clicked will not be changed.

Keep the Explain window open as you work if you think you may need information about other features in the TQ Analyst window. If the Explain window is in your way, you can easily move it by clicking and dragging its title bar or close it by clicking its Close button.

CLOSE BUTTON

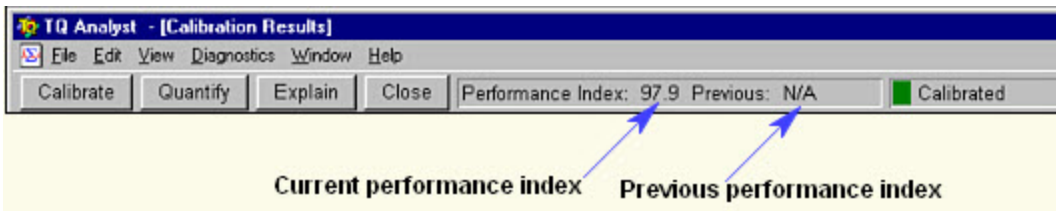
Use the Close button to close the active TQ Analyst window.



PERFORMANCE INDEX

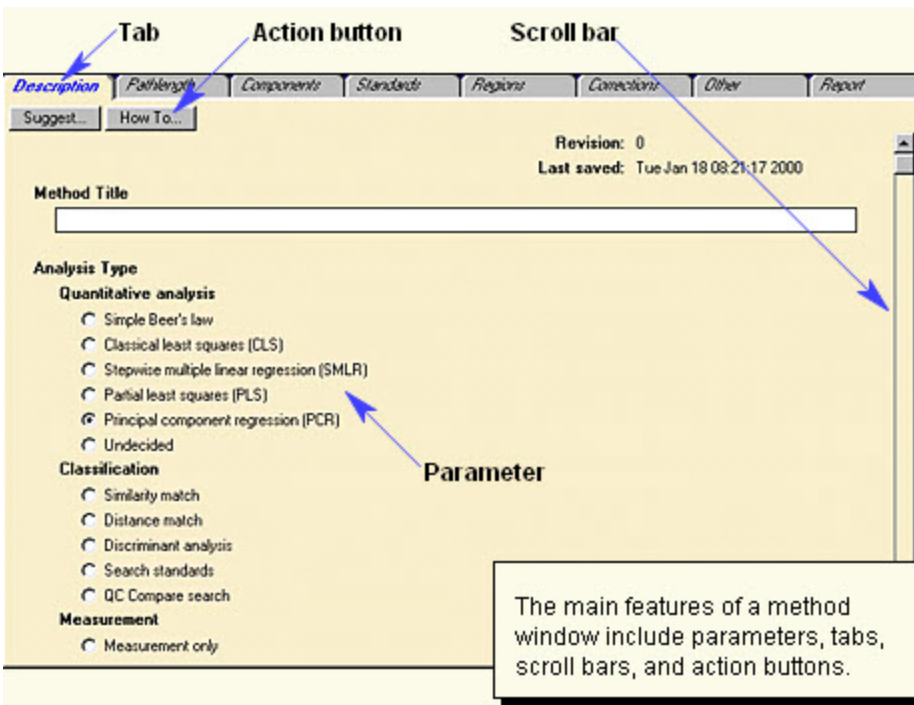
When a method is calibrated, it is assigned a performance index which appears on the tool bar. The performance index is simply a number that indicates how well the method works.

If you calibrate the same method more than once, the performance index for the previous calibration is also displayed



