

Volume

1

CHROMLAB

51 Ways to Make TotalChrom Work for You!

TotalChrom™ Tips

CHROMLAB COMMUNICATIONS

TotalChrom™ Tips Guide

On-Site operator training programs can be scheduled for your laboratory to help setup, optimize and calibrate your TotalChrom methods.

If you would like information of these hands-on operator training programs please contact *ChromLab* at 610-644-2260 or online at www.FastGCChromLab.com.

51 Ways to Make TotalChrom Work for You!

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Table of Contents

| | | | |
|------------------------------------------------------------|----|-------------------------------------------|----|
| Introduction | 2 | CHAPTER 3 – GRAPHIC EDITOR | |
| CHAPTER 1 – File Management | | 1. View Raw Data Points | 31 |
| 1. Create TotalChrom Folders | 3 | 2. Bunching Factor | 32 |
| 2. Segment Your TC Data Files | 3 | 3. Noise-Area Thresholds | 34 |
| 3. Using a TC Project Directory | 4 | 4. Component Editing | 35 |
| 4. Setup TC Quick Paths | 5 | 5. Manual Calibration | 36 |
| 5. Create of Backup Folder | 7 | CHAPTER 4 - SEQUENCE | |
| 6. Set up Default Paths | 8 | 1. Create an Auto-Calibration Sequence | 37 |
| CHAPTER 2 - METHOD | | 2. Smart Fill - Data File Names | 38 |
| 1. Method Editing - Introduction | 10 | 3. Actions – Setup Shortcut | 39 |
| 2. Inst. – Data Channels – Sampling Rate | 11 | 4. Append New Cycles | 40 |
| 3. Inst. Control – Oven/Inlets | 14 | CHAPTER 5 - REPROCESS | |
| 4. Inst. Control – Detectors | 15 | 1. Results Reprocess | 42 |
| 5. Inst. Control – Inst. Timed Events – Gas Saver Setup | 16 | 2. Batch Reprocess | 44 |
| 6. Process – Noise Threshold | 18 | CHAPTER 6 - CHROMATOGRAMS | |
| 7. Process – Area Threshold | 19 | 1. Overlay | 47 |
| 8. Process – Baseline Timed Events | 20 | 2. Auto Size | 48 |
| 9. Process - Replot | 21 | CHAPTER 7 – OTHER TIPS | |
| 10. Components – Global Info | 22 | 1. Method Editor-Component List View | 49 |
| 11. Components – Defaults | 24 | 2. Real-Time Plot | 50 |
| 12. Report Format Editor | 25 | 3. CAM Administration | 51 |
| 13. Components – Calibrate | 29 | 4. Kickoff Application | 52 |
| 14. Other – Fit Analysis(CalPlot) | 30 | | |

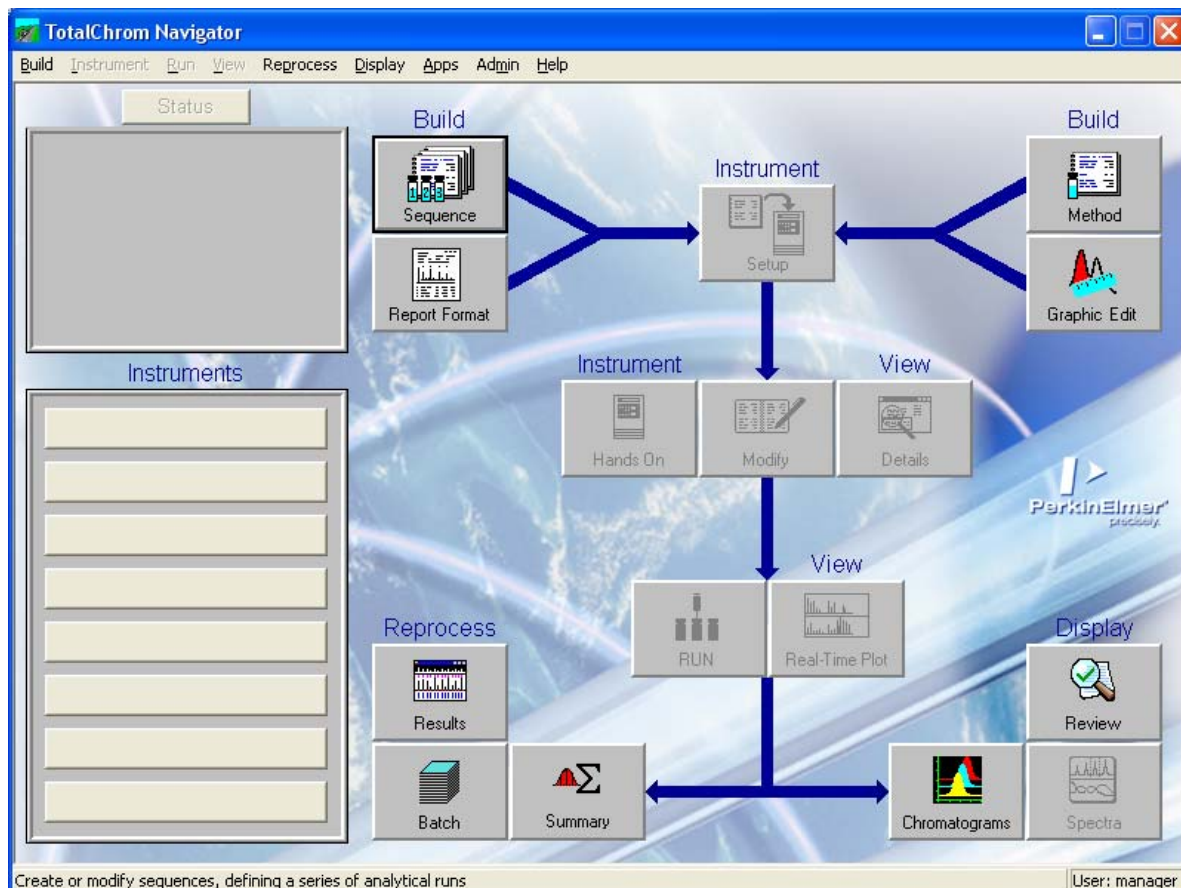
TotalChrom™ Tips

Introduction

The information and tips in this document are intended to provide some helpful ways for the user of the TotalChrom™ chromatography software to generate and optimize their methods, reports and sequences and in review of their data.

Pictured below is the **TotalChrom Navigator** screen. These system functions are accessed by a single click on the screen buttons. These functions are labeled with blue group names and can also be accessed from the drop-down menus of the same name.

For example the **Build** group for the function **Method**, **Graphic Edit**, **Sequence** and **Report Format** are also available in the **Build** drop-down menu.



Chapter 1 - File Management Tips

1. Create TotalChrom Folders

There are many ways for set up your system file structure. Here are three examples of basic TotalChrom file management structures. As a start you should create folders for Data, Methods & Report Formats and Sequences.

Tip #1- Create separate folders for your TotalChrom data, methods & reports and sequences on the C:\ drive. This will allow for shorter directory paths for easier viewing in the TC sequence screen and in report headers.

This structure will also prevent possible deletion of system files that are stored in the **PenExe** folder. It is **NOT** a good idea to use the TotalChrom **PenExe** program folder for this reason.



1. Use Windows Explorer to create new folders in the C:\ Drive.

Some examples are:

C:\TotalChrom Data or C:\TC Data
C:\TotalChrom Methods & Reports
C:\TotalChrom Sequences

Tip #2 - Always save your Method and Report Format files together in the same folder so that the TotalChrom software can always find your Report Format files.

2. Segment Your TC Data Files.

For large numbers of TC data files you may want to segment your data files by year or year & month, by instrument name or by analysis or product name as in the examples below:

C:\TotalChrom Data\2008
C:\TotalChrom Data\2008\June
C:\GC 1 – QC Lab
C:\Your Analysis or Product

Tip #3 - The more you segment your data into separate folders, the easier it will be to retrieve your data for review and reprocessing or to move you data for archival purposes.

Chapter 1 - File Management Tips



3. TotalChrom - Project Directory function.

At times it may be useful to group all of your file types into a specific folder.

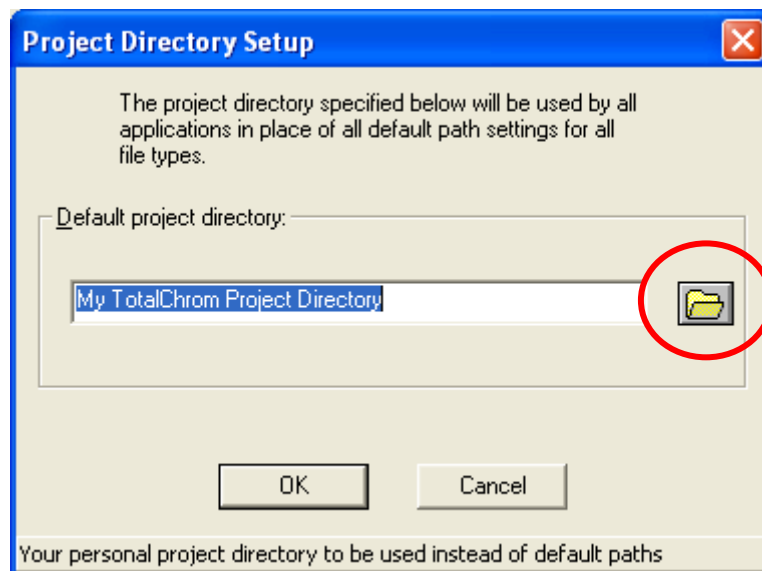
Tip #4 - Use the **Project Directory** function. This is a quick and convenient way to store and archive all the files associated with a specific project e.g. Methods, Report Formats, Data and Sequences. Check this out it may be useful for you!

Step 1. Open Windows™ Explorer and create a Project name.

Example: **C:\My TotalChrom Project Directory**

Step 2. In TotalChrom Navigator Screen

- a. Click on the **Build** drop-down menu.
- b. Select the **Configuration** function.
- c. Select **User** and then **Project Directory**.
- d. Select your previous created Project Directory using the browse button.



TotalChrom - Project Directory Setup window.

Note: You may need to use Save As to save your first file entered into a newly created project directory before your files will be automatically saved in your new project directory instead of in the TotalChrom default paths.

Chapter 1 - File Management Tips

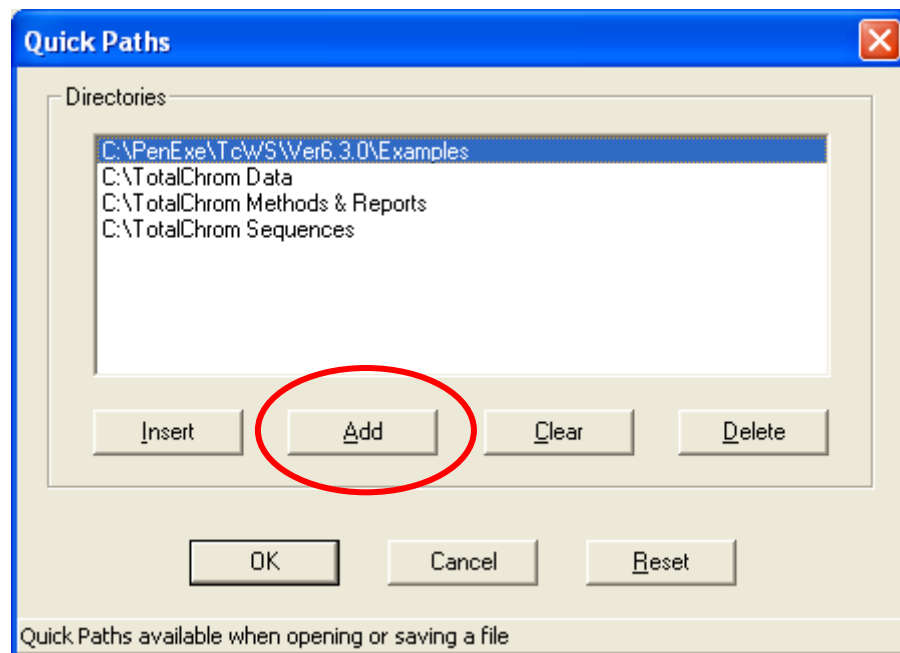


4. TotalChrom Quick Paths.

Tip #5: Setup **TotalChrom Quick Paths**. This is a quick and convenient way to easily select a directory path within TotalChrom. This can be used to save or look for data files and to look up method and sequence files.

Step 1. In the **TotalChrom Navigator Screen:**

- a. Click on the **Build** drop-down menu.
- b. Select the **Configuration** function.
- c. Select **User** and then **Quick Paths**.
- d. Use the **Add** button to find and add your most frequently used directories to **Quick Paths** list. Click **OK** when finished.



TotalChrom - Build/Configuration/User/Quick Paths window.

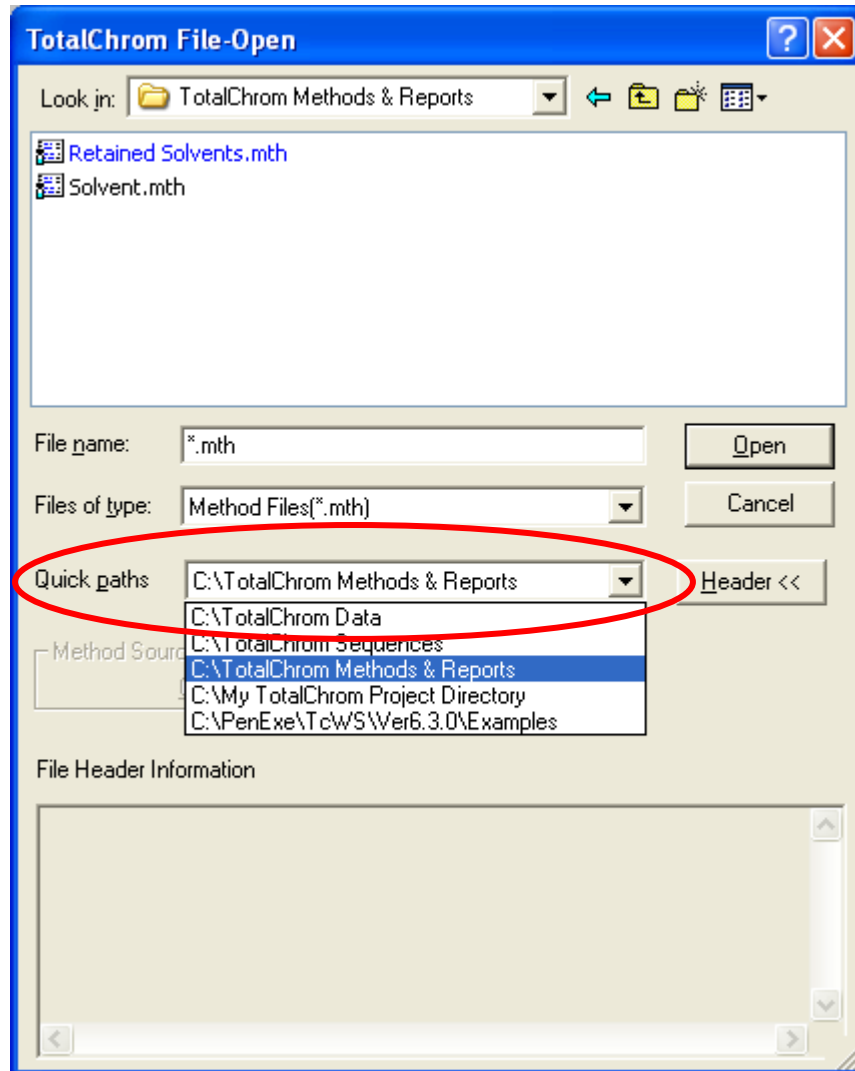
Chapter 1 - File Management Tips

4. Setup TotalChrom Quick Paths - continued.

Setting up Quick Paths for your most frequently used methods, sequences and data directories is a big time saver over the long run.

Step 2. Use the Quick paths function in any **TotalChrom File-Open** window.

- a. Click on the **Quick paths** browse button.
- b. Select the directory of interest from your list.



Using the Quick path function in TotalChrom File-Open

Chapter 1 - File Management Tips



5. Create a Backup Folder.

Tip #6 - It is highly recommended that you create a backup folder for your finished and optimized methods, report formats and sequences.

Use Windows™ Explorer to create this folder. These backup files will come in very useful if a method file is accidentally changed, lost or is corrupted.

Step 1. Open Windows™ Explorer and create a backup directory name. For example:

C:\TotalChrom Backup

Step 2. When you are satisfied that your method, report format and sequence files are finished copy them to your backup directory. You can use the Windows **Save As** function as follows:

- a. Click on the **File** drop-down menu.
- b. Select **Save As ...**
- c. Save your file to the **TotalChrom Backup** directory.

Tip #7 - It is also highly recommended that you backup all important files **off-line** in case of hard drive failure. Use removable storage media such as a flash drive, CD or floppy disk.

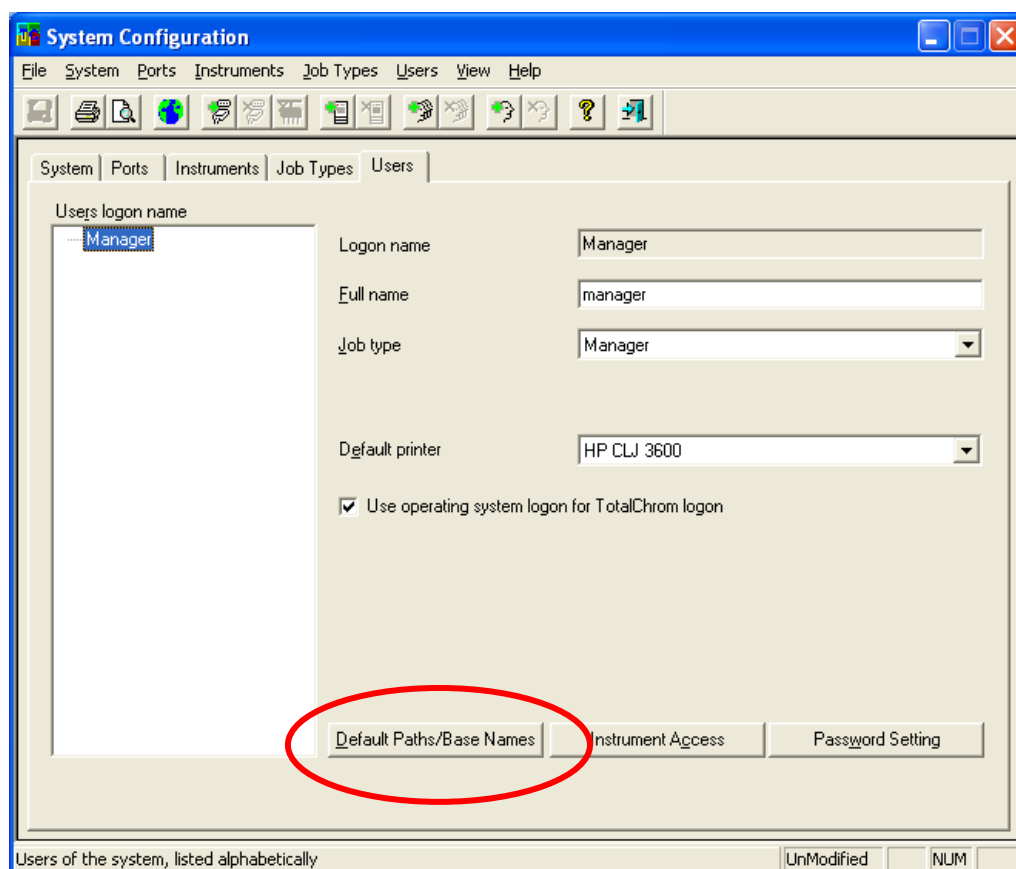
Chapter 1 - File Management Tips



6. Set up Default Paths - System Configuration

Tip #8 - If you have TotalChrom administrator (manager) privileges you can setup or change the default paths for your method, report and sequence files as needed in **System Configuration**.

