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IMACC QUANTIFY

1.0 Introduction

IMACC Quantify is a software application that allows the user to develop spectral processing methods. The processing method produced is used to analyze spectra determining the concentration of compounds present. It can also be used to reprocess/batch process a set of spectra. The saved methods can be used in the IMACC Scripting Environment to process real-time spectra.
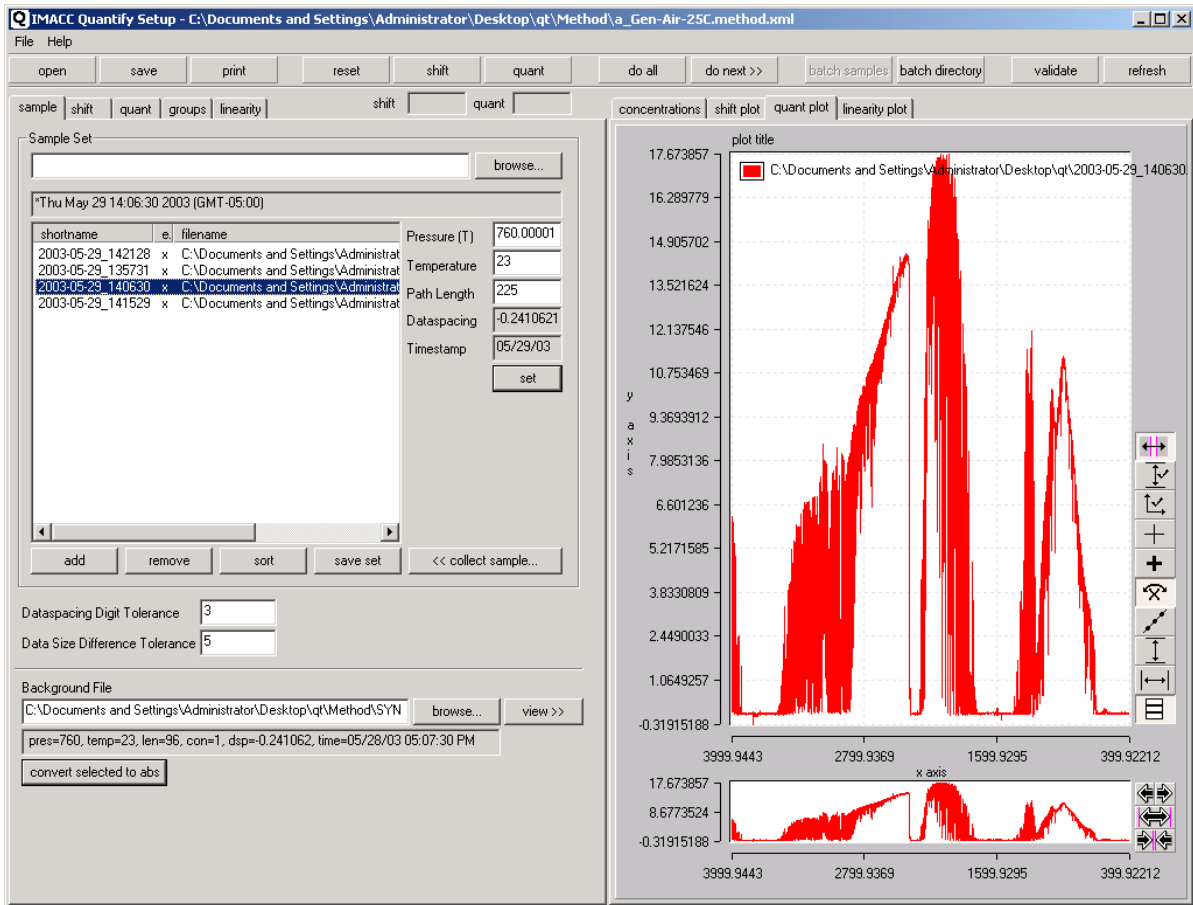
IMACC Quantify User Interface

2.0 User Interface Arrangement

The IMACC Quantify application is divided into 2 tabbed panes. The left tabbed pane is for data input and adding configuration parameters. The right tabbed pane is for output and reviewing the results of the method.

Input Configuration Tab	Corresponding Output Tab(s)
Sample Tab	Concentrations, Quantify Plot
Shift Tab	Shift Plot
Quantify Tab	Quantify Plot, Concentrations
Group & Classes Tab	Concentrations
Linearity Tab	Linearity Plot

Input Tabs
- **Sample** – Used for adding sample spectra to the method for processing. NOTE: The selected sample is the active sample for other operations.
- **Shift** – Used for defining the shift parameters for the spectra. This is used to properly align the spectral samples with the references for proper analysis.
- **Quantify** – Used for adding compound references and analytical regions to method.
- **Group & Classes** – Used for defining pseudo compounds based on weighting of analysis results or for selecting the proper analysis to report based upon concentration ranges.
- **Linearity** – Used for defining linearity coefficients to correct for Non-Beer's Law behavior in the analysis method

Output Tabs
- **Concentrations** – Used for displaying the concentration results of a method and the 2σ errors.
- **Shift Plot** – Used for displaying the results of a spectral shift of the selected spectra.
- **Quantify Plot** – Used for displaying a selected sample and selected references. This plot is also used for defining regions and windows within the region for analysis of the selected sample.
- **Linearity Plot** – Used for displaying the results of linearization for each analyte based upon a group of concentration references.
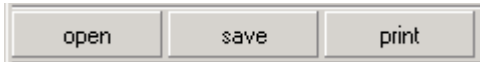
The tabs on the user interface are arranged in logical processing and development order. That is samples are shifted, Quantifyed, and linearized.