Method windows

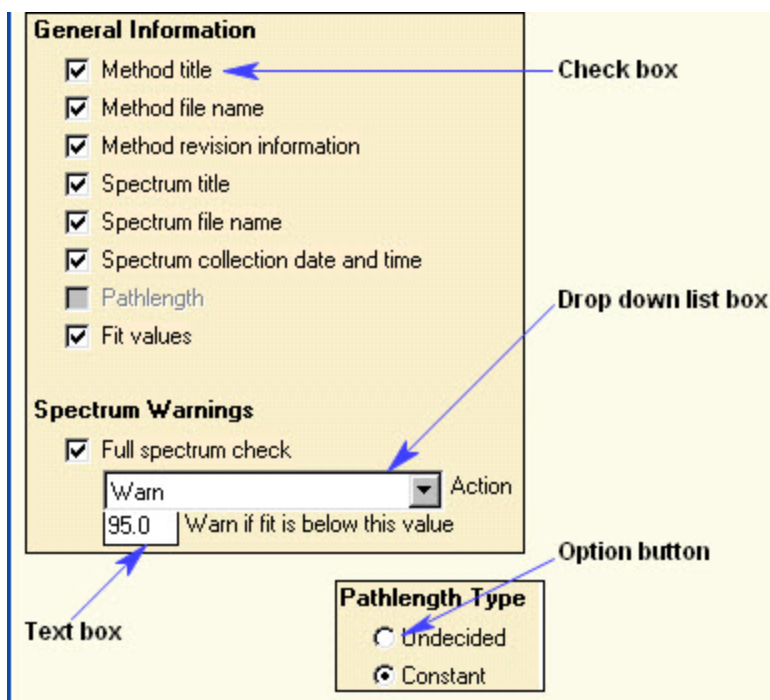
The main portion of the TQ Analyst window may be used to display method windows. A method window contains all of the information and functions needed to create a TQ Analyst method.



PARAMETERS

The method parameters specify how the method will work. There are several types of parameters, including text boxes, option buttons, check boxes and drop down list boxes.

Parameters that must be set multiple times, for each component or standard used in a method for example, are often placed in a table. You will see examples of this later in the tour.



TABS

The method parameters are grouped by function.

Each group of parameters is contained on a file card which has a tab that is always visible at the top of the method window.

When you first create or open a new method, the Description tab, which contains the first group of method parameters, is already selected.

CHOOSING TABS

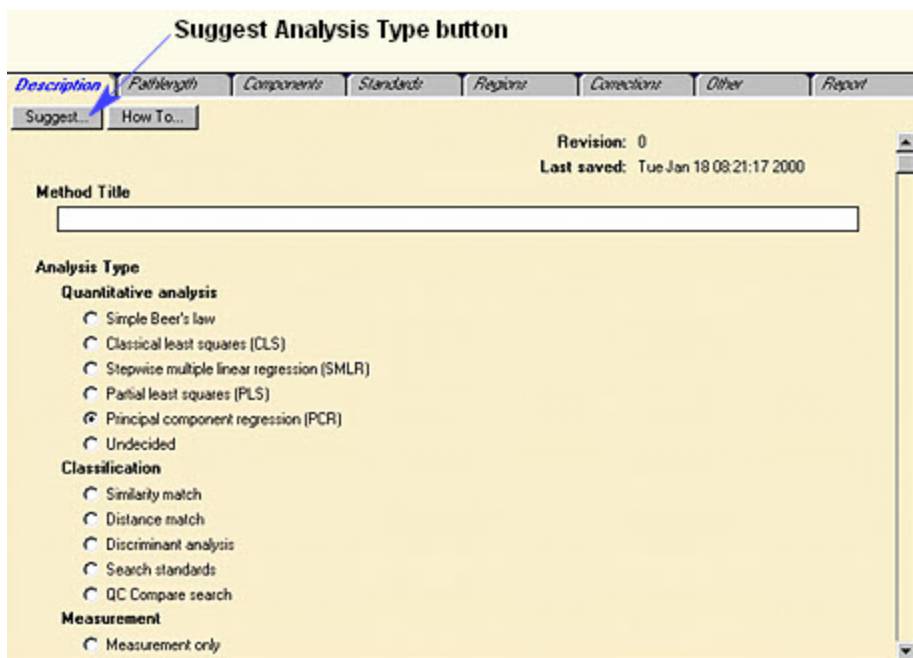
To display a group of method parameters, click the corresponding tab. The file card containing the parameters is brought to the front.

The parameters on a tab work together to specify important features of your TO Analyst methods.