- a. In the TotalChrom Navigator screen select the **System Configuration** function from the **Admin** drop-down menu.
- b. Highlight the **User - Manager** and select the **Users** tab.
- c. Click on the **Default Paths/Base Names** button. Using the browse button, select your new default data paths. Use the same path for both **Raw data** and **Result files**.



TC Navigator/Admin/System Configuration window.

Important Note: It is recommended that you do not change the paths for methods and report formats or sequences once they are setup.

Chapter 1 - File Management Tips



6. Set up Default Paths – continued

After default **Raw and Result data paths** have been created in Windows™ Explorer they can be entered here by using the browse buttons. It is highly recommended that you use the same folder for both file types.

As an example, you can add the year to your Raw and Result file data paths. **Example: C:\2008 TC Data**

The screenshot shows the 'Default Paths/Base Names' dialog box. The 'Data paths' section is circled in red. It contains two text boxes: 'Raw data path' and 'Result files path', both containing the text 'C:\TotalChrom Data'. To the right of each text box is a folder icon button. Below these are three checkboxes: 'Use instrument default paths instead of these paths', 'This user is required to use the default path (or subdirectories) for raw files', and 'This user is required to use the default path (or subdirectories) for result files'. The 'Other paths' section contains four text boxes: 'Method path' (C:\TotalChrom Methods & Reports), 'Sequence path' (C:\TotalChrom Sequences), 'Report format path' (C:\TotalChrom Methods & Reports), and 'Program path' (empty). Each has a folder icon button. The 'Default base names' section has three text boxes: 'Raw data file', 'Result data file', and 'Modified data file', each with a browse button (...). There is also a checkbox 'The user cannot edit these base names'. At the bottom right are 'OK', 'Cancel', and 'Copy From...' buttons. At the bottom left is the text 'The default path for storing raw files accessed by this user'.

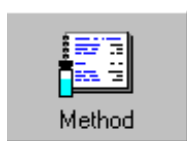
TotalChrom Default Paths/Base Names Window

Note: Consider using the Projects Directory function that is discussed in Section 3 if you need to group all of your file types together.

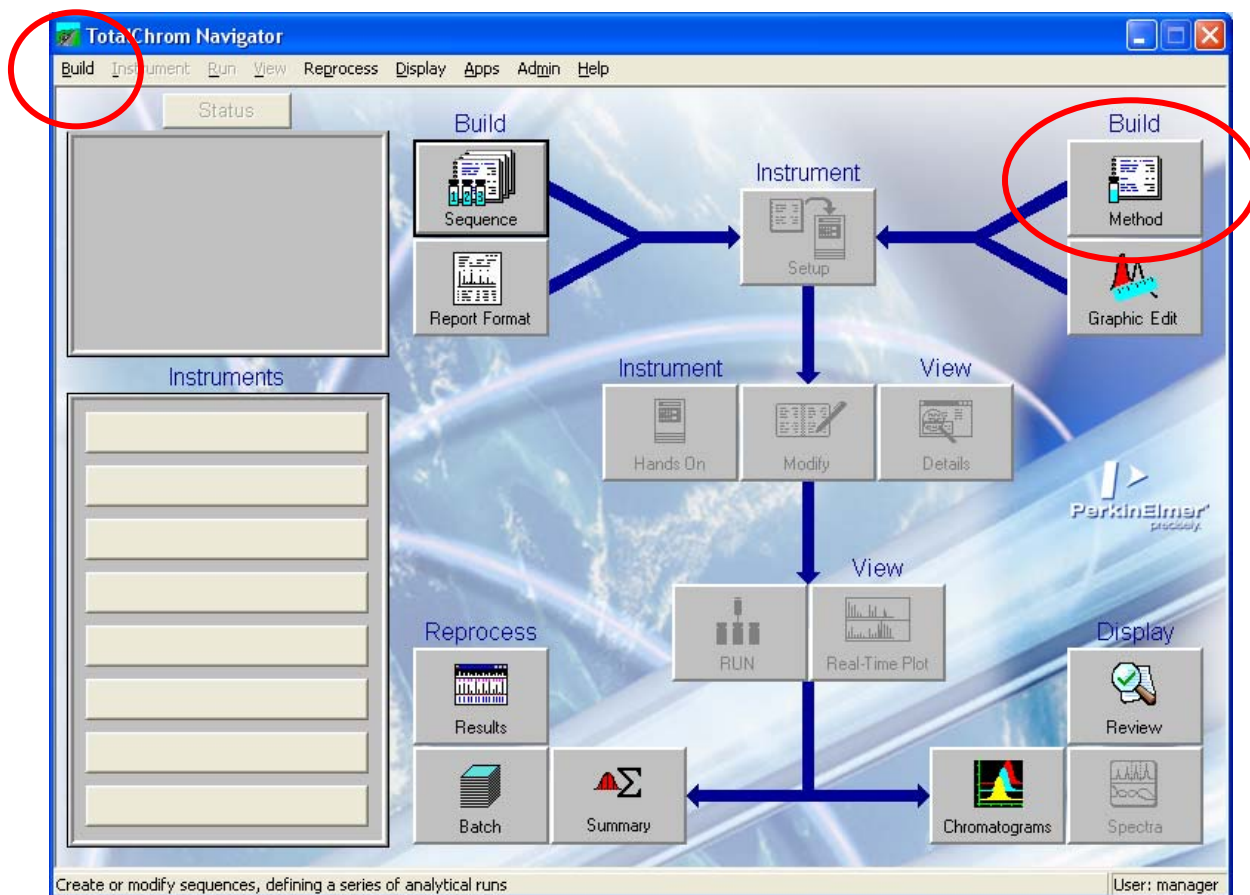
Chapter 2 – Method Tips

1. TotalChrom Method Editing - Introduction

There are many ways to edit your TotalChrom methods. Method editing can be performed either manually using the **Method Editor** functions or graphically using the **Graphic Method Editor** functions.

**1. Manual method editing.**

You can access the Method Editor functions by single clicking on the TC Navigator **Build - Method** button or by selecting Method from the **Build** drop-down menu.



TotalChrom Navigator screen - Method Editor.

Tip #9 - Use the **Review** function in the Method Editor **File** drop-down menu. This will step you through each page of the method. Don't forget to click on each of the **tabs** to review all of the method parameters.

Chapter 2 – Method Tips

2. Instrument Parameters – Data Channels

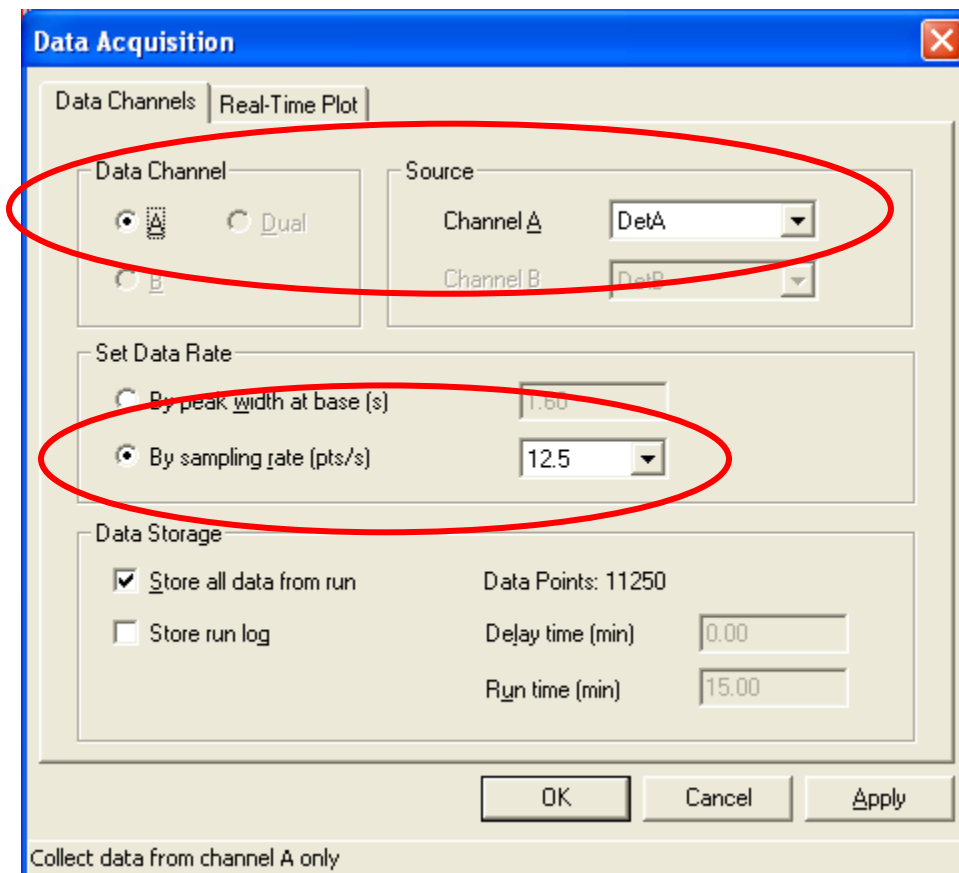
Tip #10 - Use **Data Channel-A** when only a single detector method is used even if the Source channel is the “B” detector. This will allow you to use the **Channel-A Sequence** for method setup.

Note: Setting the TotalChrom data **Sampling Rate** parameter correctly is very important for proper data acquisition and subsequent peak integration.



1. Data Channels – Setting the Sampling Rate

Tip #11 - Set the Sampling Rate so that your narrowest, and smallest, peak of interest will have at least 15 – 40 data points in the main body of the peak. Do not include peak tailing data points for this initial setting of the sampling rate.



Method Editor - Instrument – Data Channels screen.

Example: If a capillary peak is 3 - 6 seconds wide at its base, set the sampling rate to 6.25 data points/sec.

4 sec. X 6.25 data points/sec. will give 25 data points/peak.

Chapter 2 – Method Tips

2. Instrument – Data Channels - continued

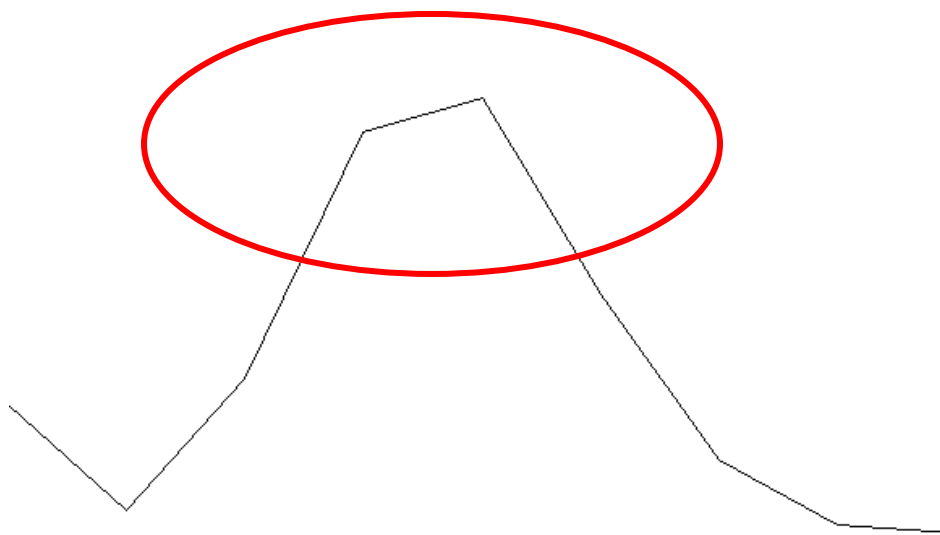
Setting the TotalChrom data **Sampling Rate** parameter correctly is very important for proper data acquisition and subsequent peak area integration.



2. Data Sampling Rate set too low.

The TotalChrom Sampling Rate is set in points/second (pts/sec) or hertz. This parameter determines the number of data points stored in the **.Raw** data files.

If the Sampling Rate is set too slow, the peak data at the crest of the peaks of interest will not be properly collected resulting in accurate and low area counts.



Example of Sampling Rate set too low. Note that the data at the crest of the peak was not collected!

Important Note: If the Sampling Rate is too low (slow) the peak crest data points may be missed causing inaccurate peak area (low) measurements.

On the other hand, setting the Sampling Rate too high (fast) and collecting too many data points will result in **.Raw** data files that are overly large and can result in peak splitting.

Tip #12 – Use the **Graphic Method Editor** to view (and count) the actual raw data points in your data file. See Chapter 3, page 31.

Chapter 2 – Method Tips

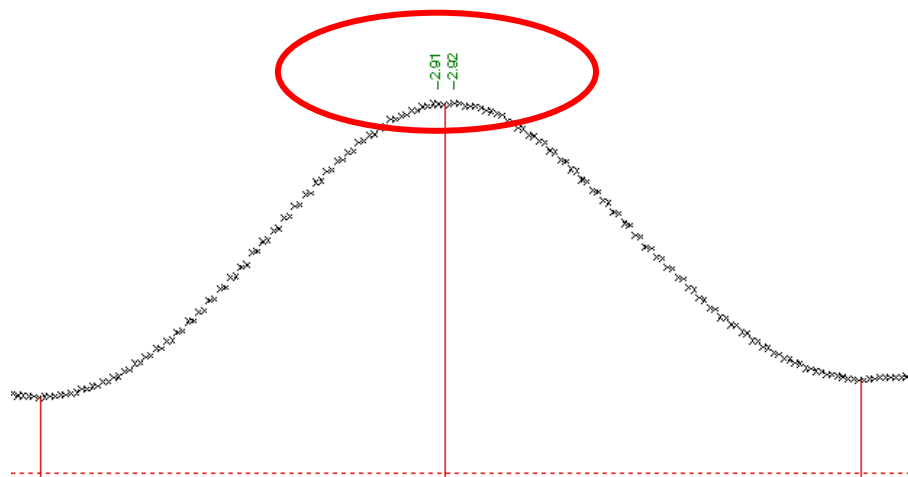
2. Instrument – Data Channels - continued



3. Data Sampling Rate set too high.

The TotalChrom Sampling Rate is set in points/second (pts/sec) or hertz. This parameter determines the number of data points stored in the **.Raw** data files.

Setting the Sampling Rate too high or over sampling can result in your method being over sensitive to detector noise that may result in peak splitting during integration.



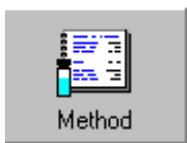
Example of the Sampling Rate set too high (fast). Note that this peak is split and will be identified as two separate peaks in the report.

Important Note: If the Sampling Rate is too high (fast) your data file size will be overly large and peak splitting may occur.

Chapter 2 – Method Tips

3. Instrument Control Options – Oven/Inlets

Tip #13 - Set the GC Oven parameters **Max. Temp** to protect your column liquid phase from being over-heated and **Equilibration Time** to stabilize the column oven temperature before the run start.



1. Setting Oven/Inlets parameters

a. Set the **Oven – Max. Temp. (°C.)** at 20 - 50° C. above the oven program final temperature, but never more than the column liquid phase max temperature.

b. Set the **Oven – Equilibration time (min)** to at least 1 or 2 minutes when using a low initial oven temperature (35 - 50° C.) to allow the oven air and column temperature to stabilize before the start of a new injection.

Instrument Control

Oven/Inlets | Carrier | Detectors | Instrument Timed Events

Program time (min)

Oven: 15.00
 Inj A: CAP: 0.00
 Inj B: NONE: 0.00
 Data end time: 15.00

Cryo

Coolant: Off
 Cut-in temp (°C): 60
 Timeout (min): 999

Oven

Max temp (°C): 250
 Equil time (min): 1.0

Heated zone setpoints (°C)

Injector A: 200 Auxiliary: 0.0
 Injector B: 0

| Oven Ramp | Rate | Temp | Hold |
|-----------|------|------|------|
| Initial | 0.0 | 50 | 2.50 |
| 1 | 20.0 | 200 | 5.00 |
| 2 | 0.0 | 0 | 0.00 |
| 3 | 0.0 | 0 | 0.00 |

OK Cancel Apply

Method Editor – Instrument – Control Options – Oven/Inlets.

Chapter 2 – Method Tips

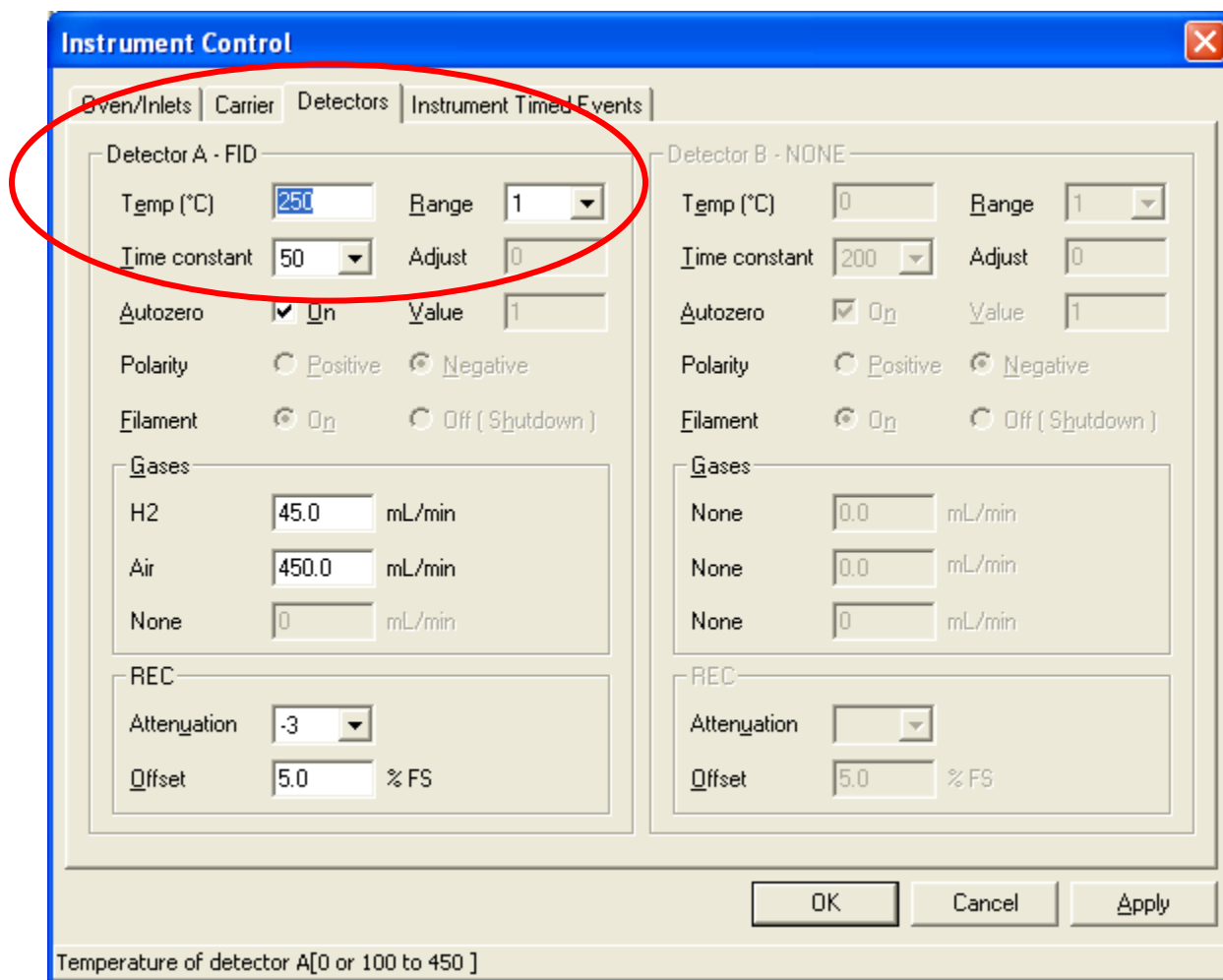
4. Instrument Control Options – Detectors

Tip #14 - The FID detector Temperature, Range and Time constant parameters must be set correctly for the column type installed.