<u>The Toolbar</u>
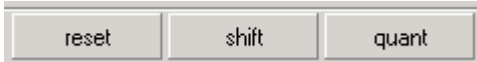
The Toolbar is used for performing major operations.

| open | save | print | reset | shift | quant | do all | do next >> | batch samples | batch directory | validate | refresh |

<div align="center">Toolbar</div>

| open | save | print |

Open – Open and load an analysis method file.
Save – Save the current analysis method to a specified file.
**Print** – Print the method's configuration.

| reset | shift | quant |

Reset – Clear user interface results.
Shift – Shift the selected sample spectrum.
Quantify – Quantify the selected sample spectrum.

| do all | do next >> |

Do All – Shift and Quantify the selected sample spectrum.
Do Next – Shift and Quantify the selected spectrum and move to the next spectrum. This is useful for stepping through a set of samples to see quantitation results.

| batch samples | batch directory |
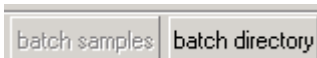
Batch Directory – Reprocess a whole directory of spectra producing a new gas concentration file.

| validate | refresh |

Validate – verify that all calculation parameters and references are valid and exist on the current computer.
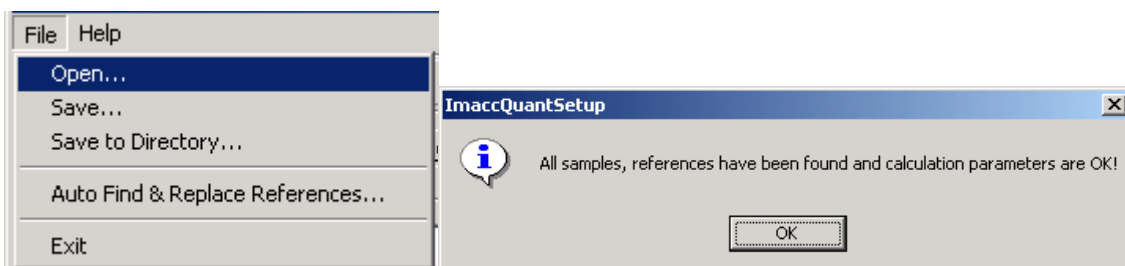**Refresh** – refresh displays

<u>Menu</u>

The file menu displays basic file loading and saving functions. The 2 operations of interest in this menu are **Save to Directory** and **Auto Find & Replace References**.

Save to Directory – Saves entire method including references and samples to a specified directory. This is useful for transferring or archiving a complete method.
Auto Find & Replace References – Searches the method for missing samples and references. Missing references and samples are automatically replaced with matching files from a directory and subdirectories selected by the user.

| File | Help |
| Open... |
| Save... |
| Save to Directory... |
| Auto Find & Replace References... |
| Exit |

ImaccQuantSetup

ⓘ All samples, references have been found and calculation parameters are OK!

OK

3.0 Sample Tab

The **Sample tab** is used to add sample spectra that you wish to work with and analyze. The usage of the buttons is as follows:

The sample set is a group of spectra. The list on this tab displays the path to the spectrum file and whether or not it has been found on the system. If it has been found there will be an 'x' in the '**exists**' column.

When a spectrum is selected its parameters will be displayed in the edit boxes to the right of the list and the actual spectrum will be displayed in the **Quantify Plot** tab.

To the right of the spectrum list there are edit fields for changing the parameters of the spectrum. You can alter **pressure** (Torr), **temperature** (C), **pathlength**. The changes will be made permanent by pressing the 'set' button.

Sample List

Sample Attribute

Spectrum plot

Samples

Spectrum List Buttons

Add – add an single beam (sgl) or an absorbance (abs,spa) spectral file. This opens a file dialog that can be used to select one or multiple spectra.

Remove – removes the selected spectrum.

Sort – sorts the list alphabetically.

Save Set – saves the set of spectra to a ".set" file so they can be retrieved as a set in the future.

Collect Sample – acquires a spectrum from the FTIR (if attached)

Browse… - the browse button allows you to load a ".set" file.

Concentrations

Other Fields

Data spacing Digit Tolerance – value that denotes how many digits of the data spacing variable in the sample spectrum must match the that of the references to be an acceptable sample.

Data Size Difference Tolerance – due to rounding errors it is possible for data from the sample to not align exactly with the reference spectra and the defined windows of analysis method. This value represents the maximum number data points you are willing to lose from the sample and still process it.

Background File – the background file that is used to convert single beam spectra to absorbance spectra.

View >> - displays the background file in the **Quantify Plot** tab window.