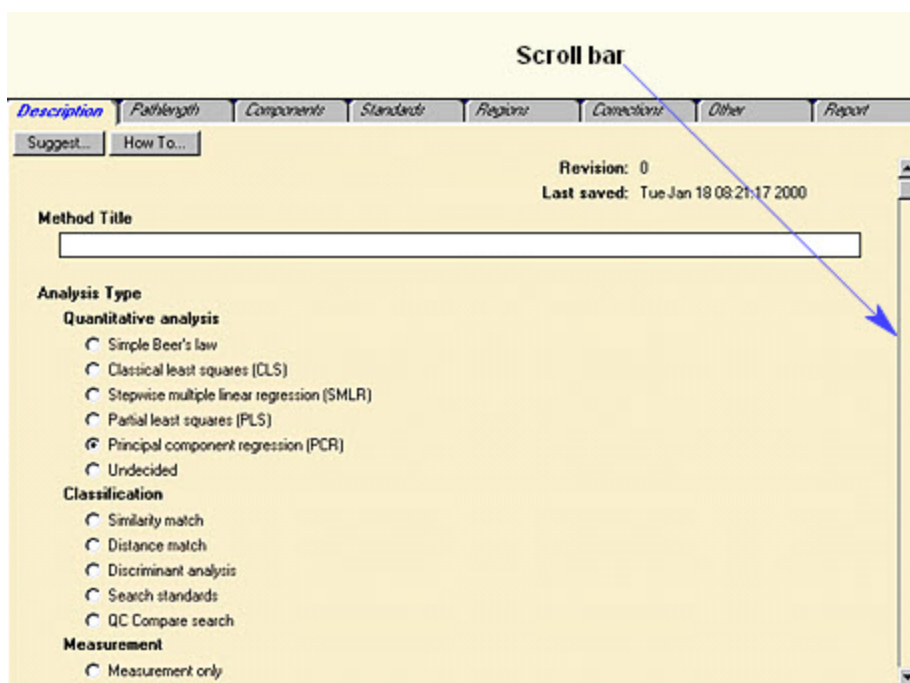
ACTION BUTTONS

When you select a tab, one or more buttons may appear below the tab name. These buttons, called "action buttons," allow you to perform tasks related to the active tab. For example, the "Suggest Analysis Type" button on the Description tab can help you set the Analysis Type parameter.



SCROLL BARS

A scroll bar may appear along the right side or bottom of the active tab when the tab contains more features than will fit in the window. You can use the scroll bars to move the tab's contents up and down or right and left in order to bring additional features into view.



SEQUENCE OF THE TABS

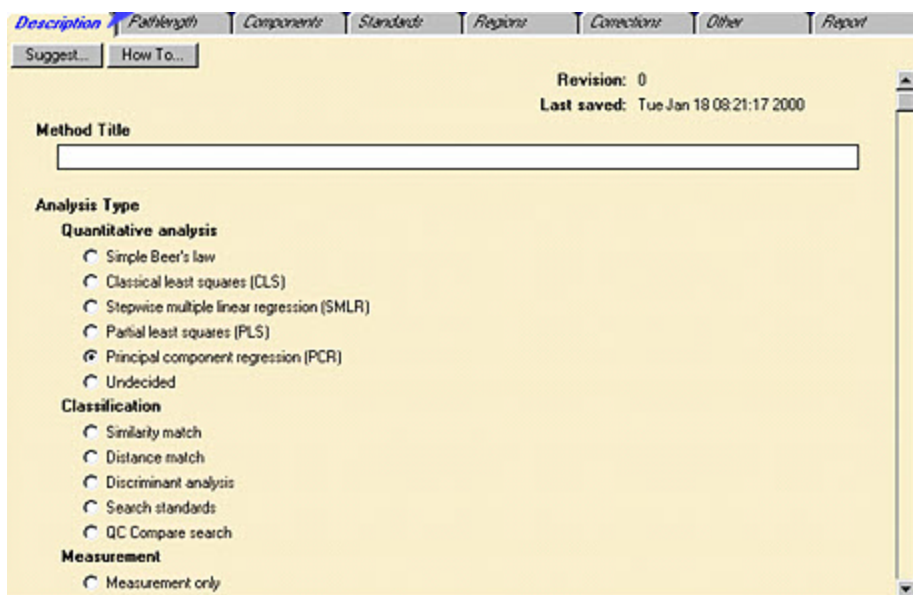
The tabs are arranged in an order that is convenient for creating a TQ Analyst method. If you select the tabs in sequence from left to right starting with the Description tab, they will lead you step-by-step through the method development process.