1. Setting up the Detector parameters.

- Set the **Detectors - Temp. (°C.)** at 20 - 50° C. above the oven program final temperature to prevent moisture and sample contamination from building up on the FID jet tip.
- Use **Range 1** for most capillary column installations, use Range 20 for packed columns.
- Set the **Time constant to 50** when using high-efficiency capillary columns that produce fast, narrow peaks to prevent signal loss at the top.



Method Editor – Instrument – Control Options – Detectors.

Chapter 2 – Method Tips

5. Instrument Control Options – Inst Timed Events

Tip #15 – Setup a Split flow gas saving mode in your method. You can modify a method to automatically reduce the split flow setting after the injection to save carrier gas. Use the **Inst Timed Events** functions for this mode of operation. **Note:** The GC must have programmable pressure control (PPC) in order to set up this feature.



Step 1. Set up Gas Saving mode Timed Events.

- a. Select the **SPL1** (or SPL 2) function with the **Event** browse button. Set the **Time** (min) to -0.5 min and the **Value** which will be your injector split flow at 50 – 100 mL/min and click on the **Add** button.
- b. Again select the **SPL1** (or SPL 2) function and set the **Time** (min) to 2.00 minutes and the **Value** back to a standby split flow rate of 15 – 20 mL/min and click on the **Add** button.

Instrument Control

Oven/Inlets | Carrier | Detectors | Instrument Timed Events

Time (min)

Event

Value

| Event | Value | Time |
|-------|-------|-------|
| SPL1 | 100 | -0.50 |
| SPL1 | 20 | 2.00 |

Valves

| | Initial Setting |
|--------|---------------------------------------------------------------|
| SPLIT | <input checked="" type="radio"/> On <input type="radio"/> Off |
| 2 NONE | <input type="radio"/> On <input type="radio"/> Off |
| 3 NONE | <input type="radio"/> On <input type="radio"/> Off |
| 4 NONE | <input type="radio"/> On <input type="radio"/> Off |
| 5 NONE | <input type="radio"/> On <input type="radio"/> Off |
| 6 NONE | <input type="radio"/> On <input type="radio"/> Off |

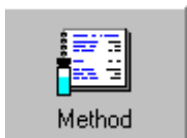
Events currently defined for this method

Method Editor - Instrument Control – Instrument Timed Events – Gas Saving mode.

Chapter 2 – Method Tips

5. Instrument Control Options – Inst Timed Events - continued

Note: When setting up the split flow gas saving mode you should also set the **Split Control – Flow (mL/min)** to a low flow rate in the **Carrier** tab screen to save carrier gas when the GC is not in the Ready state (standby).



Step 2. Set the Carrier - Split Flow for gas saving in standby.

a. Set the **Split Control - Flow (mL/min)** of the carrier gas to 15 - 20 mL/min to save carrier gas during standby.

Note: This setup can only be used on a GC equipped with programmable pressure control (PPC) of the carrier gas.

The screenshot shows the Instrument Control window with the Carrier tab selected. The Split Control section is highlighted with a red circle, showing the Flow (mL/min) set to 20.0. The interface includes a graph, a table for carrier ramps, and various control options.

| Carr. A Ramp | Rate | Setpoint | Hold |
|--------------|------|----------|--------|
| Initial | 0.0 | 2.50 | 999.00 |
| 1 | 0.0 | 0.00 | 0.00 |
| 2 | 0.0 | 0.00 | 0.00 |
| 3 | 0.0 | 0.00 | 0.00 |

Mode:
 Carrier A Control: Programmed Flow
 Carrier B Control: NONE

Split Control:
 Ratio (n:1): 7.0
 Flow (mL/min): 20.0
 Mode: Flow

Method Editor – Instrument – Control Options – Split Control – Gas saver mode.

Important Note: This split flow saving mode may cause baseline upsets if you are using a flow sensitive detector such as an ECD or TCD detector.

Chapter 2 – Method Tips

6. Process Options – Integration – Noise Threshold

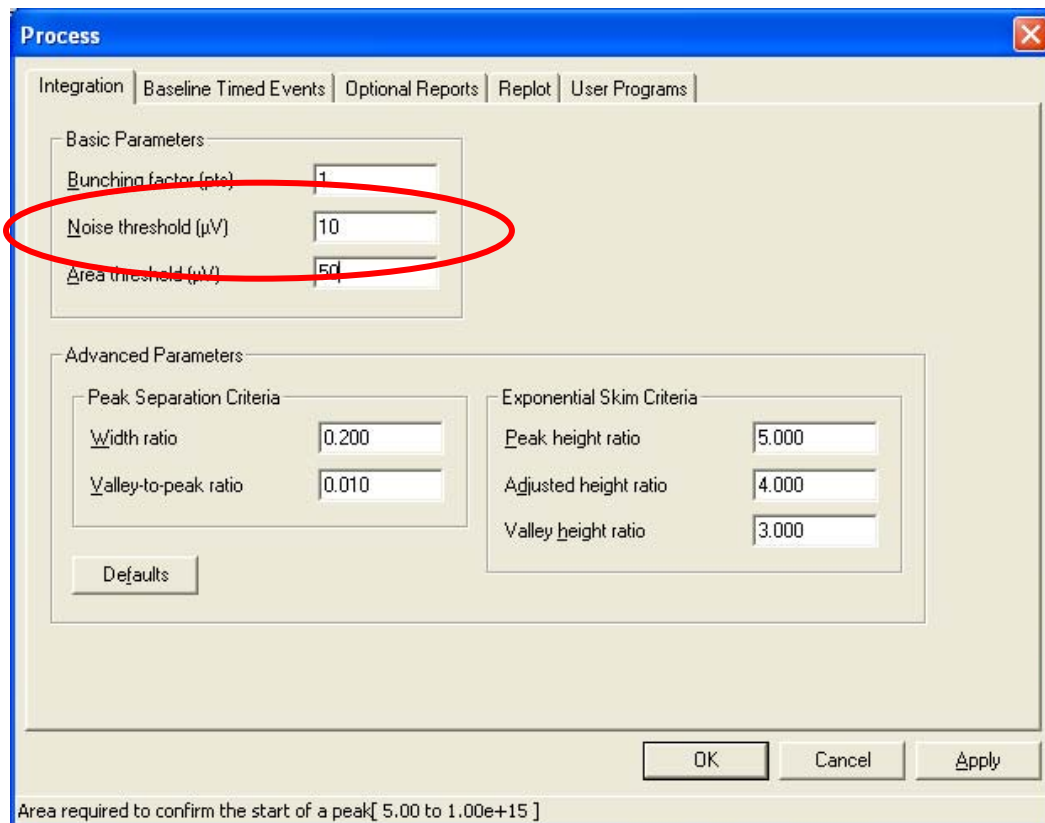
The Method **Process -Integration** parameters determine how the baseline is drawn under your peaks of interest.



1. Noise threshold parameter.

Tip #16 - The **Noise threshold** parameter controls where the start and end points are located for peak detection, i.e. where the peak baseline is drawn.

- a. **Higher numbers** for the **Noise threshold** will move the peak start and end points in toward the crest of the peak.
- b. **Lower numbers** will move the peak start and end points away from the crest of the peak.



Method – Process parameters – Integration tab – Noise threshold

Chapter 2 – Method Tips

7. Process Options – Integration – Area Threshold

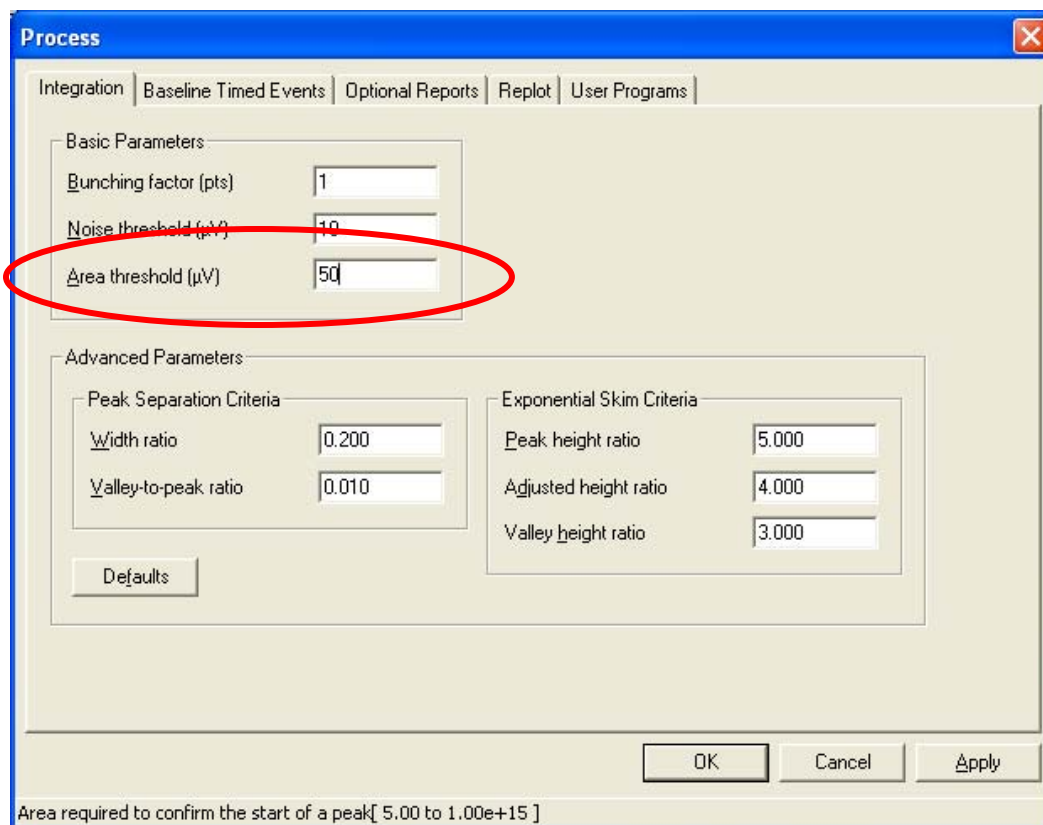
The Method **Process -Integration** parameters determine how the baseline is drawn under your peaks of interest.



2. Area threshold parameter.

Tip #17 - The **Area threshold** parameter controls whether a peak will be integrated as a peak of interest or eliminated as noise.

- a. **Lower numbers** for the Area threshold will allow integration of smaller peaks.
- b. **Higher numbers** for the Area threshold will eliminate small noise (or sample) peaks on the baseline.



Method – Process parameters – Integration tab – Area threshold

Note: A ratio of **1:5** is recommended for the Noise to Area threshold settings.

Chapter 2 – Method Tips

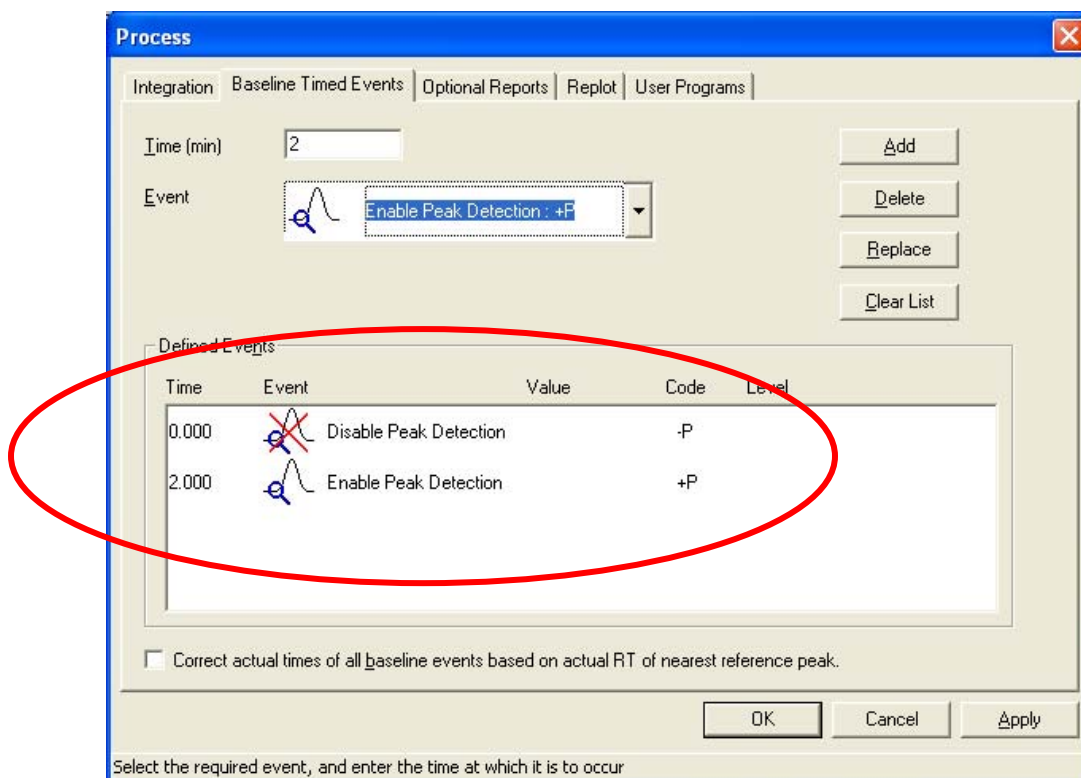
8. Process Options – Baseline Timed Events

Tip #18 - You can setup the method to automatically ignore the integration of the solvent peak and other baseline upsets using the **Process -Baseline Timed Events** functions.



3. Locking out integration of the solvent peak.

- a. Click on the **Process** drop-down menu.
- b. Select **Baseline Timed Events**.
- c. Select the **Disable Peak Detection** (-P) function with the **Event** browse button. Set the **Time** to 0 (zero) (min) and click on the **Add** button.
- d. Select the **Enable Peak Detection** (+P) function with the **Event** browse button. Set the **Time** to after the crest of the solvent peak and click on the **Add** button.



Method Editor - Process Menu – Baseline Timed Events – Peak Detection.

Note: Use Timed-Events sparingly and only when necessary. As the column ages component retention times may shift unlike the timed events that are at fixed times in the method.

Chapter 2 – Method Tips

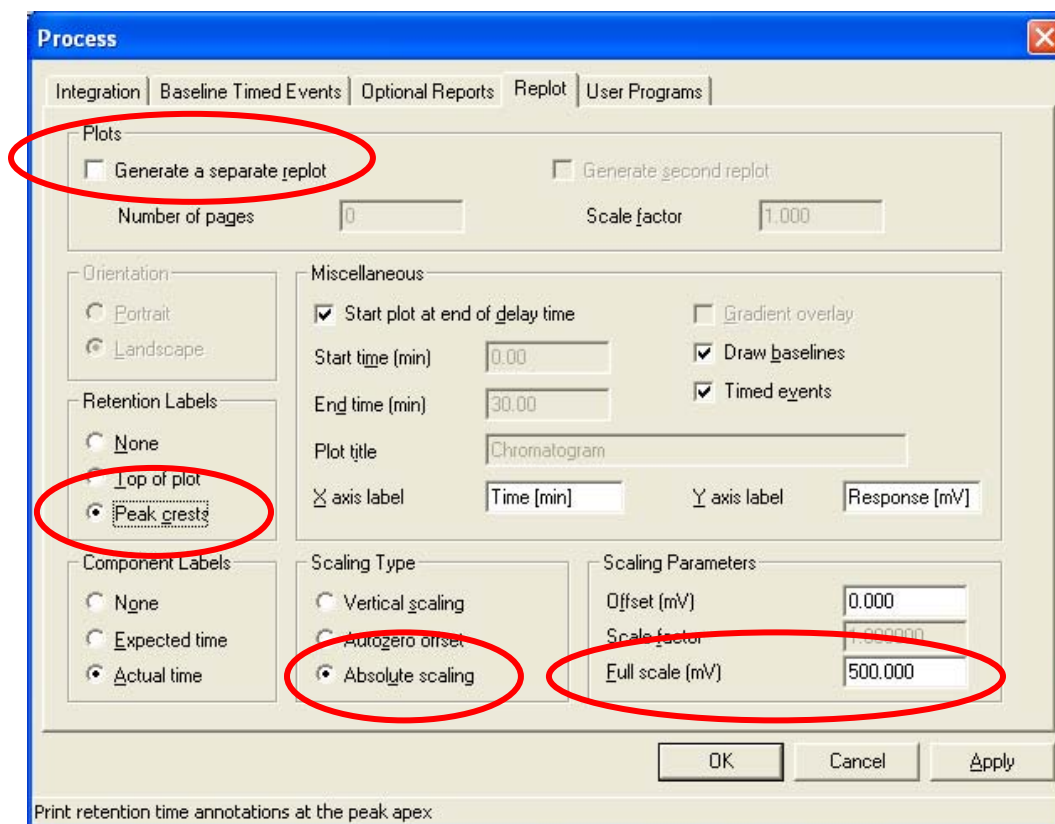
9. Process Options – Replot

Tip #19 - The method replot parameters for your chromatogram printout can be modified from the default options in **Process - Replot**.



4. Replot Settings Optimization.

- a. Uncheck the **Generate a separate replot**. **Note:** Be sure to add **Print a Plot with Report** in the Report Format file that is associated with your method.
- b. Set the **Retention Labels** to **Peak crests**.
- c. Set the **Scaling Type** to **Absolute scaling**, and set the **Full scale (mV)** for your desired plot display. This will fix the vertical axis of the chromatogram replot so that you can visually compare chromatograms.



Method Editor – Instrument – Control Options – Split Control – Gas saver mode.

Important Note: Always check that your largest peak of interest is on scale at or below 500 mV. This will prevent the clipping of your peaks and loss of data.

Chapter 2 – Method Tips

10. Components – Global Information

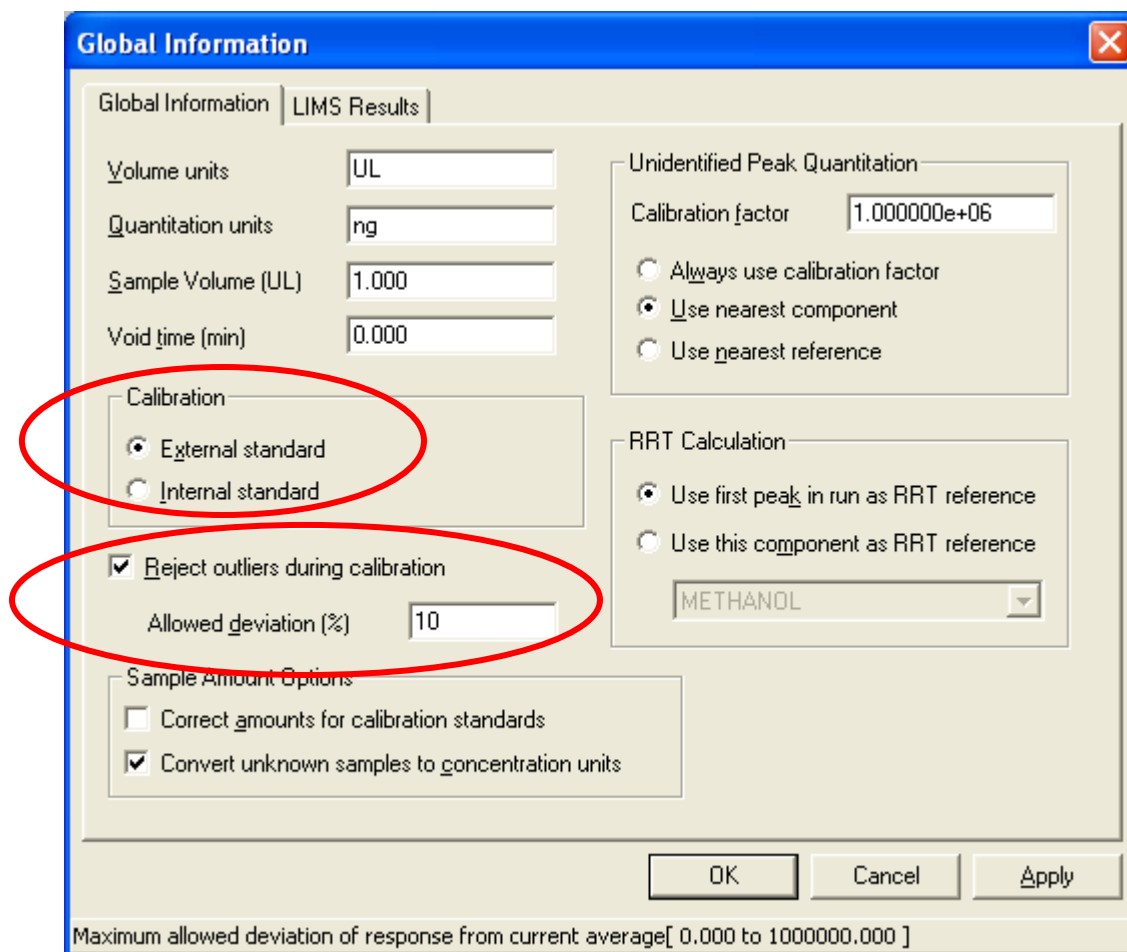
The method Global Information options must be selected for method calibration type and auto-calibration.