Convert selected to ABS – displays the resulting conversion of single beam to absorbance in the **Quantify Plot** tab window.

Any selected sample spectrum can be viewed on the **Quantify Plot** tab.

4.0 The Shift Tab

The shift tab and the corresponding shift plot can be used to properly align the sample with a standard wavenumber base. This shift uses cross correlation between the data and a reference standard. The peak of the correlation plot represents the position where the two spectra are in optimum alignment. It is this peak that is used to shift the data to force alignment. However the spectrum is not just moved. The data spectrum is shifted relative to the fixed laser sampling grid of the FTIR. As a result the shape of the lines will change based upon the sampling dictated by the sampling grid.

Shift Reference – typically a H20 absorbance spectrum, but any spectrum containing the lines you wish to shift to. These should be well established line positions. .

Start, Stop – the spectral range that is used when doing the cross correlation between the selected sample and the shift reference.

Max Delay – is a cross correlation parameter which represents the maximum shift of the data from it original position to start the correlation (typically 5). It is the maximum delay.

Interpolate Count – how many orders of interpolation are to be used to more accurately determine the exact position of the cross correlation peak (typically 7).

Shift Count – how many times you wish to perform the shift operation (typically 3). Each shift will make a finer and finer correction. A fit to better than 0.001 cm^{-1} should be possible.

Save shifted spectrum – saves the shifted spectrum

Deltas – displays the amount of shift performed for each iteration of the shift routine.
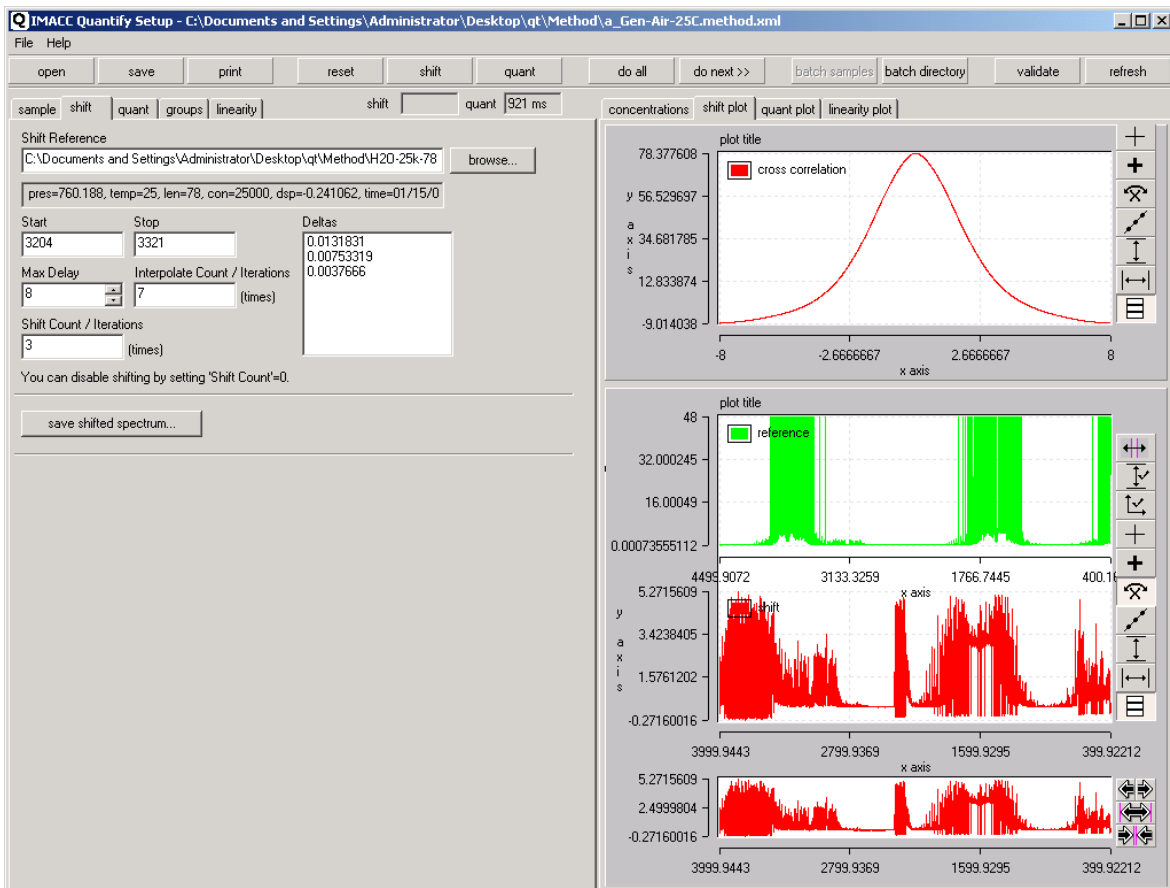
5.0 The Quantify Tab

The `Quantify Tab` and its corresponding `Quantify Plot` tab are used to define references, analysis regions and sub windows within an analysis region.

`Reference Set` – the references that are to be used in analyzing the spectra.