Start with the parameters on the Description tab. Then continue with the Pathlength tab and so on until all of the parameters have been set.

Description tab

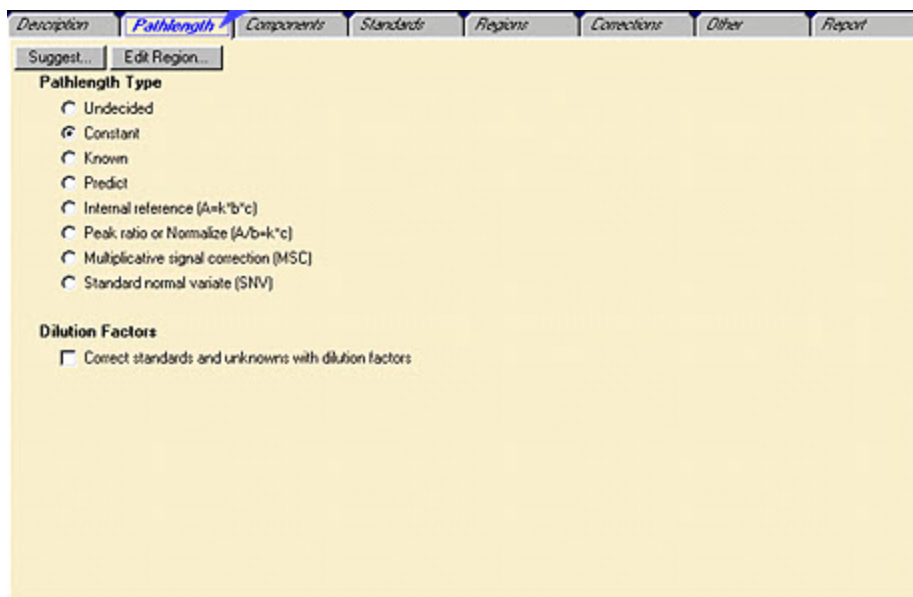
Use the parameters on the Description tab to enter general information about your method.

A method can be described by its title, developer, revision number, revision date, and analysis type. A longer description can also be entered, if needed.



Pathlength tab

The parameters on the Pathlength tab define how the active method will determine sample pathlength or thickness. Sample pathlength is important to most analytical experiments because the intensities of the peaks in a sample spectrum are determined by the sample's thickness as well as its composition.



Components tab

The Components tab provides a convenient table for entering information about the components in a quantitative method, such as the component names and concentrations. For classification

and spectral measurement methods, the components tab is replaced by the Classes or Measurements tab.

Assess Feasibility...

Concentration Limits

- Use analysis limits
- Use acceptance limits

Concentration Constraints

- Force concentration values in Quantity result to sum to a constant (typically 100%)

Component Interaction

- None (use for measuring sample properties)
- Some (use for measuring component concentrations)

Components Table

Index	Component Name	Abbrev.	Unit	Digits	Analysis Low	Analysis High	Uncertainty Li
1	Glucose	Glu	wt %	2	0.00	3.00	10
2	Benzoic acid	BA	wt %	2	0.00	3.00	10
3	Propanediol	Pro	wt %	2	0.00	5.00	10
4	Glycerol	Gly	wt %	2	0.00	4.00	10
5							

Standards tab

The Standards tab has a table for specifying the standards that will be used to calibrate, validate, or correct the components in a quantitative method.

For classification methods, the standards define the properties of each class. Spectral measurement method do not use standards.