1. Calibration type selection.

a. In the window you can choose between the **External** or **Internal standard** calibration calculations.

Tip #20 – Select the **“Reject outliers during calibration”** feature to automatically reject calibration results that deviate by more than the allowed % entered for this option. This is very useful for method calibration runs that are added to a long sample analysis sequence or auto-calibration sequences.



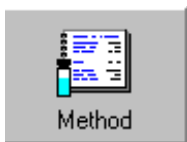
Method Editor – Component – Global Options – Calibration type/Reject outliers.

Chapter 2 – Method Tips

11. Components – Component Defaults

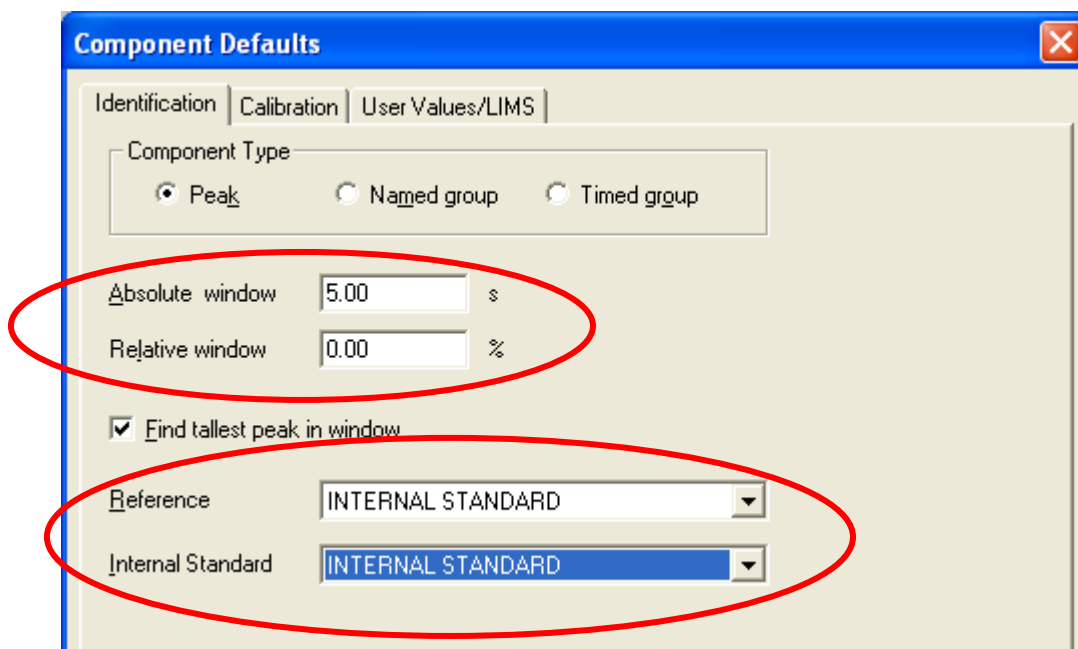
Tip #21 - The Component Defaults values for component identification and calibration may be added. Entering these before adding any components to the method will greatly speed up data entry of a component list with multiple entries.

Note: These default values must be entered **BEFORE** any components are added to a new method. If these default values are not entered before entering components they will not be applied automatically.



2. Component Defaults - Identification

- Enter an Absolute window value for component ID. This value is in seconds around both sides of the crest of each component.
- Turn off the Relative window to remove this parameter from the component ID calculations to simplify the ID window calculation.



Method Editor – Component Defaults – Component ID windows and References.

Tip #22 – Check the “**Find tallest peak in window**” function so that the ID software will find the tallest peak in the window as apposed to the default which is the peak closest to the middle of the window.

Chapter 2 – Method Tips

11. Components – Component Defaults - continued

Note: Remember that any default values must be entered **BEFORE** any components are added to a new method.



2. Component Defaults - Calibration

a. Select the Calibration Type, use **Avg calibration factor** for a single level calibration. Select **Use curve** for multi-level calibration methods.

b. Enter the calibration **Level** names, **Amounts** and choose whether to **Include** or to **Force** the origin.

Component Defaults

Identification | Calibration | User Values/LIMS

Calibration Type

Use calibration factor
 Avg calibration factor
 Calibrate by reference
 Use curve

Response

Area
 Height

Curve fit type: 1st Order

Scaling: None

Weighting: None

Purity (%): 100.0000

Origin Treatment

Include
 Force

| | Level | Amt. | Area (µV·s) |
|---|---------|-----------|-------------|
| 1 | Level 1 | 1.000000 | 0.000000 |
| 2 | Level 2 | 2.000000 | 0.000000 |
| 3 | Level 3 | 5.000000 | 0.000000 |
| 4 | Level 4 | 10.000000 | 0.000000 |
| 5 | Level 5 | 20.000000 | 0.000000 |

OK Cancel Apply

Use a calibration curve to calculate amounts

Method Editor – Component Defaults – Calibration using multiple levels.

Tip #23 – To prevent results calculated by using a curve fit from giving negative values, choose **Force** for the **Origin Treatment**.

Chapter 2 – Method Tips

12. Report Format Editor

The **Report Format Editor** is used to build the Report file (.RPT) that controls what data is included in the printed report.

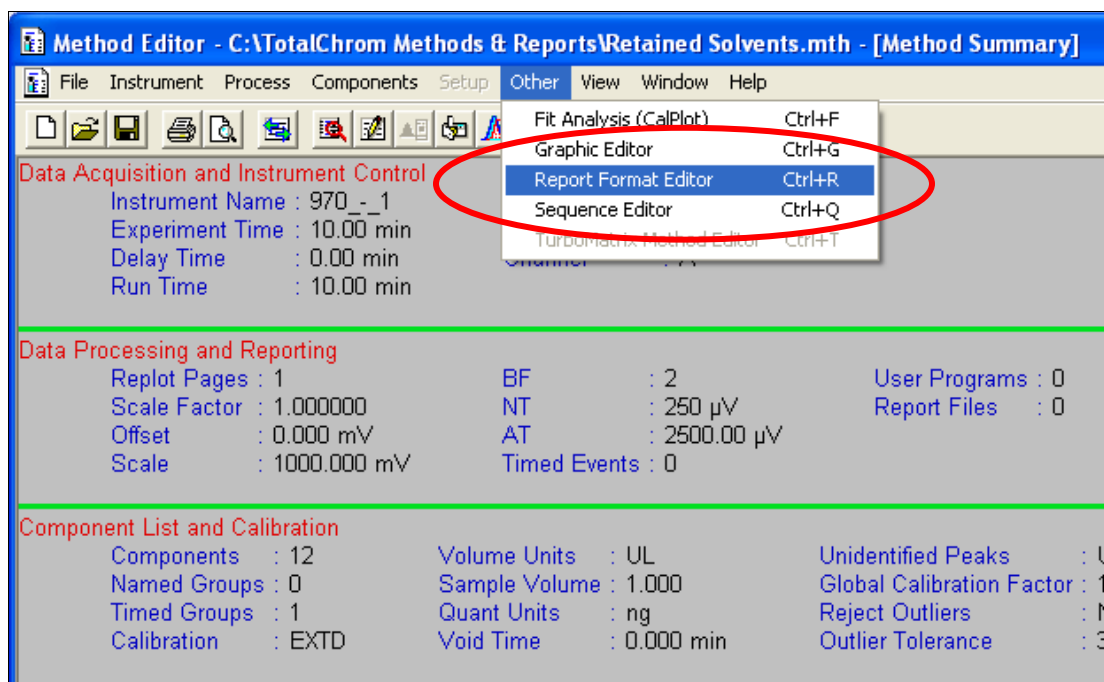
Tip #24 - It is a good practice to use the **same file name** for the Report file as was used for the Method file and to store it in the **same directory** as the Method file.

Note: If TotalChrom can not find the method Report file it will use the Default Report.



1. Using Report Format Editor.

- a. Generate a method with components and calibration information.
- b. Click on the **Other** menu in the Method Editor window and choose the **Report Format Editor** function.
- c. The Report Format displayed for a new method is the **Default Report**.



Method Editor – Other – Report Format Editor

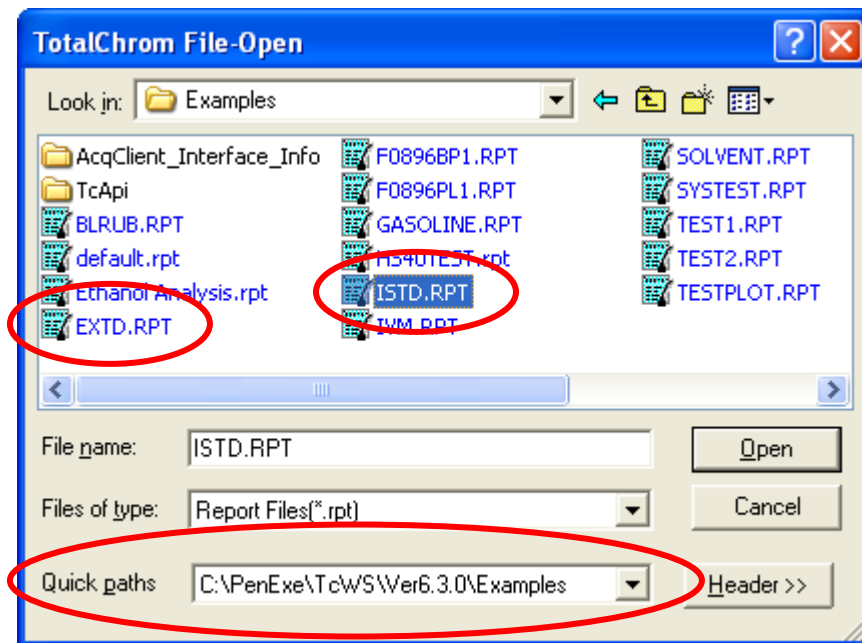
Chapter 2 – Method Tips

12. Report Format Editor - continued

Tip #25 - An easy way to create a new external or internal standard Report Format file is to use the templates stored in the TotalChrom Examples directory.

**2. Using Report Format templates.**

- a. Click on the **File** drop-down menu in the Report Format Editor window.
- b. Select the **Open** function.
- c. Click on the **Quick paths** browse button and select the TotalChrom Examples directory path: **C:\PenExe\TcWS\Ver6.3\Examples**.
- d. Select the **ISTD.RPT** for internal standard calibration report format or **EXTD.RPT** for external standard calibration report format.



Report Format Editor – File – Open – TotalChrom Examples Directory

Chapter 2 – Method Tips

12. Report Format Editor - continued

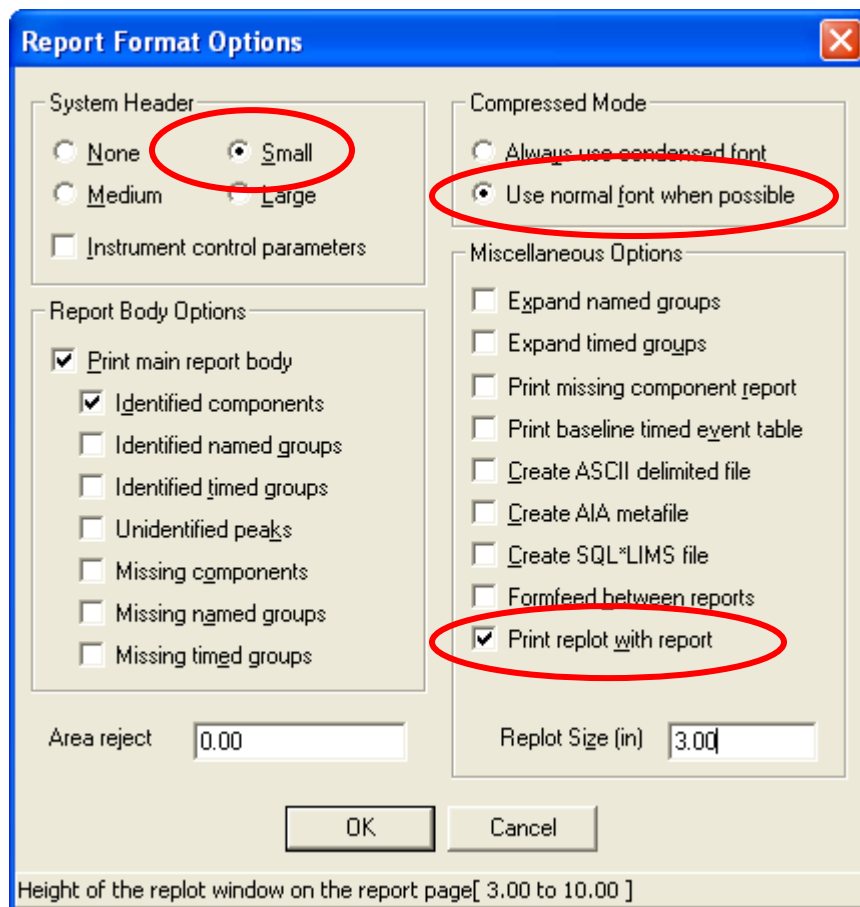
Tip #26 - When using the templates stored in the TotalChrom Examples directory be careful not to modify the template file itself or it will not be available for the next user. **Save the Examples template to your method name and path before editing this file.** Do not overwrite the template files!

**2. Using Report Format templates - continued.**

a. Use **File/Save as** to save the Examples template format with the method name that you are developing.

The following modifications to the default report are suggested.

- Select the **Options** drop-down menu and select **Small** for **System Header**.
- Select **Use normal font when possible** for **Compressed Mode**.
- Check the **Print replot with report** in **Miscellaneous Options** to create a one-page report with the chromatogram on the same page as the results.



Report Format Options

Chapter 2 – Method Tips

12. Report Format Editor - continued

Tip #27 - All of the fields and columns in a Report Format file can be edited by the user. Simply click on a field and edit it as desired.



3. Editing the Report Format file.

- a. **Delete** all the extra columns in the report format until the report font is no longer compressed.
- b. Click on the format **Title** and enter your report name.
- c. Click on a column label to modify a column label name.
- c. Change the number of **Digits** to display after the decimal point in a data column with the **Replace** command.
- d. The columns may be rearranged using the **Move** command.
- e. Click on **File** and **Save** the modifications to your report format file.

Report Format Editor - C:\TotalChrom Methods & Reports\Solvent.rpt

File User Notes Report Edit Options Help

INTERNAL STANDARD REPORT

| 1 | 2 | 3 | 4 | 5 |
|--------|----------------|--------------------|-------------------------|------------|
| Peak # | Ret Time [min] | Peak Area [uV-sec] | Component Name | Raw Amount |
| 000 | 00000.00 | 000000.00 | XXXXXXXXXXXXXXXXXXXXXXX | 00000.0000 |

Raw Amount

Current column: 5

Column number: 5

Column width: 10

Digits: 4

Column label: Raw

Second label: Amount

Calculate total for this column

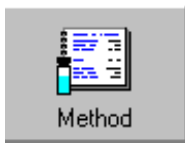
Location of this column across the page[1 to 6]

Report Format Editing

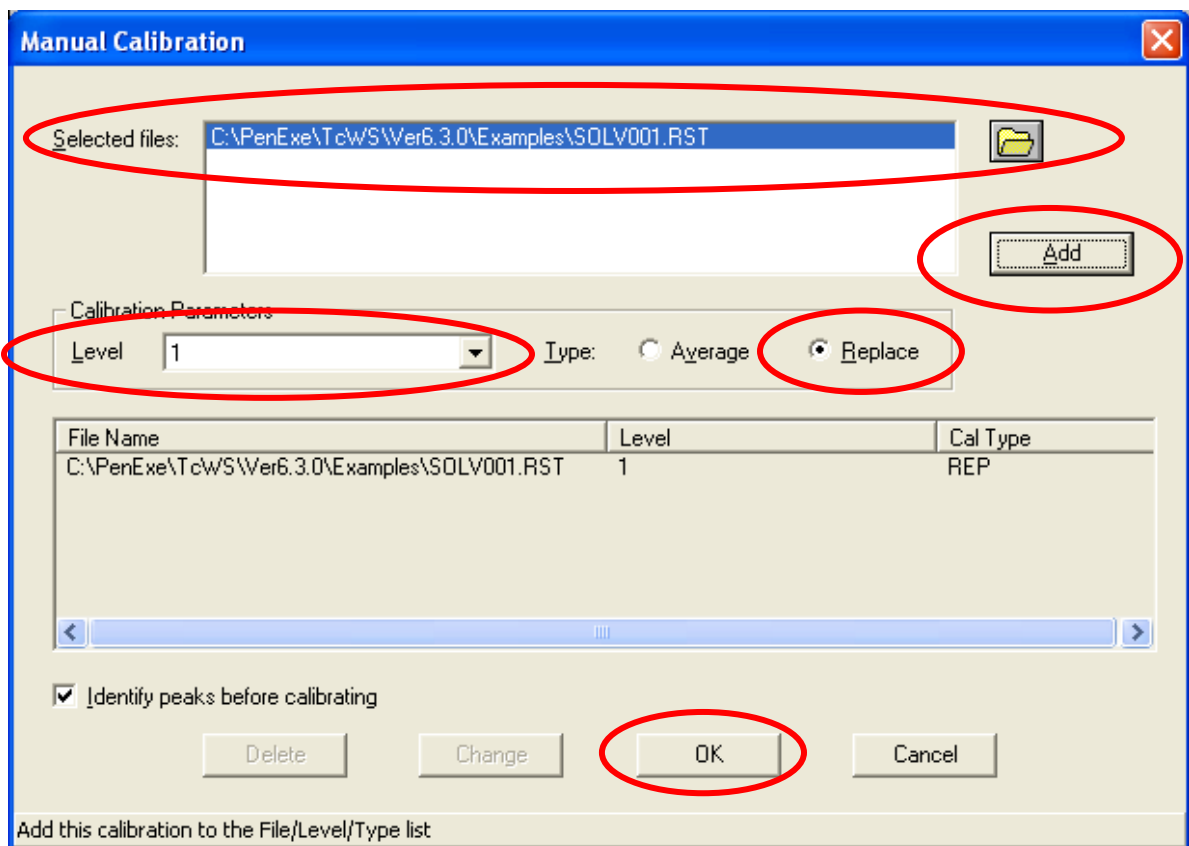
Chapter 2 – Method Tips

13. Components – Calibrate

Tip #28 - The **Components - Calibrate** function allows the user to calibrate a method manually. This function is very useful for initial calibration of the method to check that all parameters are entered correctly.