Reference Set Buttons
`Add` – adds a reference file (spa,abs) and its corresponding compound to the analysis procedure.
`Remove` – removes the selected reference and the corresponding compound
`Sort` – alphabetically sorts references
`Save Set` – saves groups of references in a .set file for rapid inclusion in the future

The reference list contains a column "`exists`" if the reference is in the specified path on the computer system you are using, an 'x' will appear in this column, if not you will need to locate it or add it. If the checked box by the reference code name is selected the reference will be plotted on the `Quantify Plot` above the data plot for the sample selected. Multiple `spectra can be selected`.

You may alter the attributes of the references using the following fields.

Reference Attribute Edit Fields
`Code Name` – name that you wish for this references. This code name will be used when reporting the concentration results of the method on a sample.
`Pressure` – pressure of the reference (Torr)
`Temperature` – temperature of the reference (Centigrade)
`Concentration` – concentration of the reference (ppm)
`Path Length` – The path length used in collecting the referenced (m).
`Dataspacing` – the dataspacing of the reference.
`Timestamp` – Date & Time stamp showing when the reference was acquired.
`Set` – assigns the new values to the reference file and writes them to the spectral header record

Divider Bars
Divider bars are useful graphical tools for defining regions and windows. To show a divider bar press '`add divider bar`'. The whole divider bar can be moved by selecting the center of the bar and

dragging it. Or a divider bar can be expanded or contracted by selecting the edge bars and dragging them.
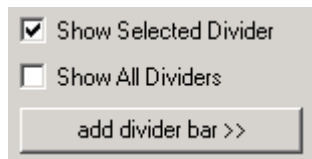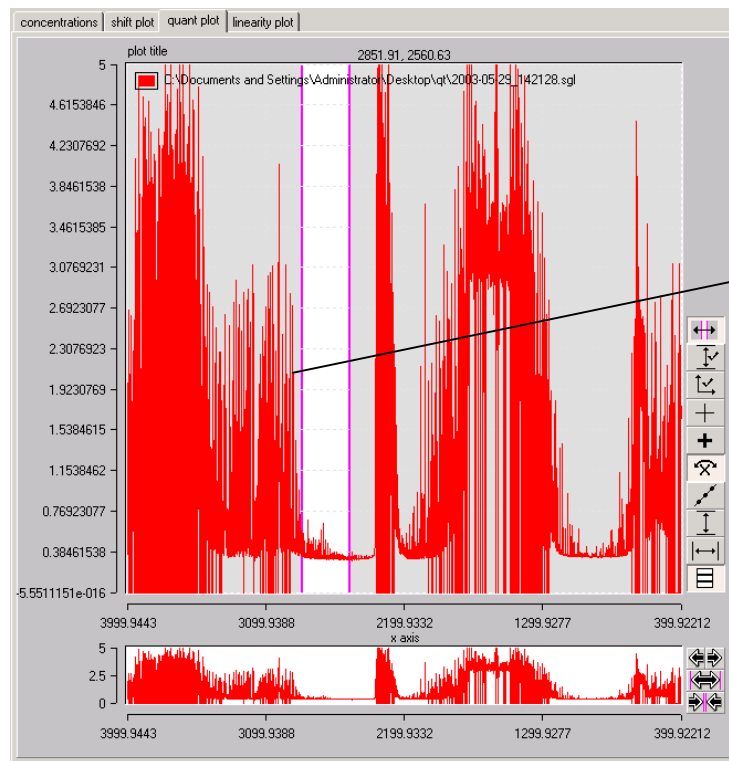

Divider Bar

Divider Controls
Show Selected Divider – displays the divider bars for the selected window or region.
Show All Dividers – displays all of the selected windows or regions.
Add Divider Bar – inserts a divider bar.

The divider bars can be used to define a region/window and then add it or update an existing one. The buttons: **add new region, update selected region, add new window, update selected window**, can be used to perform these functions with the coordinates (start-stop points) defined by the divider bar at the time.

Divider Bar Plot

Regions List
Lists the regions in the sample spectrum that are to be used to do the analysis.
Add – shows an add dialog for adding a new region manually
Remove – removes a selected region
<< Add New Region – uses the divider bars adds a the selected divider bar area
<< Update Selected Region – uses the divider bars and updates the selected region
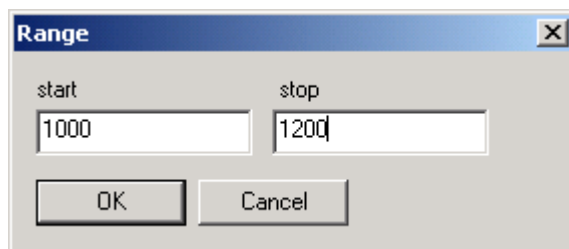
Adding Region / Window Range

Windows List
Lists the windows within a selected region that are to be used for analysis data outside the windows is ignored.
Add – shows an add dialog for adding a new window manually
Remove – removes the selected window
<< Add New Window – uses the divider bars and adds a new window.
<< Update Selected Window – uses the divider bars and updates the selected window