Standards

- Show spectrum titles
- Show spectrum file names
- Allow spectral processing
- Show processed spectra in View Standards
- Restrict Y-axis range in unprocessed spectra for calibration and diagnostics
 Start End

Standards Table

Index	Display	Spectrum Title	Usage	Glucose wt %	BA wt %	Pro wt %	Glycerol wt %
1		pls example; standard 1	Calibration	1.94	0.99	1.92	2.17
2		pls example; standard 2	Calibration	1.26	0.50	4.01	2.47
3		pls example; standard 3	Validation	2.59	0.57	1.49	3.04
4		pls example; standard 4	Calibration	0.36	2.01	2.69	1.41
5		pls example; standard 5	Validation	1.55	0.77	2.54	2.79
6		pls example; standard 6	Calibration	1.13	1.12	4.14	0.86
7		pls example; standard 7	Validation	2.25	0.39	3.03	1.61
8		pls example; standard 8	Validation	2.22	0.70	3.59	0.75
9		pls example; standard 9	Calibration	1.69	1.12	2.91	2.46
10		pls example; standard 10	Calibration	1.36	0.90	2.87	2.22

Regions tab

Use the Regions tab to specify the spectral peaks or regions that will be used for the analysis. If no regions have been selected, TQ Analyst starts the Suggest Regions wizard when you open the Regions tab. To see the suggested peaks or regions for a method, click the Edit Regions button on the Regions tab.

Regions Table

Index	Region Type	Location	Baseline Type	Point 1	Point 2	Offset
1	Spectrum Range	1,735.62 - 977.73	None			
2						