**1. Using the Method Calibration function.**

- a. In the **Components** drop-down menu click on **Calibrate**.
- b. Select a calibration standard data file that was previously run using the browse button.
- c. In the **Calibration Parameters** box, select the **Level** name, Calibration **Type – Average** or **Replace** and click on the **Add** button.
- d. Click on the **OK** button to perform the method calibration.



Method Editor – Components - Calibrate – Manual Calibration.

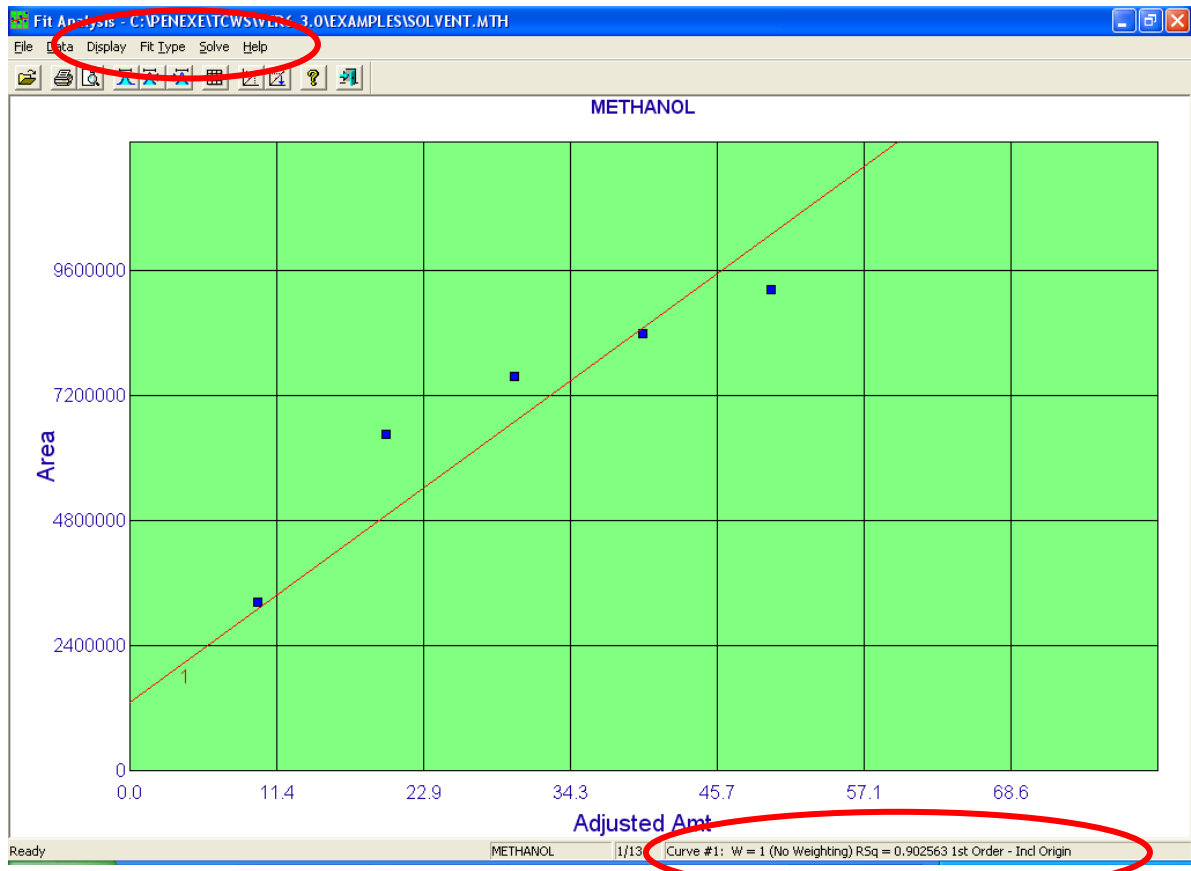
Chapter 2 – Method Tips

14. Other – Fit Analysis (CalPlot)

Tip #29 - When performing a multi-level calibration you can review the calibration curve data stored in the method using the **Fit Analysis** function to check for out-laying data points and curve linearity (R-Squared results).

**1. Calibration Review – Fit Analysis.**

- a. In the **Other** drop-down menu, click on **Fit Analysis (CalPlot)**.
- b. The R-Squared results are displayed in the bottom right-hand corner of the window.
- c. The calibration curve information may also be reviewed by selecting **Fit Type** drop-down menu and selecting **Curve Info**.



Method Editor – Other – Fit Analysis (CalPlot).

Chapter 3 – Graphic Method Editor Tips

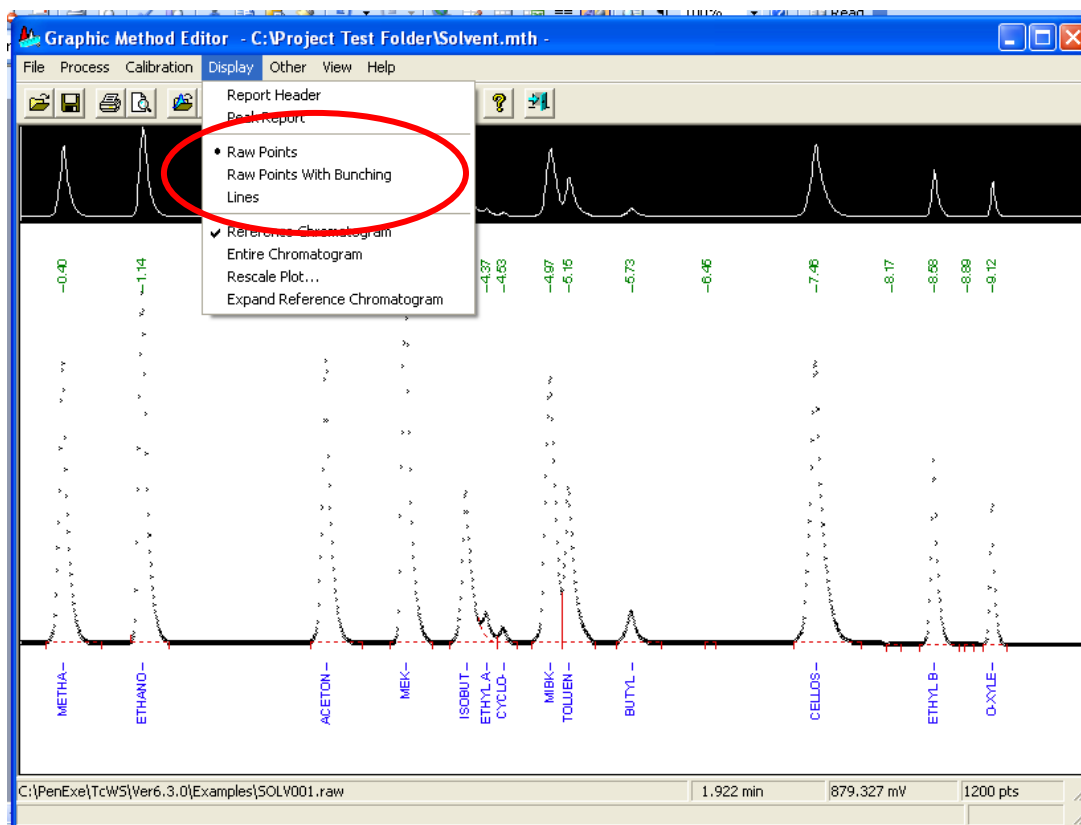
1. Graphic Method Editor

Tip #30 - Use the Graphic Method Editor - **Display** functions to view the actual data points collected in any raw data file. This function will allow you to optimize the data sampling rate parameter for acquiring data.

**1. Display Raw Data Points**

In the **TotalChrom Navigator** screen single click on the **Graphic Edit** button. Click on the **Display** drop-down menu and select the **Raw Points** function.

Your raw data files will now be displayed showing the actual data points.



Graphic Method Editor – Display - Raw Points screen.

Tip #31 - One way to access the **Graphic Editor** is from the Method Editor screen. Using this technique, you will not need to re-select your method file name in the Graphic Editor.

Click on the **Other** drop-down menu in the Method Editor and select **Graphic Editor**.

Chapter 3 – Graphic Method Editor Tips

2. Graphic Method Editor - Bunching factor

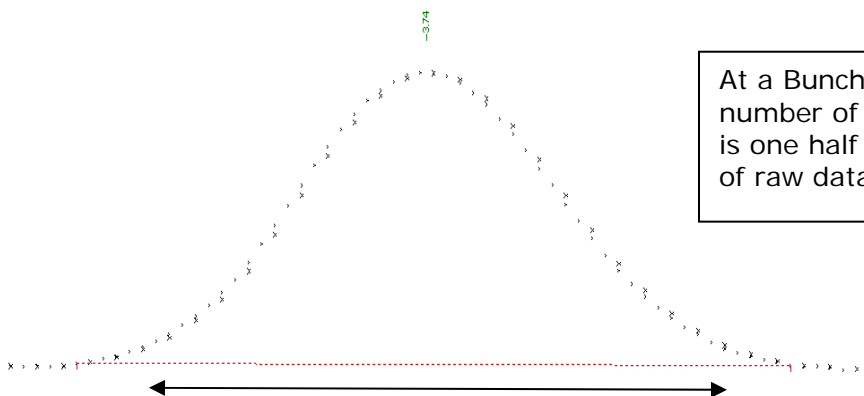
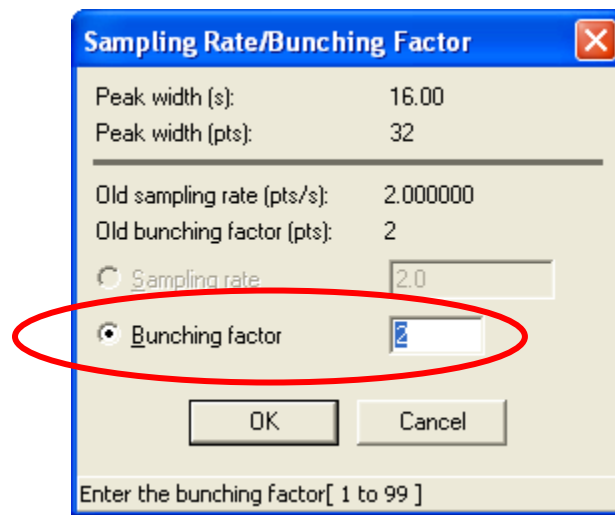
Tip #32 - You can optimize the bunching factor applied to the data points collected in a raw data file using the Graphic Method Editor.



1. Bunching Factor – manual optimization

The TotalChrom Bunching factor is used to generate average data points which in turn will help to remove baseline noise and spikes.

Tip #33 - It is recommended that the maximum Bunching factor never exceed a value of **3 – 5** points. Reduce the Sampling Rate value if higher bunching factors are indicated.



At a Bunch factor of 2 the number of bunched points is one half of the number of raw data points.

Graphic Method Editor – Display - Raw Points with Bunching

Tip #34 – The optimum points/peak is 15 - 40 bunched (averaged) points.

Bunch factor values of 2 or 3 (average of every 2 or 3 data points) can also be used to improve the baseline placement and peak integration results.

Chapter 3 – Graphic Method Editor Tips

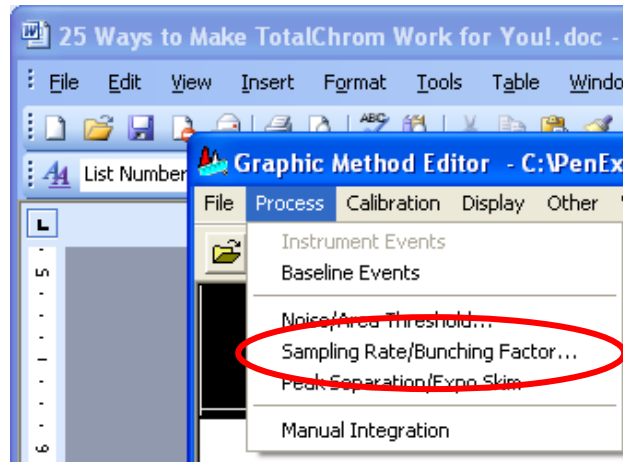
2. Graphic Method Editor - Bunching factor – continued

Tip #35 - You can optimize the Bunching Factor automatically with the **Process - Sampling Rate/Bunching Factor** function.



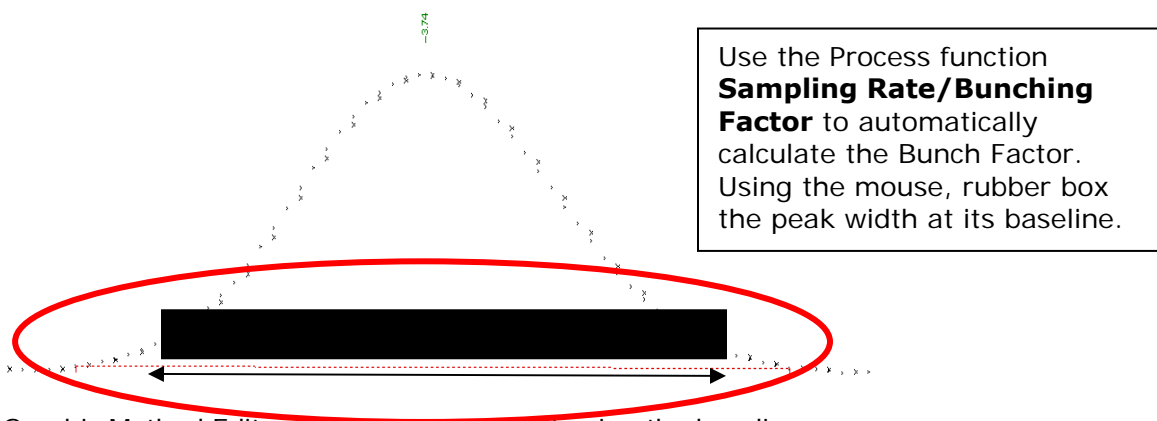
2. Optimize the Bunching Factor automatically.

a. Click on the **Process** drop-down menu and select the **Sampling Rate/Bunching Factor**.



Graphic Method Editor -Process Menu – Sampling Rate/Bunching Factor.

b. Using the mouse, rubber box the narrowest peak of interest at its baseline. **DO NOT** include peak pre/post tail area.



Graphic Method Editor – Process – Rubber boxing the baseline.

Important Note: If a bunch factor higher than 2 or 3 is calculated to achieve 20 – 40 bunched points it is better to reduce the Sampling Rate parameter.

Chapter 3 – Graphic Method Editor Tips

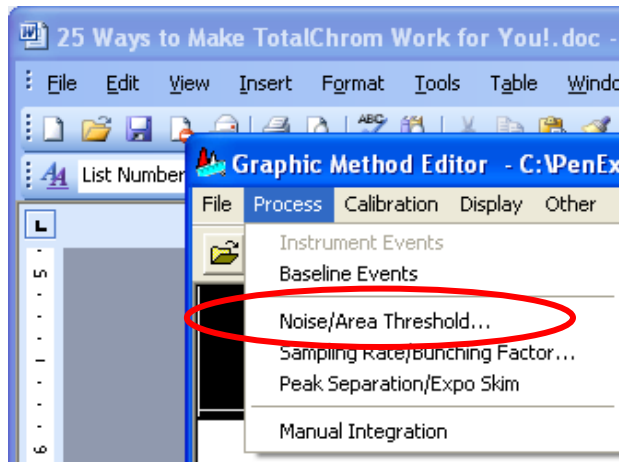
3. Graphic Method Editor – Noise/Area Threshold

Tip #36 - You can optimize the Noise and Area thresholds automatically to remove excessive numbers of noise peaks from the chromatogram with the **Noise/Area Threshold** function.

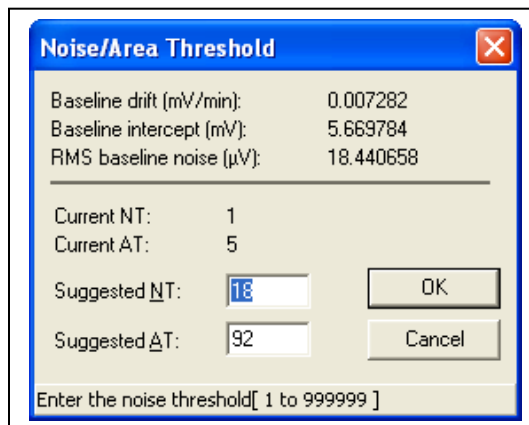
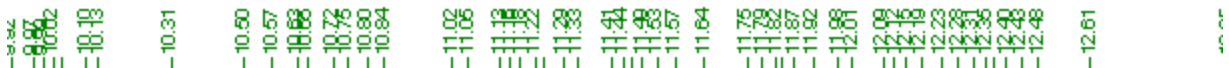


1. Optimize the Noise/Area Thresholds.

a. Click on the **Process** drop-down menu and select **Noise/Area Threshold**.



b. Using the mouse, rubber box to highlight a section of baseline noise. **DO NOT include peaks.**



Process Menu – Noise/Area Threshold.

Note: A ratio of 1 to 5 is recommended for the Noise and Area Thresholds.

Chapter 3 – Graphic Method Editor Tips

4. Graphic Method Editor – Component Editing

Tip #37 - A fast and easy way to update or even generate a method component list is by using the Graphic Editor **Calibration – Edit Components** functions.



1. Graphic Component Editing

- Click on the **Calibration** drop-down menu and select **Edit Components**.
- Using the mouse, rubber box to highlight a section of chromatogram to update.
- Click on a component that was not identified correctly due to a retention time shift. The peak will be enclosed in a dotted line box.
- In the **Name** window click on the browse button to open the list of your component names. Select the component name of interest and click on the **Next** button.

Graphic Method Editor - C:\Project Test Folder\Solvent.mth -

Type Re-Identify Return Help

Peak : 3
Retn time : 12.606
Area : 49341.60
Height : 8080.58

RRT Ref. Ref. ISTD

Name: ACETONE
Reference: MEK
ISTD: ISOBUTANOL
Absolute win: ETHYL ACETATE
Relative win: CYCLO-C6
MIBK
TOLUENE
BUTYL CELLOSOLVE

Find tallest peak in window

Update calibration

Level:
Amount:

Calibration type
 Average Replace

C:\PenExe\TcW5\Ver6.3.0\Examples\F86A195.raw 14.117 min 9.955 mV 1217 pts
Use Next/Prev or Return to accept changes. Click on another peak to cancel changes. **MODIFIED**

Graphic Method Editor - Calibration – Edit Components

Chapter 3 – Graphic Method Editor Tips

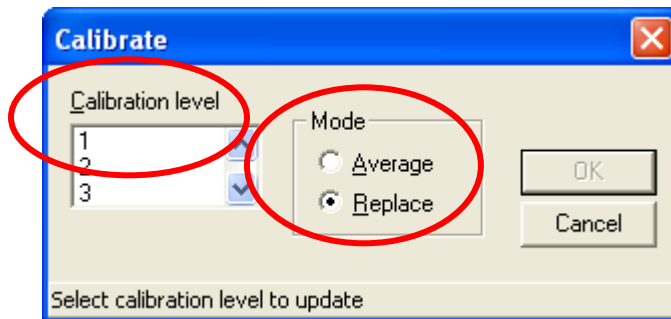
5. Graphic Method Editor – Calibration

Tip #38 - One easy way to manually calibrate a method is with the Graphic Method Editor **Calibration - Calibrate** function.



1. Manual Calibration.

a. Click on the **Calibration** drop-down menu and select **Calibrate**.



Calibration – Calibrate

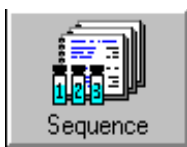
- b. Select the **Calibration level**.
- c. Select the **Mode**, either **Average** or **Replace**.
- d. Click on the **OK** button. The method is calibrated with the parameters selected.
- e. Click on the **File, Save** to save your calibration.