Compounds List
Lists the compounds that will be included in the analysis of spectra for the selected region/windows.
Add – shows an add dialog for adding a compounds to the selected region. The dialog containing all of the current compounds in the method (except those already selected) is displayed. Placing a check by the compounds you wish to add will add them to the selected region.
Remove – removes a compound from the region.
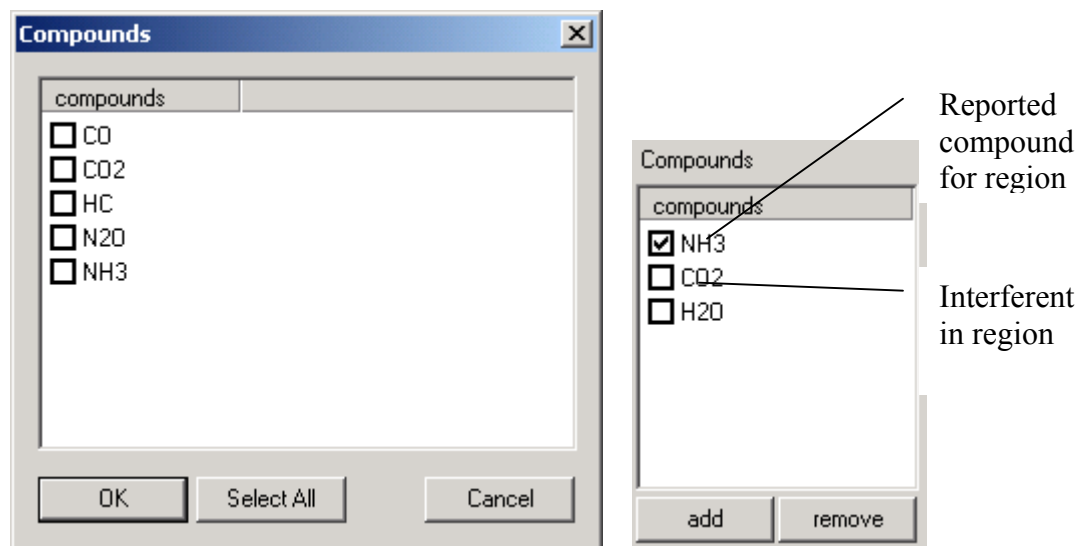
Adding Compounds & Selecting Reported Compounds

Placing a check by the compound in the compound list defines the what compound will be reported in the concentration list (an analyte). The other unselected compounds represent the interferents in the selected region so they are analyzed for but are not reported.

Once you have defined the references, regions and windows you can process a spectrum selected in the sample list by pressing `Quantify` or `do all.` The results are displayed on the `concentrations tab`.

`Quantify` – processes the selected spectrum without shifting the selected spectrum.
`Do All` – processes the selected spectrum with pre-shifting of the selected spectrum.
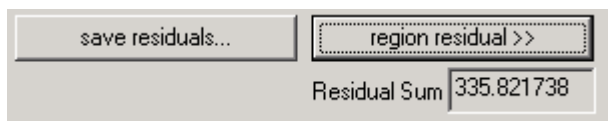

Residuals
One way of determining how well you have fit the data spectrum in a region is to observe the spectrum with the calculated concentrations of each compound removed. This is displayed by the residual buttons.

`Save Residuals`… - saves all residual values to a CSV file for further processing or analysis.
`Region Residuals` – displays the selected spectrum on the `Quantify Plot` showing the selected region's gas concentrations subtracted from the spectrum in that region/windows.
`Residual Sum` – displays a numeric value to give you an idea of whether or not you are improving the calculation by adjusting the region's windows and compounds.

Residual

Special Features
`Interpolate Count` – performs interpolation on the references and the sample spectra increasing the number of data points in the same manner as zero padding of the interferogram would. This operation increases the number of data points in the regions by a factor of 2^n. A value of 0 disables this feature where as a value of 3 increases the number of data points 8 times.

`Use Dynamic References` – enables reference selection from the group of references listed on the `linearity tab` `for each specie.` This reduces the error in the calculation by properly substituting a reference that more closely matches the actual feature in the data spectrum. After dynamic reference selection the spectrum is reanalyzed with the new references.
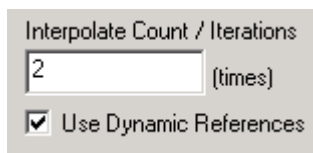
Special Features

6.0 Linearity Tab

The `Linearity Tab` and the corresponding `Linearity Plot` are used to define a function which will accurately calculate a gas concentration when the compounds observed concentration falls far from the defined reference for the analysis method. Under these circumstances the references may not follow Beer's law over the large interpolation range required. This function corrects for the non-Beer's law behavior.

Reference standards (spectra) with known concentrations of specific compounds are added to a compound's set and these are chosen to span the desired concentration range for the compound. Selecting an `order` computes coefficients for that order of a polynomial fit to the data. These coefficients allow for correction of CLS computed concentrations for any non-linearity present over the total range spanned. The plot displays the actual concentrations (ppm*m) versus the CLS calculated concentrations (ppm*m). The red curve is the fit to data for all spectra in the set. Coefficients are assigned to each compound corrected and used when you `Quantify` or `do all`.