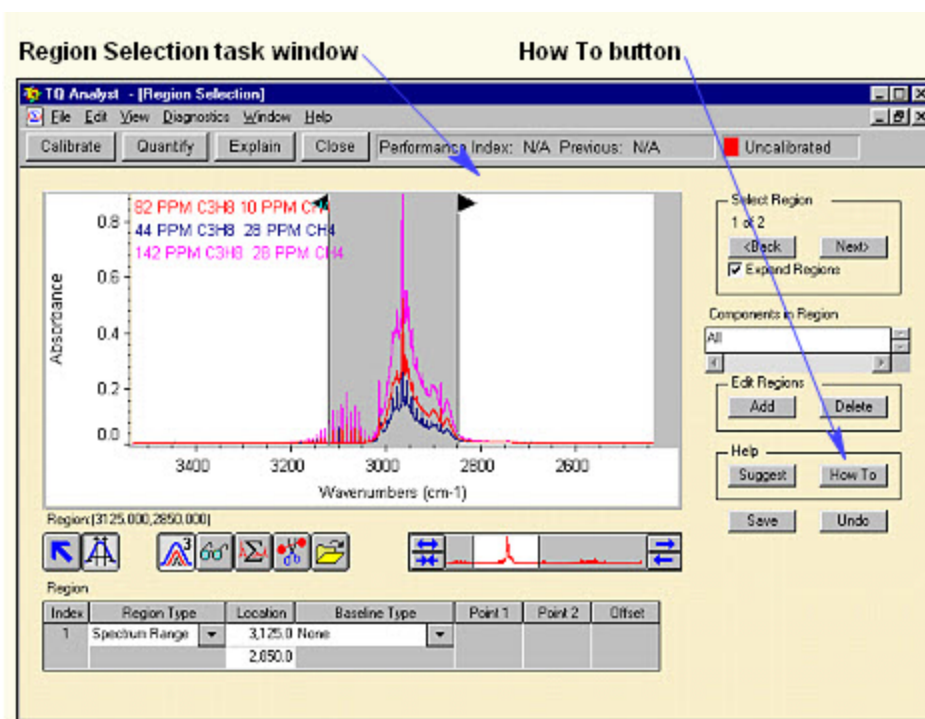
Components in Regions Table

Index	Measurement Location / Range	Glu	BA	Pro	Gly
1	1735.62 - 977.73	+	+	+	+

Viewing and editing regions

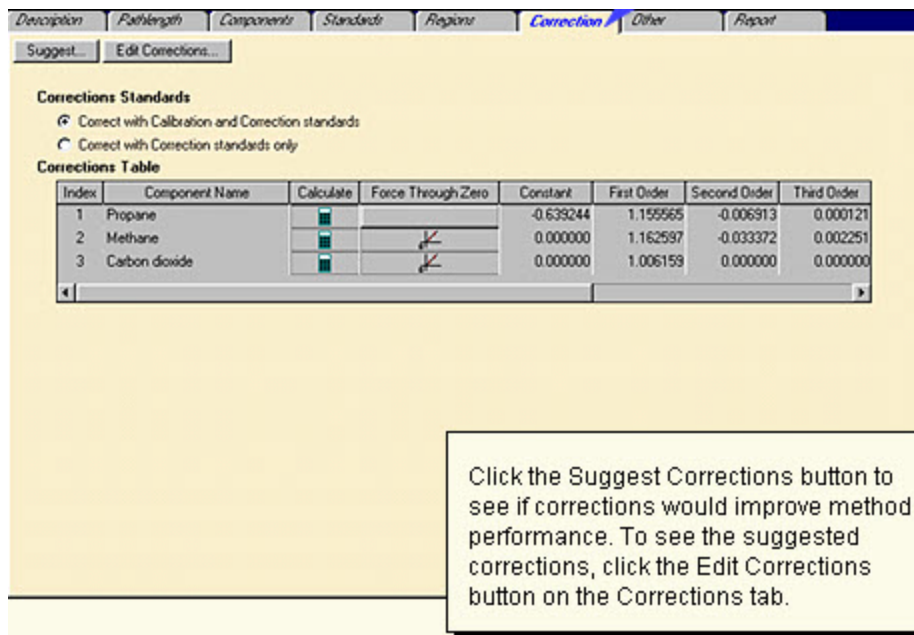
When you click Edit Regions, the Region Selection task window appears on the display.

Click the How To button in the task window to display the associated help information. Follow the instructions in the help window to learn how to edit the regions in your method.



Corrections tab

The Corrections tab can be used to set up a linearity or bias correction for one or more components in a method. When you use the method to analyze for a "corrected" component, a correction factor is extracted from the curve and applied to the component results before they are reported.



Viewing and editing corrections

When you click Edit Corrections, the Corrections task window appears on the display. Click the How To button in the task window to display the associated help information. Follow the instructions in the help window to learn how to edit the corrections curves in your method.

Corrections task window **How To button**

Performance Index: 98.0 Previous: 97.9 Calibrated

Act. x path. -0.4% Diff.

Uncorrected x Pathlength Actual x Pathlength

Corrections Standards

Index	Spectrum Title	Uncorrected	Actual	Corrected	% Differenc
1	82 PPM C3H8 10 PPM CH4	82.091	82.000	82.295	0.3
2	65 PPM C3H8 19 PPM CH4	64.891	65.000	64.938	-0.0
3	62 PPM C3H8 20 PPM CH4	61.984	62.000	61.910	-0.1
4	59 PPM C3H8 21.5 PPM CH4	58.775	59.000	58.788	-0.3
5	44 PPM C3H8 29 PPM CH4	43.760	44.000	43.057	-0.3
6	33 PPM C3H8 32.5 PPM CH4	32.778	33.000	33.104	0.3
7	2.0 PPM C3H8 49.5 PPM CH4	2.308	2.000	1.992	-0.3