Important Note: Check to be sure that the data file currently being viewed in the Graphic Method Editor is a calibration standard run before using the **Calibrate** function.

Chapter 4 – Sequence Editor Tips

1. Sequence Editor – Auto-Calibration Sequence

Tip #39 - You can automatically calibrate your method with a sequence setup for auto-calibration. This is a fast and easy way to re-calibrate your method when using an autosampler to inject your samples.



1. Create an Auto-Calibration Sequence

- a. In the TotalChrom **Navigator** screen, click on the **Sequence** button.
- b. **Load** or **Create** a Sequence that uses the method you wish to calibrate automatically.
- c. The example below shows a three injection sequence which will generate average response factors for all components in the method.
- d. **Save** your auto-calibration sequence with the method name included in the auto-calibration sequence name for easy identification.

Example Name: Retained Solvent Auto-Calibration.seq

| Row | Type | Name | Vial | Method | Rpt Fmt File | Data | Calib Rpt | Cal Level | Update R1 |
|-----|-------------|------------|------|-------------------|-------------------|-------------|-----------|-----------|-----------|
| 1 | Cal:Replace | Cal Std #1 | 1 | retained solvents | retained solvents | Cal Std_001 | Short | Level 1 | Yes |
| 2 | Cal:Average | Cal Std #2 | 2 | retained solvents | retained solvents | Cal Std_002 | Short | Level 1 | Yes |
| 3 | Cal:Average | Cal Std #3 | 3 | retained solvents | retained solvents | Cal Std_003 | Short | Level 1 | Yes |
| 4 | | | | | | | | | |
| 5 | | | | | | | | | |
| 6 | | | | | | | | | |
| 7 | | | | | | | | | |

Sequence Editor – Auto-calibration sequence for average response factors.

Important Note: Double check to be sure that the sample vials in the autosampler tray positions to be analyzed are indeed the calibration standards to be run before using this auto-calibration sequence. **A method that is calibrated with the wrong samples will give erroneous results.**

Chapter 4 – Sequence Editor Tips

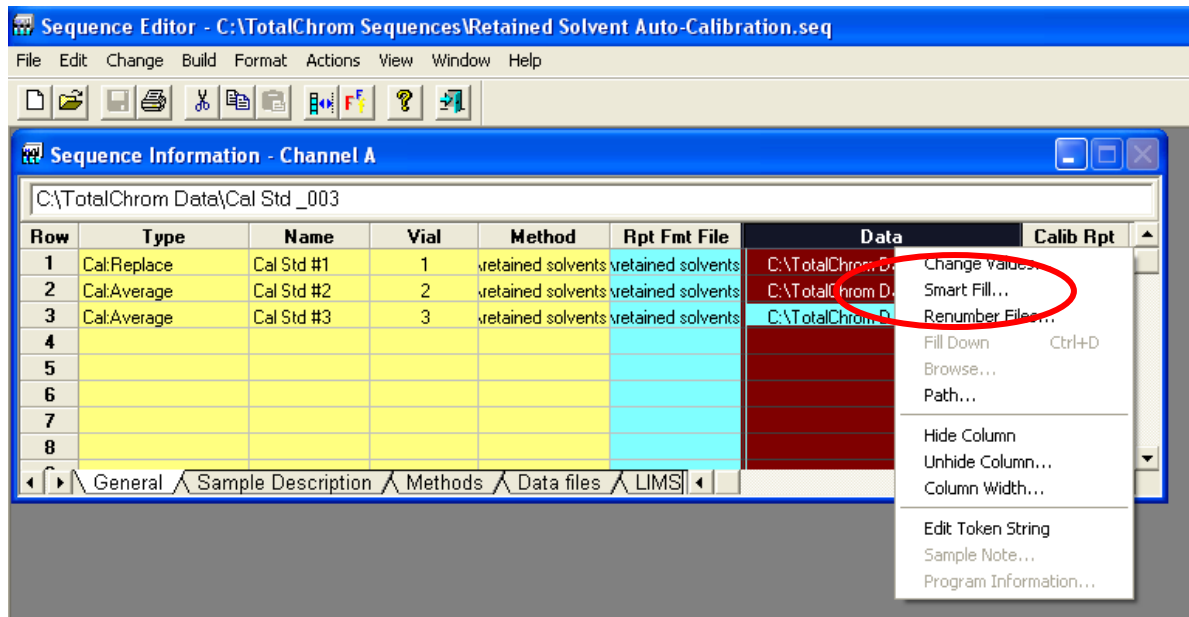
2. Sequence Editor – Smart Fill

Tip #40 - Use the **Smart Fill** function to easily update or change the data file names in your sequence. This is a fast way to re-name your data files with unique names so that they can be located easily for future reference.

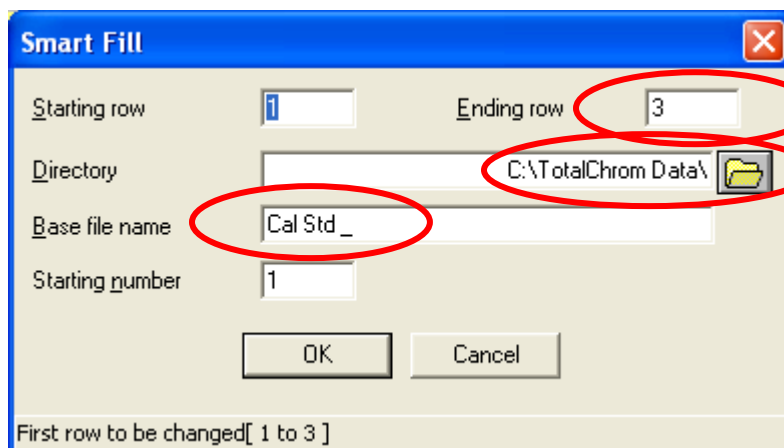


1. Use Smart Fill to edit Sequence Data File Names.

- a. **Load** or **Create** a Sequence.
- b. **Right click** in the **Data** column and select **Smart Fill**.



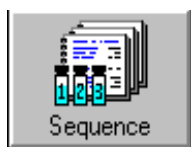
- c. Enter the **Starting Row, Ending Row, Directory** and Edit the **Base file name** as necessary to give your data files unique names.



Chapter 4 – Sequence Editor Tips

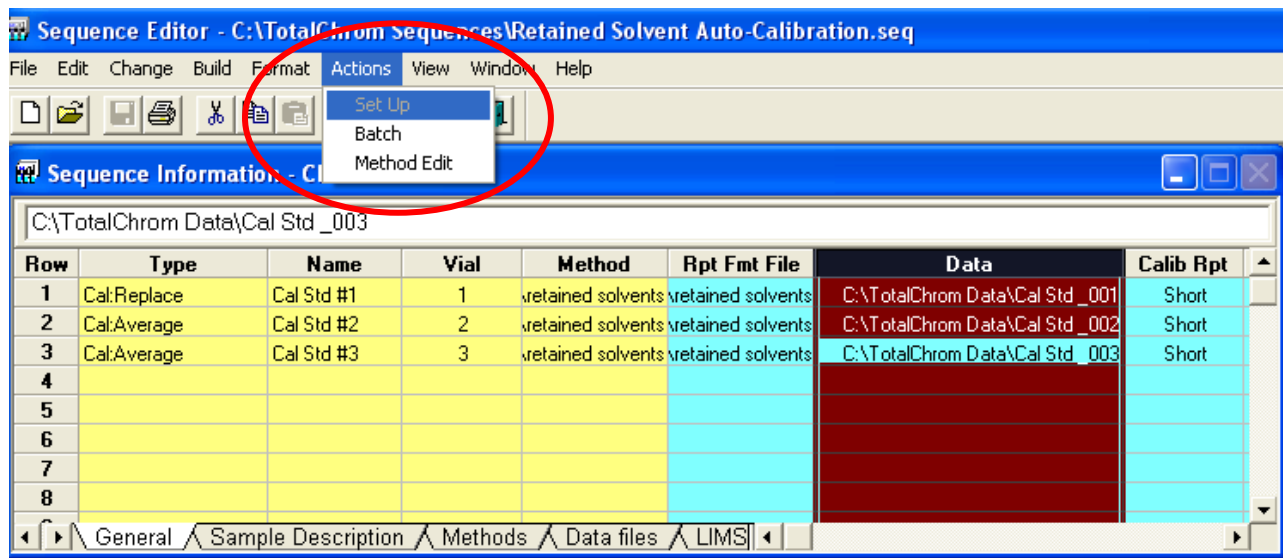
3. Sequence Editor Shortcuts – Actions - Setup

Tip #41 - The shortcut for sequence setup is located in the Sequence Editor **Actions** drop-down menu. With this shortcut the sequence file will not need to be re-selected. This is a fast and easy way to set-up your sequence without leaving the sequence screen.



1. Using the Actions - Set-Up function.

- Click on the **Actions** drop-down menu in the **Sequence Editor** screen.
- Select the **Set Up** function.



Sequence Editor – Actions – Set Up function.

2. Using additional Actions menu shortcuts.

You can also use the sequence Actions menu to open Batch or the method editor.

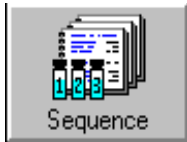
- Click on the **Batch** function to get to Batch reprocess your data files.
- Click on the **Method Edit** function to return to your method for additional modifications or manual calibration.

Chapter 4 – Sequence Editor Tips

4. Sequence Editor Shortcuts – Build – Append New Cycles

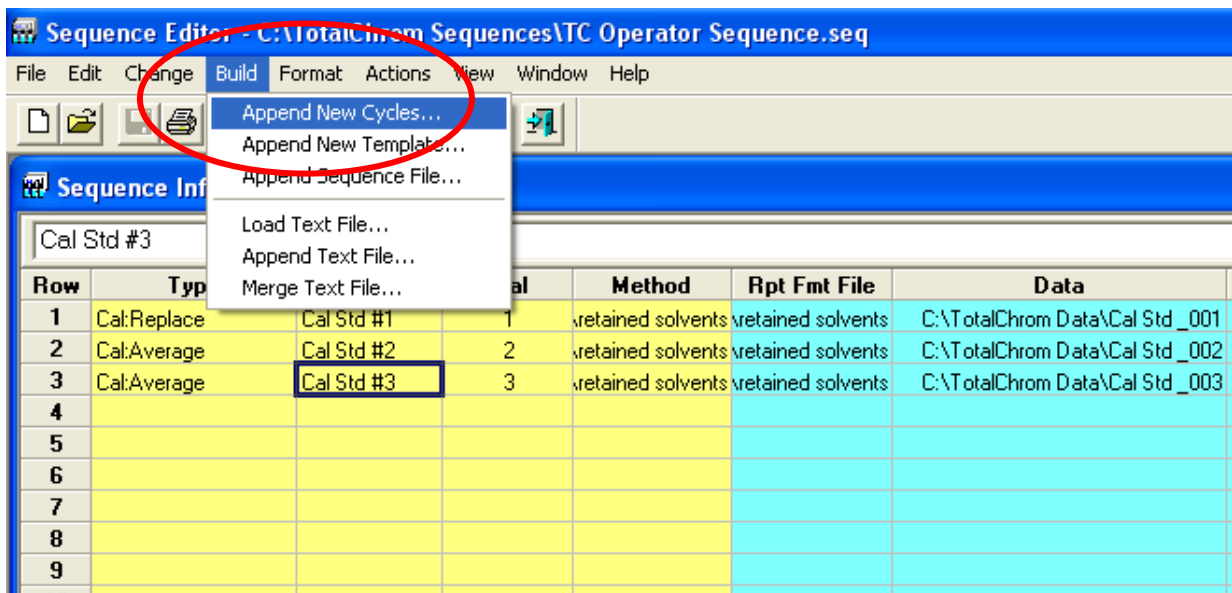
Tip #42 - The shortcut for adding new cycles (Sample rows) to a sequence is located in the Sequence Editor **Build** drop-down menu. This is a fast and easy way to append additional samples to your sequence.

Remember that a **"Cycle"** in TotalChrom is really synonymous for **Row #** during the initial running of the sequence.



1. Using Build - Append New Cycles function.

- Click on the **Build** drop-down menu in the **Sequence** Editor screen.
- Click on the **Append New Cycles** function.



Sequence Editor – Build – Append New Cycles (samples) function.

Chapter 4 – Sequence Editor Tips

4. Sequence Editor Shortcuts - Append New Cycles - continued

This shortcut will add new sample rows using the current method and report files and will automatically increment the data file names.

Note: The **Vial** number is not automatically incremented in the sequence when using this function. This will need to be changed manually or by clicking on Smart Fill in the vial column.



2. Set the Append New Cycles parameters.

- Click the **Type** browse button to select your sample type.
- Enter the **# of cycles** (sample rows) to be added.
- Type in your new sample name in the **Name** field.
- Click the **Add + Close** button to add the new cycles to your sequence.
- Review** the added sample rows and update the name and vial number, as necessary.

Append New Cycles

Identification | Files | Quantitation

Sample

Type: Sample

Name: New Samples

Number pattern: #

Study:

Vial: 4

Injection site: A

Actual number: 4

Rack: 1

Method: c:\penexe\tcws\ver6.3.0\tc data\retained sol

Add + Close Close Add

Vial number for this sample [0 to 100]

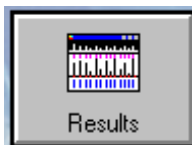
Sequence Editor – Build – Append New Cycles (samples) function.

Chapter 5 – Reprocess Tips

1. Results Reprocess

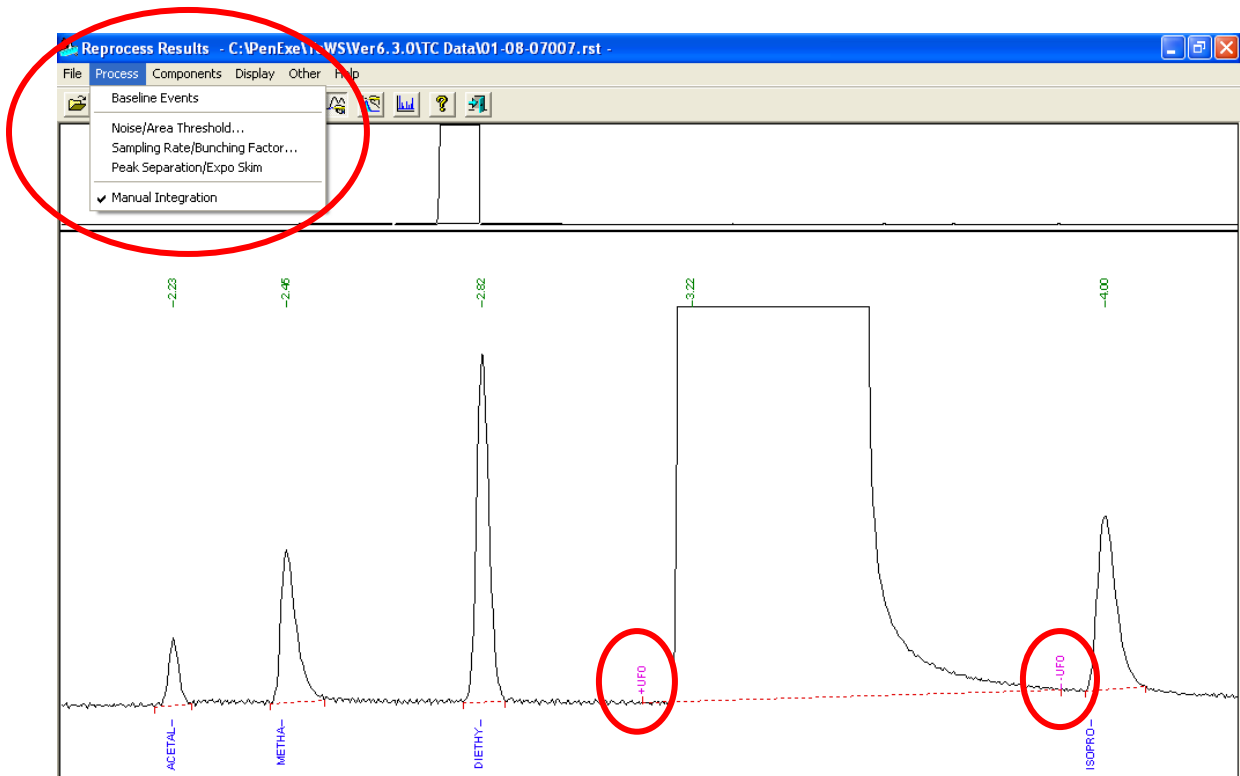
Tip #43 - Results Reprocess can be used to review an individual data file. You use these functions to manually preview, print, draw a component baseline, optimize the integration parameters and display the results from a data file.

Note: Results Reprocess changes to a data file DO NOT affect the stored method integration values!

**1. Manual Integration.**

Use manual integration to re-draw the baseline under a peak of interest.

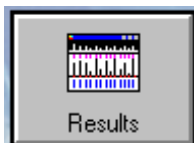
- Click the **Process** drop-down menu.
- Select **Manual Integration**.
- Place the **+** cursor on the baseline, in front of the peak of interest, click and drag the new baseline to a point after the peak.
- Review your new peak area in either **Display/Peak Report** or with **File/Print Preview Report**.



Reprocess Results – Process – Manual Integration.

Chapter 5 – Reprocess Tips

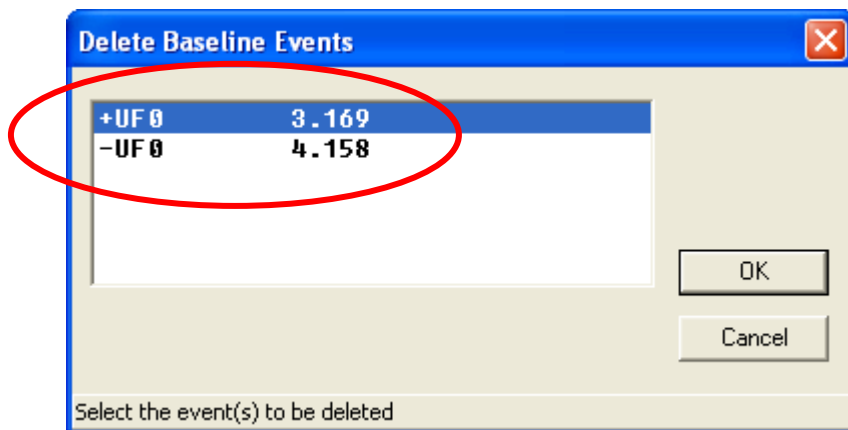
1. Results Reprocess - continued



2. Delete Baseline Events.

While using the manual integration to re-draw the baseline you may need to delete the manual baseline events during optimization of the baseline.

- Click the **Process** drop-down menu.
- Select **Baseline Events**.
- Click on the **Delete Events** function.
- Click on the **OK** button.
- Redraw the manual baseline as necessary.



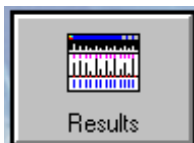
Reprocess Results – Process – Delete Baseline Event.

Important Note: Use caution whenever adding baseline events to a method. These events are fixed in time and DO NOT move automatically. Therefore, if a component retention shifts in time, as for instance when a column ages, fixed events may cause the baseline to be drawn incorrectly and improperly integrated!