Linearity Interface

<u>Settings</u>
`Order` – order of the polynomial fit
`R^2` – R^2 for the fit defining the accuracy of the fit
`Force Through Zero` – forces the calculation to pass through zero
`Dynamic References` – marks this compound as a dynamic reference. If this is checked and the
`use dynamic references` on the `Quantify tab` is checked the Quantify process will swap
references dynamically to more closely match the reference to the actual observed concentration.
Spectra in the linearity list are available for choice. This reduces CLS errors.
`Minimize Percent Error` - when checked minimizes the percent of error in the curve fit otherwise
it minimizes the absolute difference value. This will improve the fit to smaller values.
`Generate Coefficients` – when `dynamic reference` is selected this button will generate
linearization coefficients for each linearity reference spectrum based on the current order setting. This
assures that when a reference is selected dynamically that is specific linearity function is also selected.
When each reference spectrum in the set is selected with the mouse, its fit and its unique coefficients
are displayed. By stepping through the set it is easy to determine if a reference has a problem which
produces an undesirable fit for that reference.
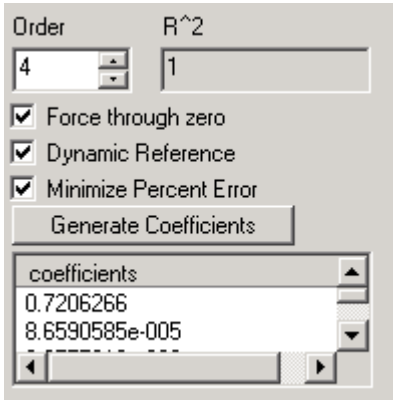
Each spectrum within the reference set can have varying orders, intercepts, etc. if desired. This is
done by selecting the reference in the reference list and adjusting the settings.

Linearity Settings

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7.0 Groups & Classes Tab

The **Groups & Classes Tab** allows you to define new printout parameters that are defined by multiple compounds and their weightings.

This can be used to:
1) report a value for a compound based on the PPM values observed for other defined "compounds" and specified concentration validity ranges. For example CO2 can select from CO2-LO, CO2-MD, and CO2-HI which might be analyzed in separate regions.
2)
```
CompoundA = CompoundB (if range) | CompoundC (if range) | …
```

3) report a new parameter value based on a weighted sum of other analytes.
4)
```
CompoundA= CompoundB*weightB + CompoundC*weightC + …
```

Group Class List
Add – adds a new compound
Remove – removes selected compound
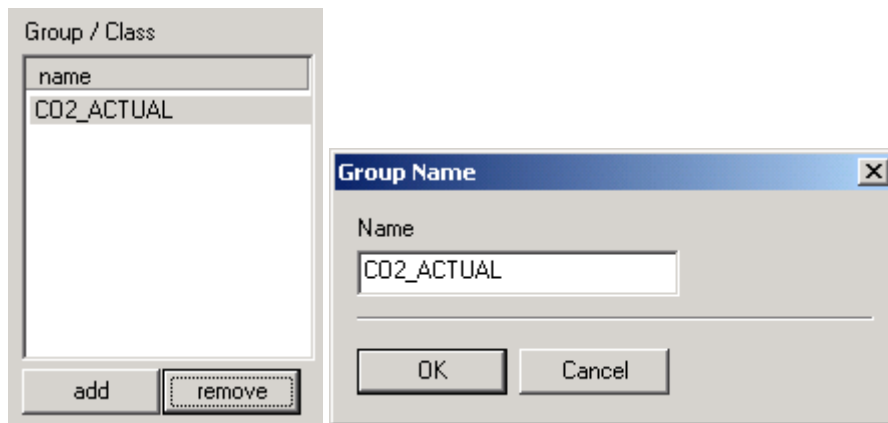
Group Class List, Adding a Group

Compounds and Parameters List
Add – adds a compound and parameters to the selected Group
Remove – removes a compound from the selected Group
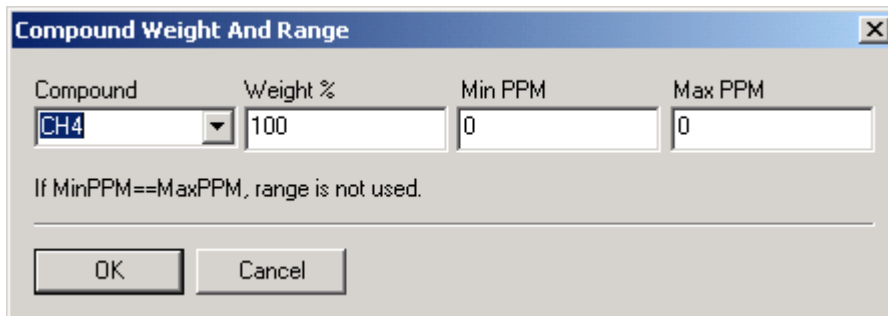
Adding a compound to a Group / Class

8.0 Plot Usage

The plot is a useful tool for viewing spectral data. This section explains the plot and its tools.