Performance Index

Propene

Current: 98.6

Previous: 99.5

Help

How To Suggest

Save Changes

Coefficients

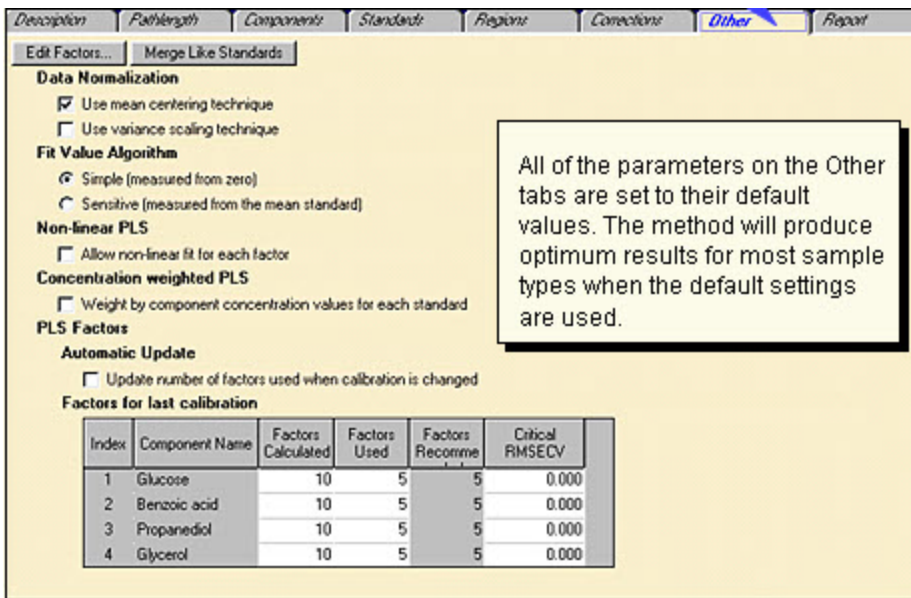
Constant	First Order	Second Order	Third Order	Fourth Order	Fifth Order
-0.638244	1.152665	-0.006913	0.000121	-0.000001	0.000000

Calculate coefficients after each calibration

Other tab

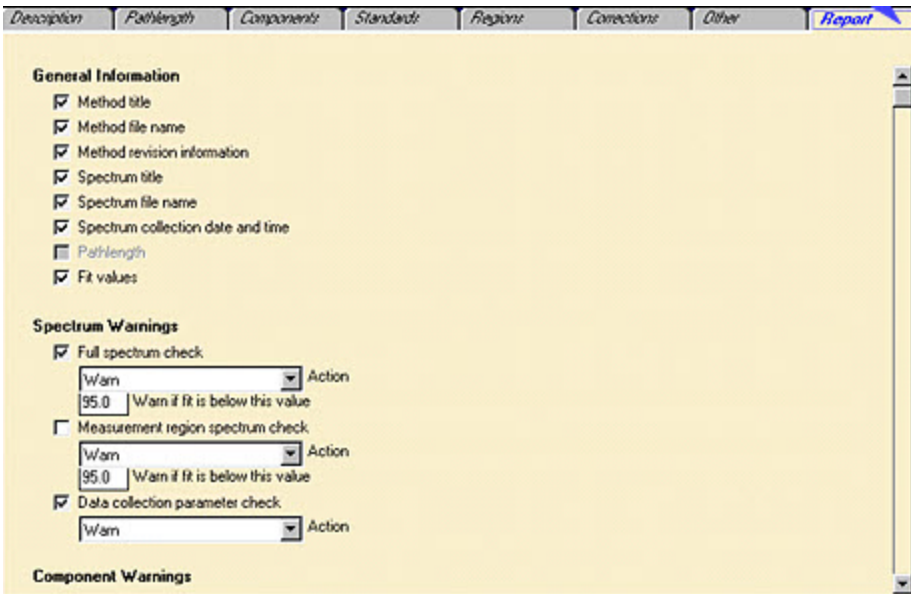
Use the parameters on this tab to customize the way your method calculates or reports the analysis results.

The Other tab is displayed for all analysis types except Simple Beer's Law and Measurement Only. The parameters that appear on the Other tab are different for each analysis type.



Report tab

The parameters on the Report tab allow you to choose the information you want to include in your sample reports, including any spectrum or component warnings.



TQ Analyst Professional Edition

The Analysis Type parameter on the Description tab defines the kind of results the method will produce when you use it to analyze a sample. If you have the Professional Edition of TO Analyst,

the algorithms that are typically used for predicting component concentrations are provided plus a number of others for classifying spectra based on a set of standards. You can also set up a method that simply measures a peak height or area or takes the ratio of two spectral peaks.

Analysis Type

Quantitative analysis

- Simple Beer's law
- Classical least squares (CLS)
- Stepwise multiple linear regression (SMLR)
- Partial least squares (PLS)
- Principal component regression (PCR)
- Undecided

Classification

- Similarity match
- Distance match
- Discriminant analysis
- Search standards
- QC Compare search

Measurement

- Measurement only

TQ Analyst EZ Edition

The EZ Edition of TQ Analyst includes the features needed to create and run the common quantitative and classification experiments. If you purchased the EZ Edition, some of the features described in this tour are not available in your software.