Chapter 5 – Reprocess Tips

2. Batch Reprocess

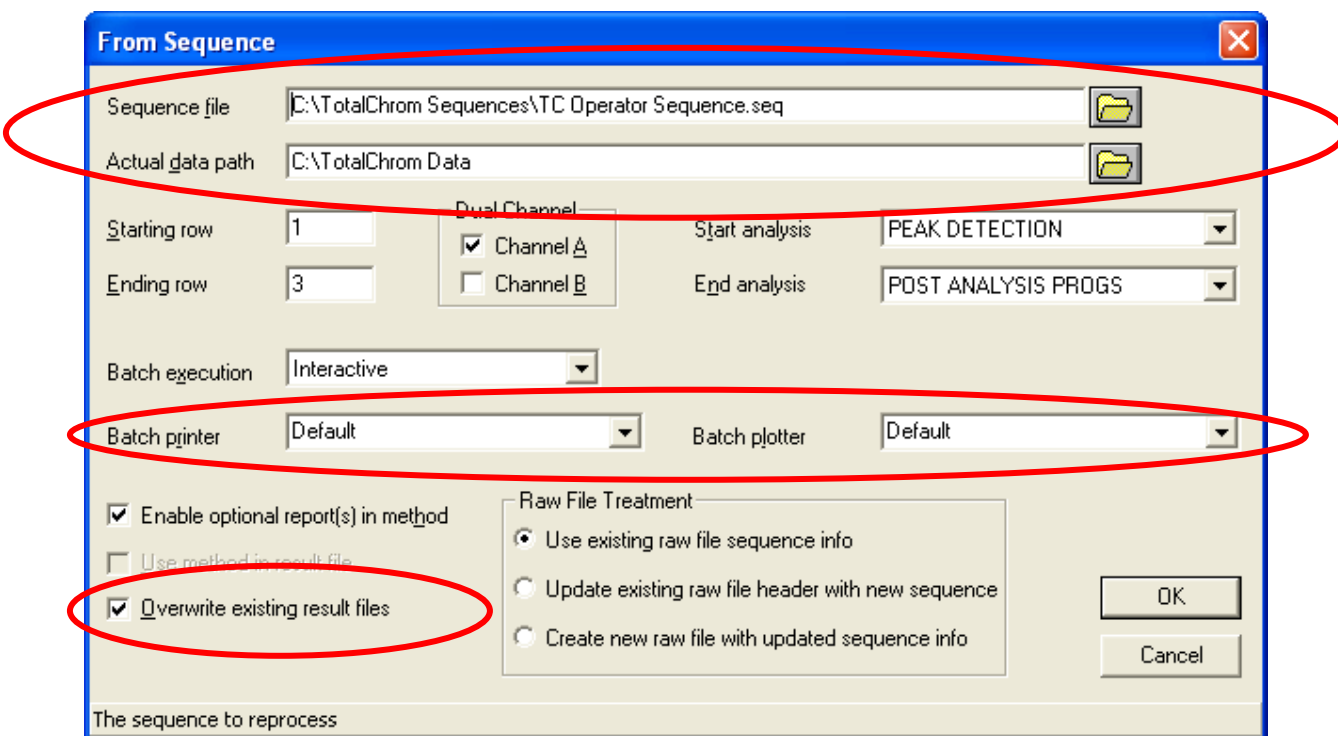
Tip #44 - Batch Reprocess can be used to automatically re-integrate an individual data file, a group of data files with the same name prefix or a sequence.



1. Batch Reprocess

Batch Reprocess is usually performed after method integration parameters have been optimized in the method either manually or by using the Graphic Method Editor.

- In the **TC Navigator** screen click on **Batch** Reprocess.
- Click on the **Three Vial Icon** or click on **File/Sequence**.
- Select your **Sequence file** using the browse button.
- Choose your **Actual data path** with the browse button.
- Check the **Overwrite existing result files** option.



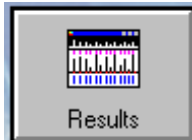
Batch reprocess – From Sequence

Note: Select **None** for the **Batch printer** to reprocess the data files only, without reprinting the results.

Chapter 5 – Reprocess

2. Batch Reprocess – continued

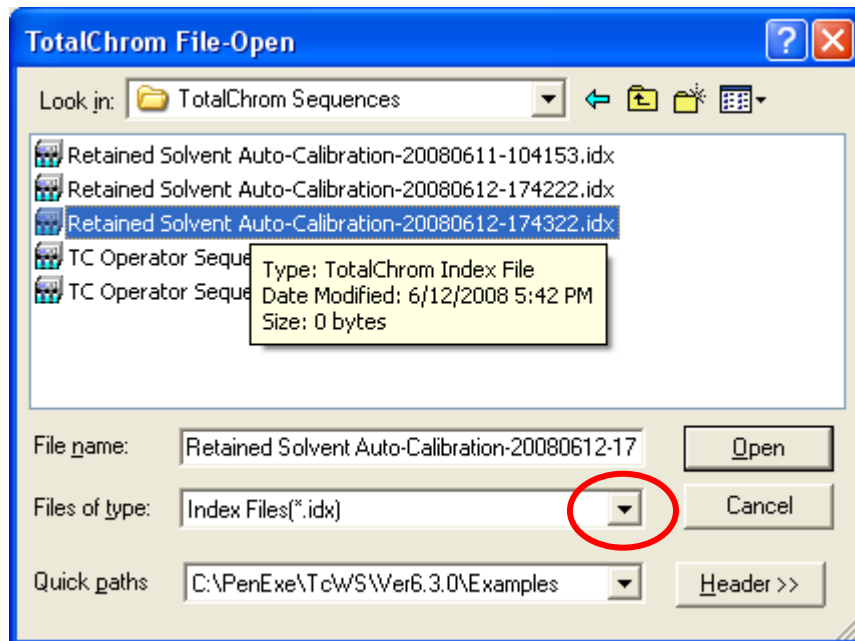
Tip #45 - If you reuse the same sequence over and over again as a template to collect data for numerous runs it may be easier to find your data using a sequence index file. A sequence index file is created each and every time a sequence is run.



1. Using Sequence Index (*.idx) Files.

Locate the sequence index files as follows:

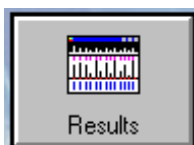
- a. In the Batch - **From Sequence** window click on the **Sequence file** browse button.
- b. The **TotalChrom File-Open** window is displayed.
- c. Click on the **Files of type:** browse button and select **Index Files[*.idx]** files.



Batch Reprocessing – From Sequence – Files of type

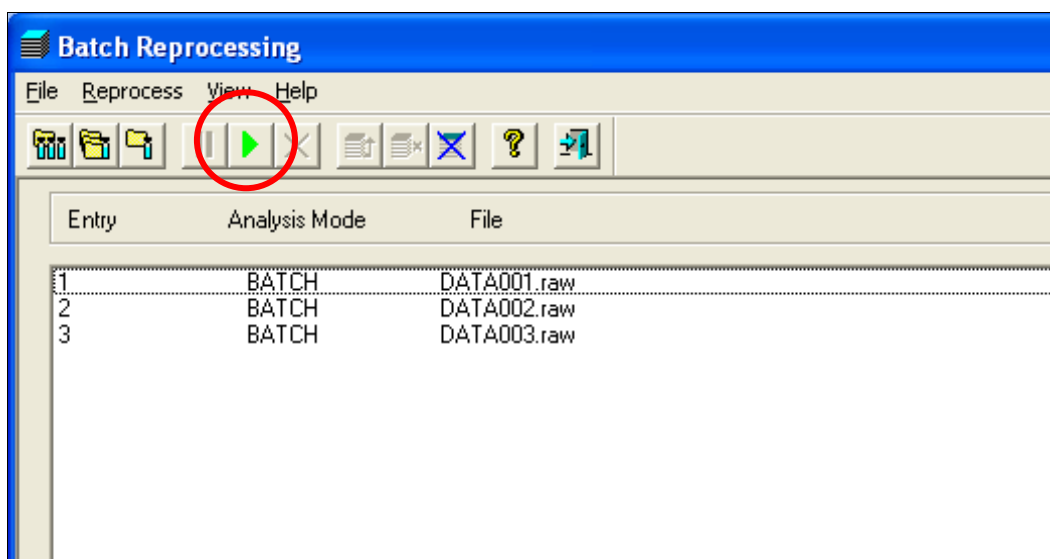
Chapter 5 – Reprocess

2. Batch Reprocess – continued



3. Start Batch Reprocessing.

- Review the data files in the Batch Reprocessing window that is displayed.
- Click on the green - **Start icon** to start the reprocessing of the selected files.
- The data files selected will be reprocessed and the results printed if a new printout is called for by selecting a printer on the Batch screen.



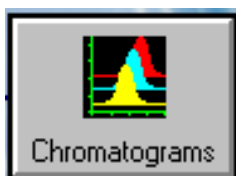
Batch Reprocessing – Start

Chapter 6

Chapter 6 – Chromatograms

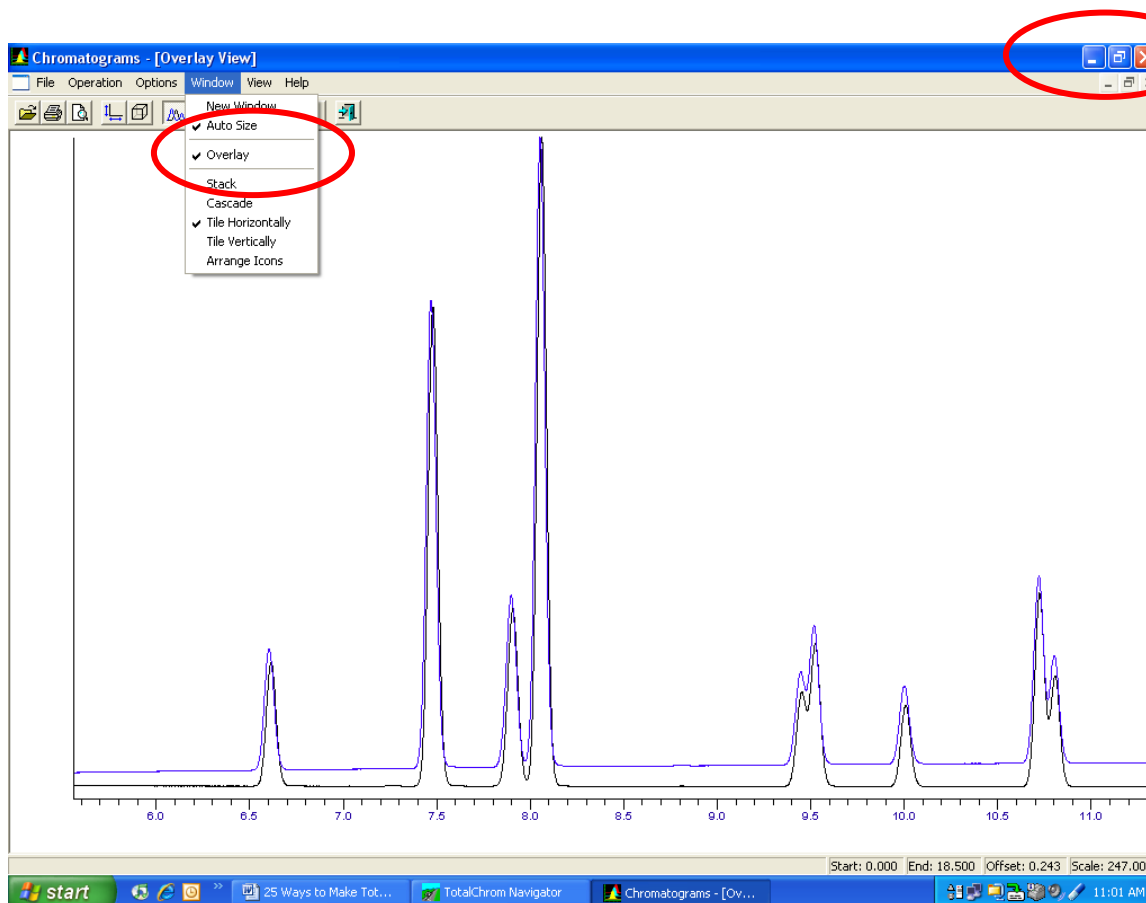
1. Chromatograms - Overlay

Tip #46 - Using **Chromatograms – Overlay** you can select two or more chromatogram files and overlay them for visual inspection.

**1. Using Chromatograms - Overlay.**

Locate the data files of interest in the **File - Open TotalChrom Multiple-File-Open** window.

- Use **shift-click** or the **control click** to select two or more files.
- Click on the **Window** drop-down menu and check (✓) the **Overlay** function.
- Maximize** the **Overlay View** to see the overlay in full screen.

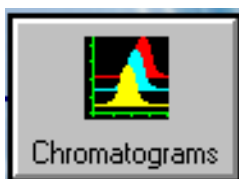


Chromatograms – Overlay

Chapter 6 – Chromatograms

1. Chromatograms – Auto Size

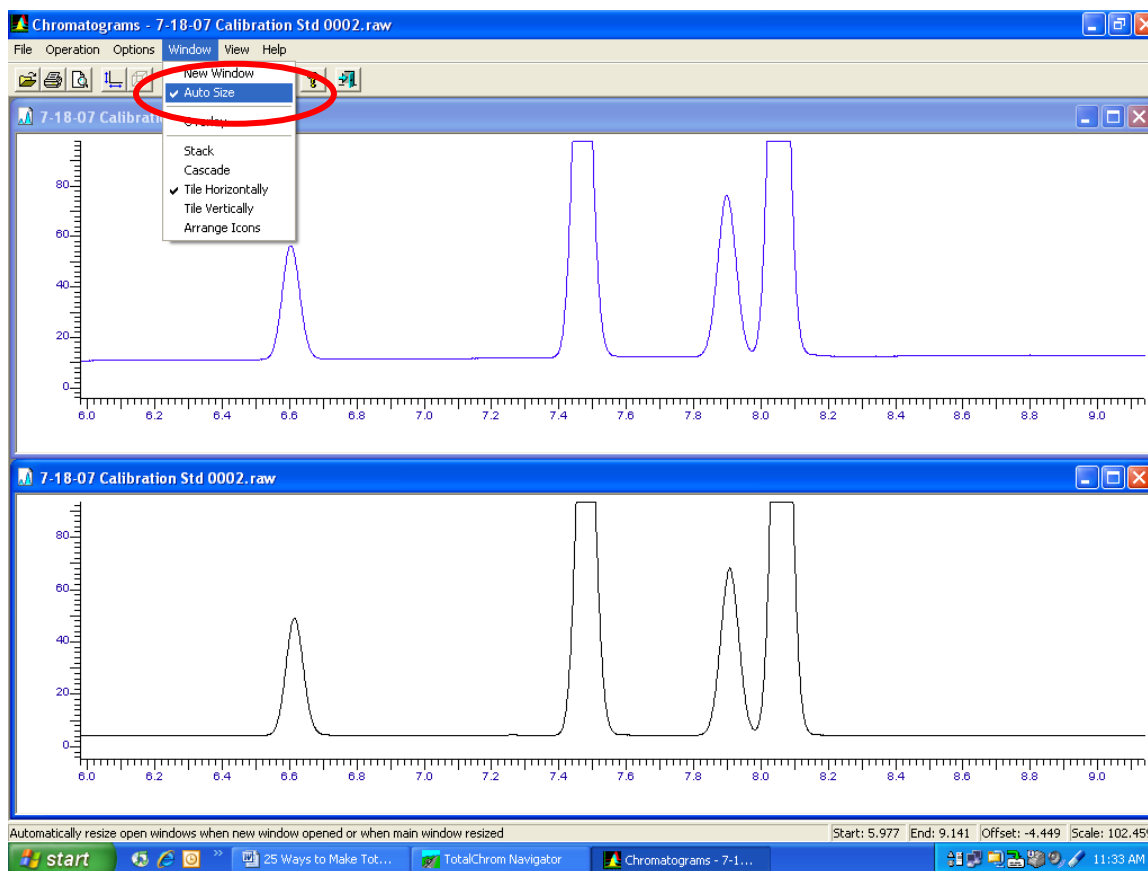
Tip #47 - With **Chromatograms – Auto Size** you can expand all selected chromatograms displayed to see the chromatogram details more easily.



2. Using Chromatograms – Auto Size.

Select the data files of interest in the **File - Open TotalChrom Multiple-File-Open** window.

- Click on the **Window** drop-down menu and check (✓) the **Auto Size** function.
- Use the rubber box function, **left-click and drag** to expand a section of interest in one chromatogram.
- Right-click** in a chromatogram to **Undo** the expansion.



Chromatograms – Auto Size

Chapter 7

Chapter 7 – Other Tips

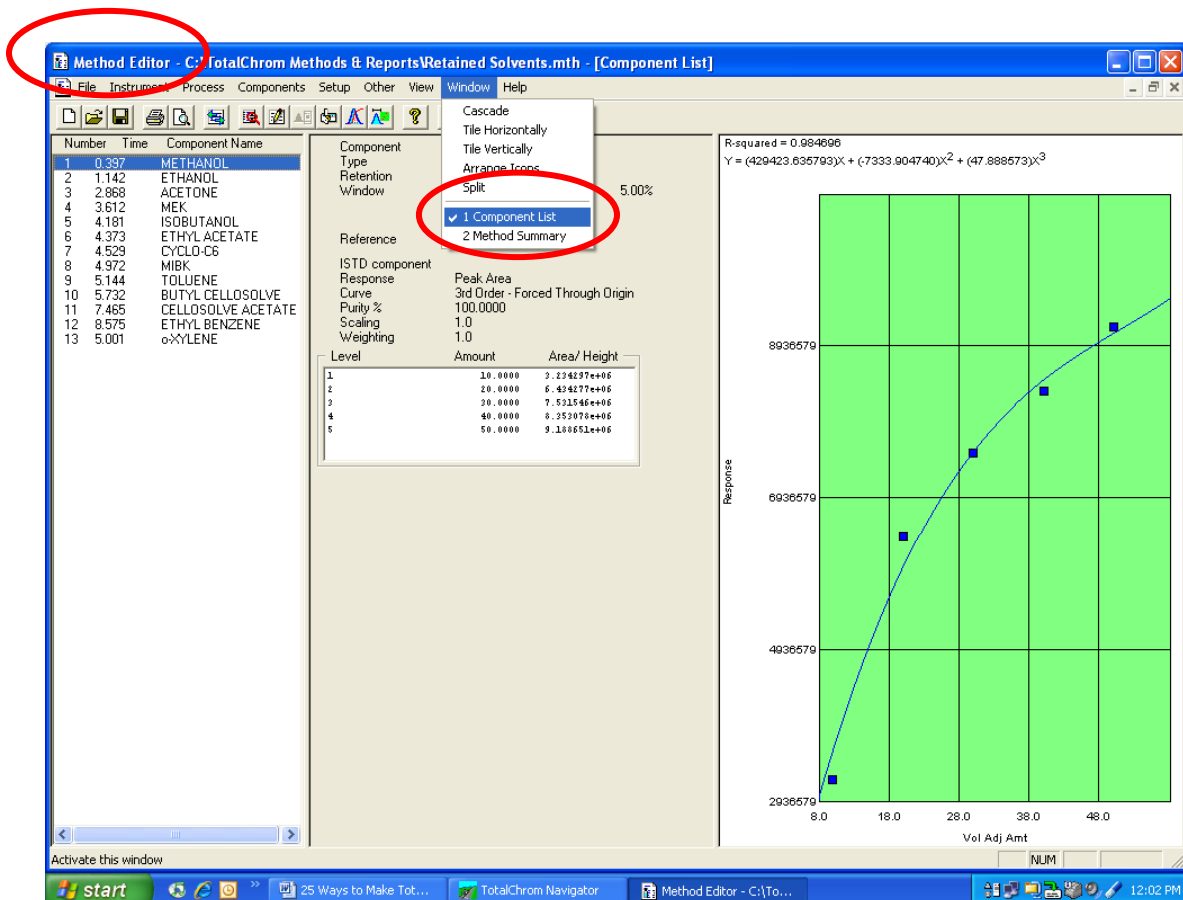
1. Method Editor – Component List View

Tip #48 - Using the **Method Editor - Component List** view you can display the method component list, the calibration parameters and the calibration curve together on the screen to more easily review the calibration results.