Plot Window

Plot Toolbar
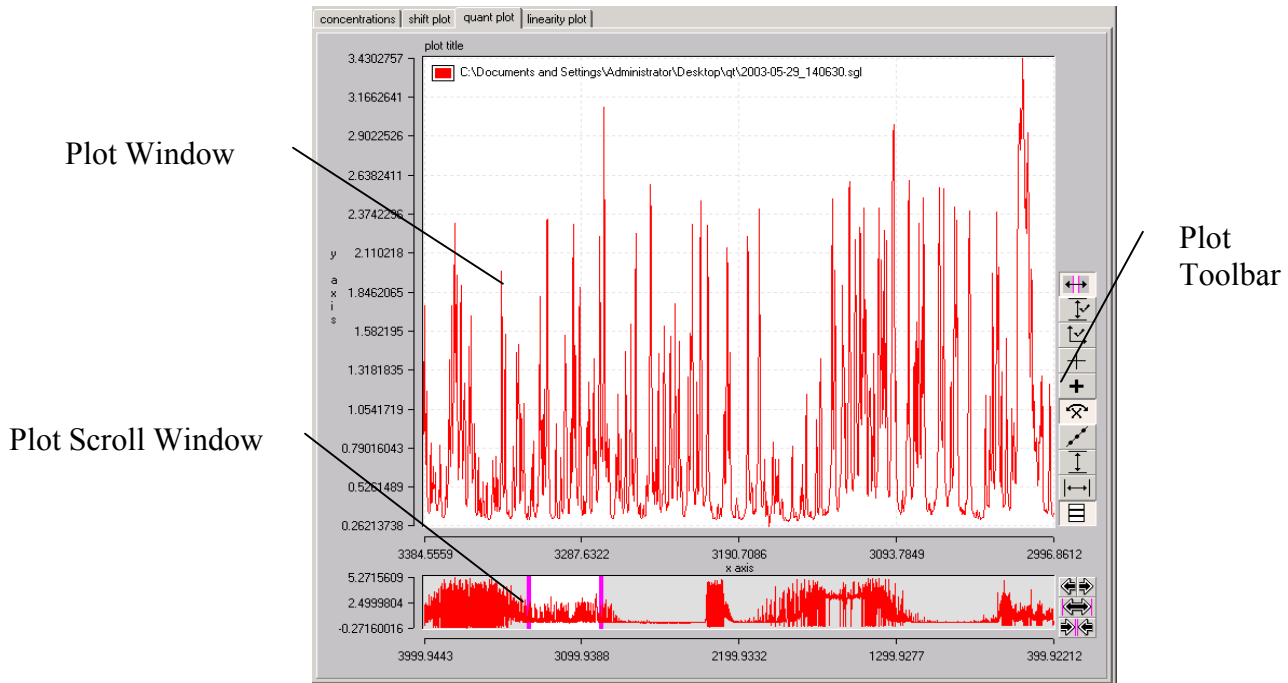
Plot Scroll Window


Plot Toolbar

Fix Auto Scroll X – scrolls all plots together in x-axis values.

Fix Auto Scale Y – auto-scales plots to max and min y values independently in each window.

Fix Axes X & Y – sets common x and y scales of all plots to the selected plot

Guides – displays horizontal and vertical guides that can be moved to check alignment of data

Cursor Value – shows current datapoint value on selected plot

Flip X – flips the X axis reversing the plot direction

Show Points – displays individual data points in the plot

Auto Scale Y – scales selected plots in Y value

Auto Scale X – scales selected plot in X-value

Stack Plots – stacks or overlaps plots – toggle button

Scroll Window – scrolls the viewing window left or right

Stretch Window – stretches the plot within the viewing window, expanding it.

Shrink Window – shrinks the plot within the viewing window, compressing it.

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Zoom Box – A left-click of the mouse held down and dragged in any plot window will create a zoom box. When the mouse button is released the contents of this box will be enlarged to fill the plot window.
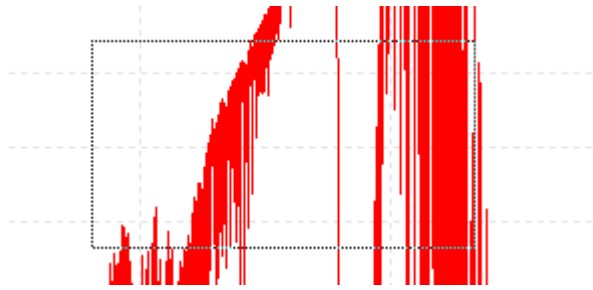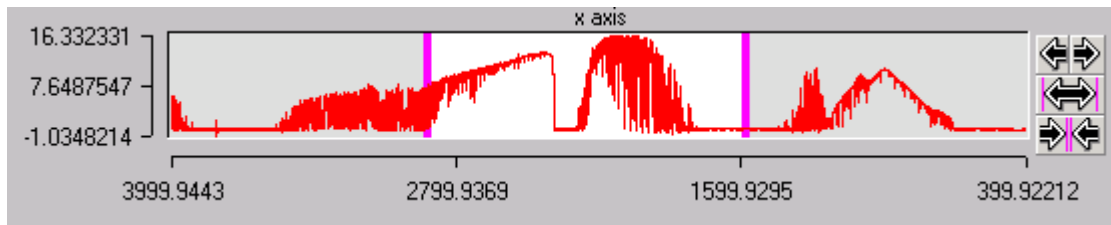