Analysis Type

Quantitative analysis

- Simple Beer's law
- Classical least squares (CLS) for peak heights and areas

Classification

- Similarity match
- Search standards
- QC Compare search

Measurement

- Measurement only

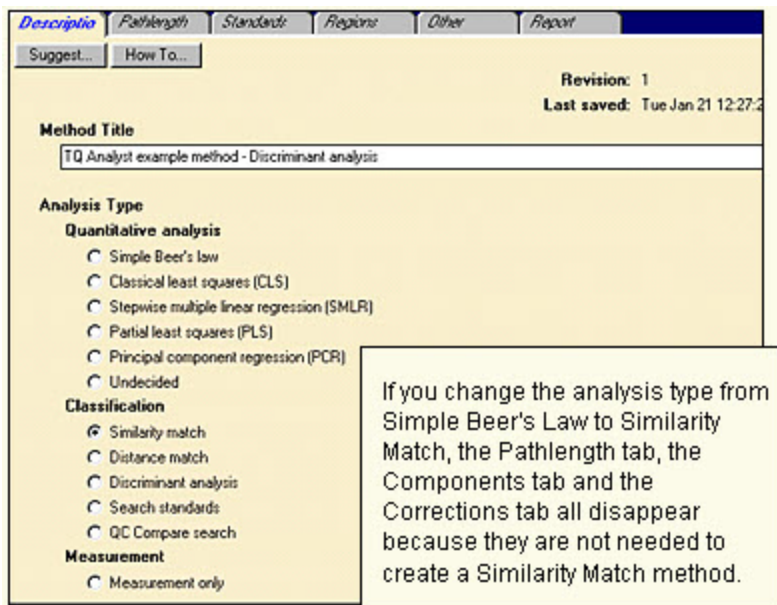
Selecting the analysis type

If you want information about one of the options for Analysis Type, click the Explain button on the TO Analyst tool bar and then use the mouse to select the option.

If you're not sure which analysis type is appropriate for your samples, set the Analysis Type to "undecided" and run the Suggest Analysis Type wizard. You must select the analysis type before you can calibrate a method.

Changing the analysis type

You are free to change the analysis type at any time, even after the method is calibrated. Each time you change the analysis type, the main TQ Analyst window is reconfigured so that only the method tabs and parameters which are needed to develop the type of method you selected are displayed on the screen.



A note about method parameters

Your method must contain valid settings for all of the method parameters before it can be calibrated.

When you create a new method, the method parameters are automatically set to their default values. You can change any of the parameter settings or use the default settings.

TQ Analyst wizards

You may have noticed that many of the method tabs contain a "suggest" button. The "suggest" features allow you to take advantage of Tq Analyst's built-in advisors for expert instruction on how to proceed with the tasks on the active tab. We've eliminated the guesswork from method design. If you're wondering which settings will give you the best answers, ask the TQ Analyst wizards for help.

Using "suggest" wizards

If a "suggest" wizard is available for the parameters on a particular tab, the suggest button will appear when the tab is selected.

To start the wizard, click the Suggest button.

The guidance you receive from a wizard depends on the tab that is currently active. For example, when the Suggest Standards button on the Standards tab is pressed, the wizard fills in the Standards table with the names and concentrations of the standards you should prepare and collect.

Other suggest wizards can help you select the proper analysis and pathlength type, choose spectral regions for the analysis, select factors for a partial least squares (PLS) or principle component regression (PCR) analysis, and decide whether to use a correction curve.

The wizards are designed to help you make the right choices each step of the way.

Where to go next

Now that you have reviewed the highlights of TQ Analyst, you are ready for the next phase of your training.

If you want a quick preview of the ins and outs of a particular analysis type, run the example method by choosing Example Methods from the TQ Analyst Help.

To create your first method

If you are already familiar with the basic techniques for sample analysis, you are ready to start building a method.

The first step is to create a new method file by choosing New Method from the File menu. When you create a new method file, the Description tab is automatically selected and all of the method parameters are set to their default values.