Zoom Box
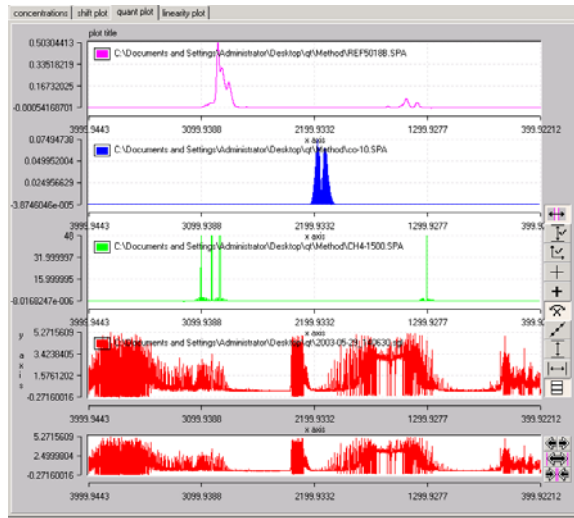
Stacked Plots

The small Scroll Window at the bottom of all plots can be used to define the visible X region of the plot. The purple divider bars can be dragged to stretch or shrink the visible region. If you click in the center of the divider bars the whole visible region can be dragged with the mouse without changing its width.

Scroll Window

9.0 Batch Reprocess

Batch reprocess is used to process all spectral files in a selected `Sample Directory`. The loaded method is used to analyze the spectra and the results are both displayed on the concentrations tab and written to a file if `Output Concentration File` is specified. The `Background File` spectrum is used to convert single beam spectra to absorbance spectra before analysis.

The **Sample Directory** is the directory containing spectra to be processed. Wild cards can be used to limit the spectra processed. For example a manual addition of *.sgl to the path wil process only single beam spectra with an sgl extent.

The **Output Concentration File** is the file to which the gas concentration results should be written. If it does not exist it will be created.

The Checkboxes
`Shift` – If checked the method shifts the incoming files against the selected shift reference prior to analysis
`Quantify` – Quantifys the spectra with the loaded method (if this is not chosen the spectra can be batch shifted and saved)
`Ignore Errors` – will not notifiy you when an error is encountered during analysis (this is helpful if a large number of spectra are being processed).
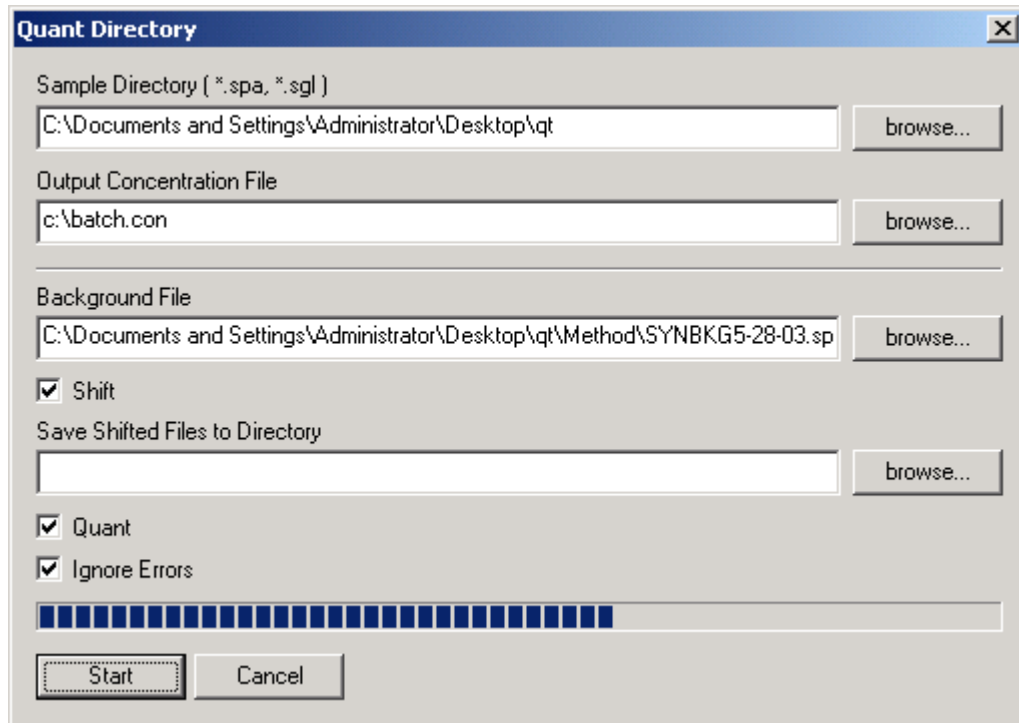
Quantify Directory

The **Blue Progress Bar** shows the percentage complete for the selected spectra.

NOTE: If the **Concentrations Tab** is selected data will be displayed as it is generated.