1. Using Method Editor – Component List View.

- Open the **Method Editor** screen.
- Click on the **Window** drop-down menu and select **Component List**.



Method Editor – Component List screen

Chapter 7 – Other Tips

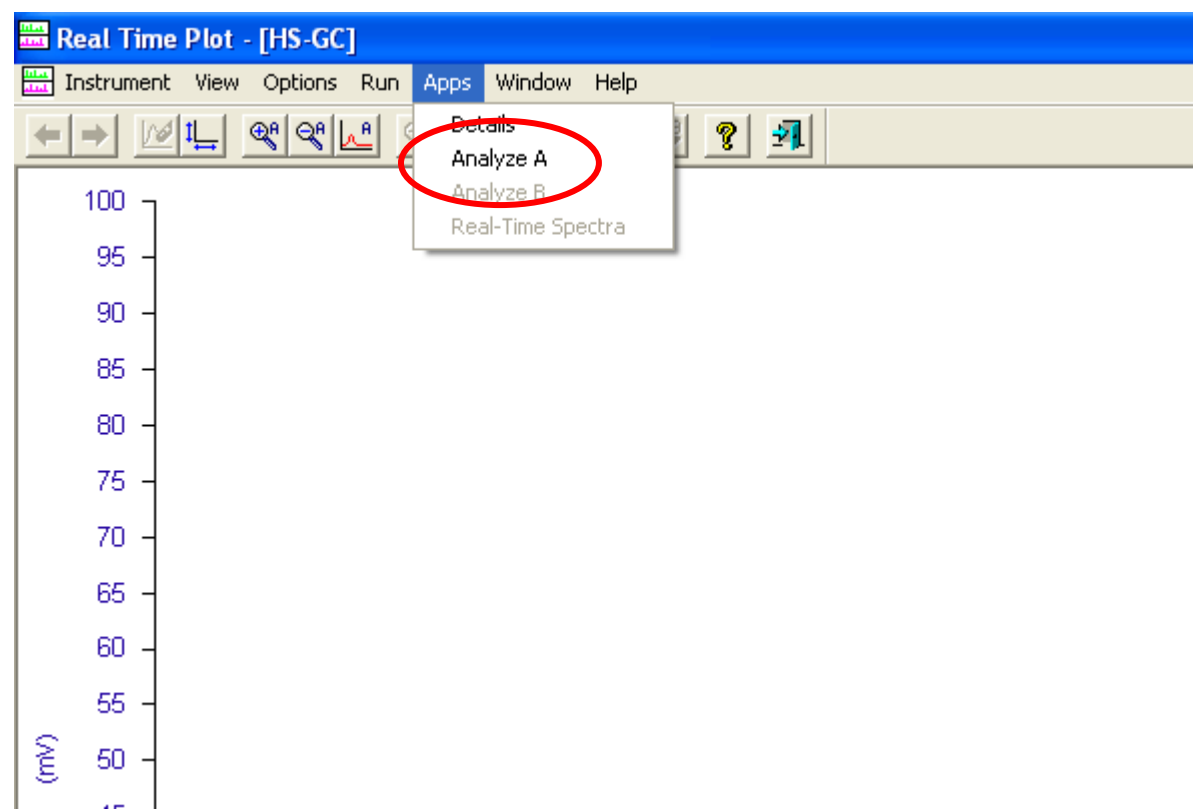
2. Real-Time Plot

Tip #49 – In the Real Time plot mode you can capture the data that has been collected up to that point in the run for review and optimization in the Graphic Method Editor.



1. Using Real-Time Plot – Review Application

- a. Open the **Real-Time Plot** screen.
- b. Click on the **Apps** drop-down menu and select **Analyze A**.
- c. Your data will appear in the Graphic Method Editor screen.



Real Time Plot – Apps – Analyze A

Chapter 7 – Other Tips

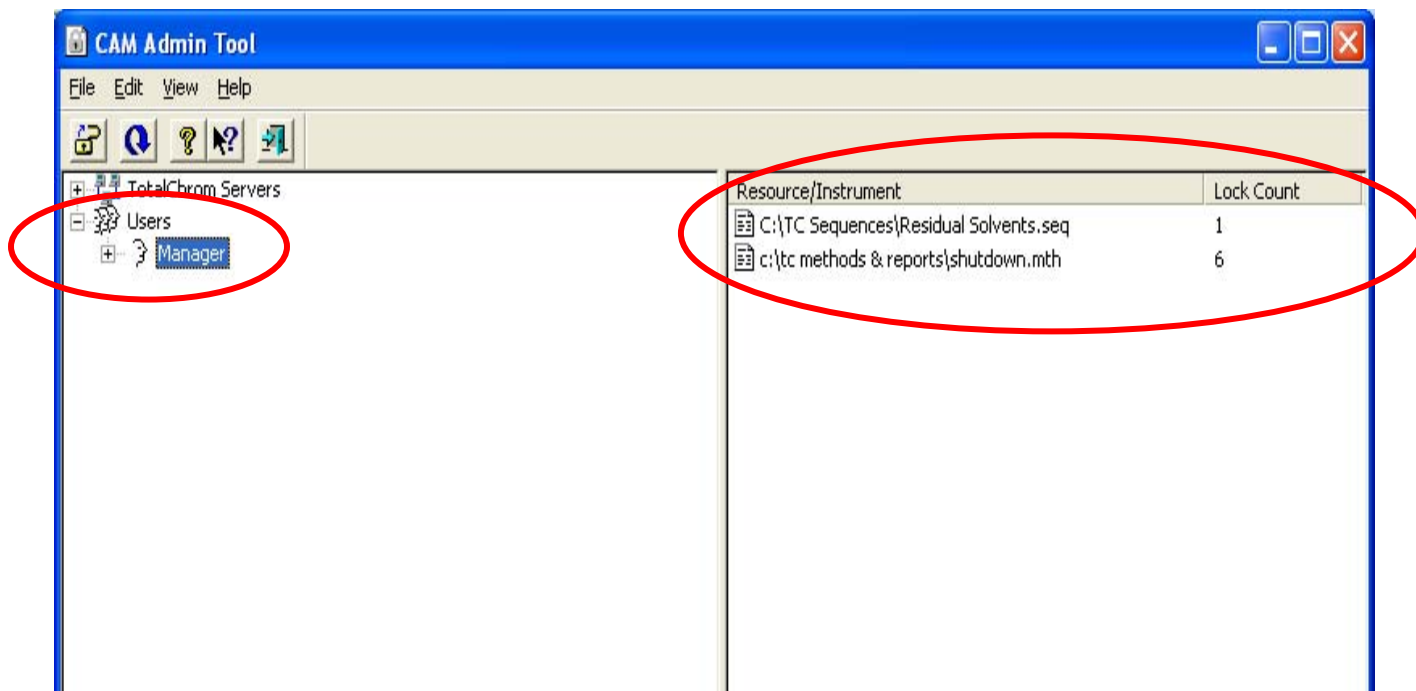
3. Unlocking Methods and Sequences

Tip #50 – If opening a method or sequence displays an error message that will only allow you to open the file as a read-only file you must remove the system "locks".

1. Using CAM Administration to remove Method locks

Use the following steps to remove method or sequence locks.

- In the **Admin** drop-down menu and select **CAM Administration**.
- The **CAM Admin Tool** screen is displayed.
- Open the current TotalChrom User by clicking on the + box to the left of **Users**.
- If any sequences or methods are displayed in the right side of the screen, click on the **Unlock icon** on the left side of the icon bar to remove the locks.
- Click on **File – Exit** to close the CAM Admin Tool.



CAM Administration Tool – Used to remove method or sequence locks

Chapter 7 – Other Tips

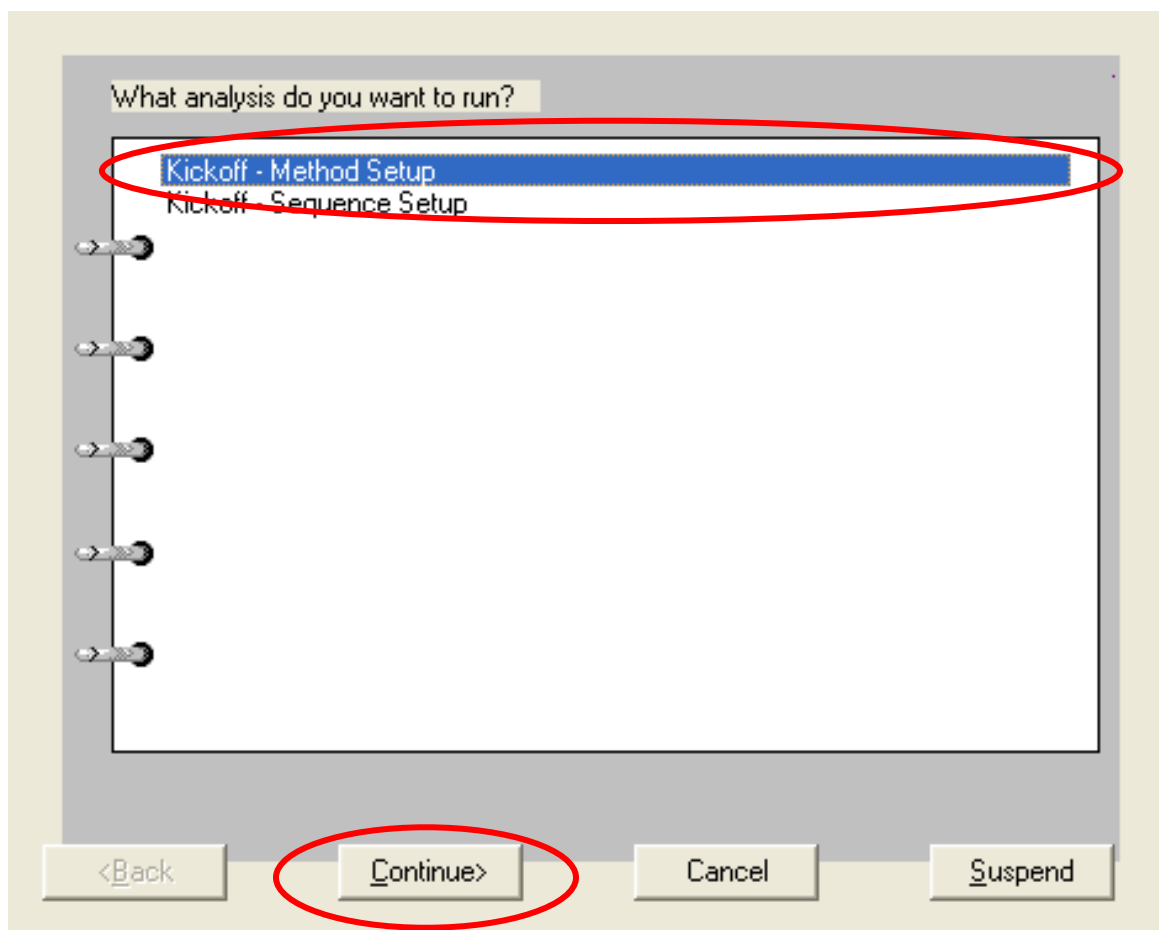
4. Kickoff – Simplified User Interface

Tip #51 - TotalChrom includes a Simplified User Interface (SUI) application called **Kickoff™**. After configuration this application will allow the user to setup TotalChrom methods or sequences quickly and easily. The user will have see any Method, Sequence or the standard Setup functions.

1. Using Kickoff – First screen.

- a. In the **Navigator** screen click on the **Apps** drop-down menu.
- b. Select **Kickoff**.
- c. Highlight the analysis you want and press the **Continue**.

Note: This and the following Kickoff screens are an example of a Kickoff - **Method Setup**.



Kickoff - Simplified Use Interface Application – First screen.

Chapter 7 – Other Tips

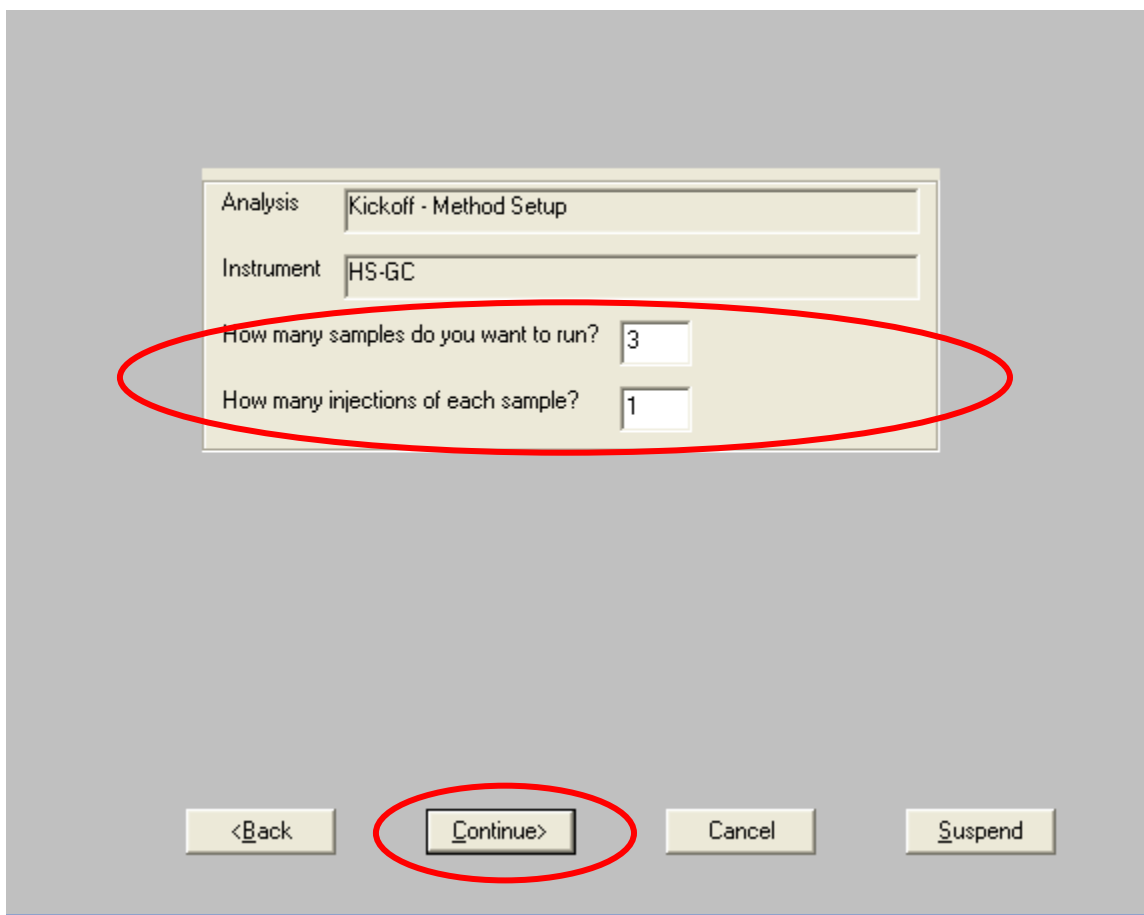
4. Kickoff – Simplified User Interface - continued

The Kickoff application is very easy to configure and use. The Kickoff Analysis name can be configured to the original method or sequence name for ease of use.

2. Using Kickoff – Second screen.

In the analysis screen enter the sample information.

- a. **How many samples do you want to run?**
- b. **How many injections of each sample?**
- c. Click the **Continue** button to proceed to the next screen.



The screenshot displays a software dialog box for configuring a Kickoff analysis. The dialog box has a light beige background and is set against a grey background. It contains the following elements:

- Analysis:** A text field containing "Kickoff - Method Setup".
- Instrument:** A text field containing "HS-GC".
- How many samples do you want to run?:** A numeric input field containing the value "3".
- How many injections of each sample?:** A numeric input field containing the value "1".

At the bottom of the dialog box, there are four buttons: "<Back", "Continue", "Cancel", and "Suspend". The "Continue" button is circled in red, indicating it is the next step in the process.

Kickoff - Simplified Use Interface Application – Second screen.

Chapter 7 – Other Tips

4. Kickoff – Simplified User Interface - continued

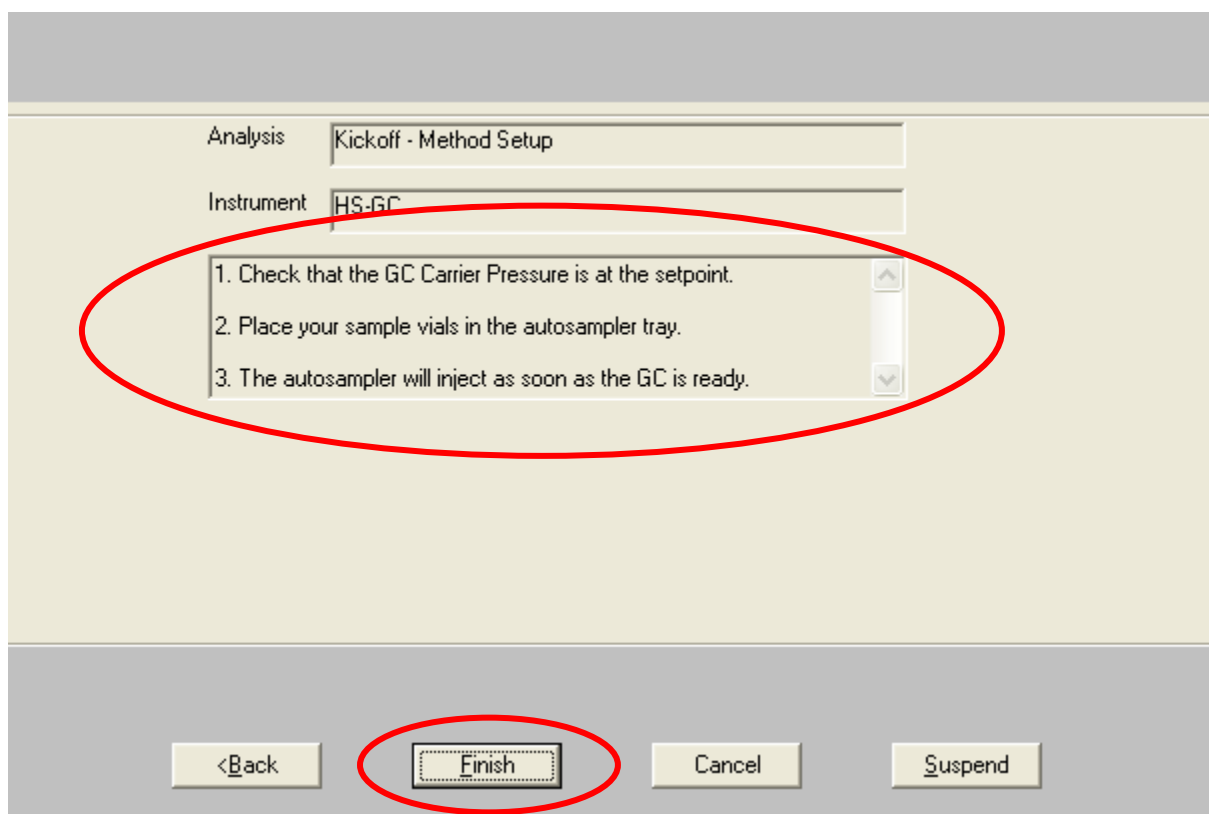
The Kickoff application is very easy to configure and use. The Kickoff Analysis name can be configured to the original method or sequence name for ease of use.

3. Using Kickoff – Third screen.

In the final Kickoff - Method setup screen customizable prompts are displayed for the user.

a. Click on the **Finish** button to complete the Kickoff setup.

Note: When using Kickoff – Method setup the **data file name** is automatically generated using the **Kickoff name** appended with the **date and time** of each injection. The data file is automatically stored in the default Data Directory.



Kickoff - Simplified Use Interface Application – Third screen.

Chapter 7 – Other Tips

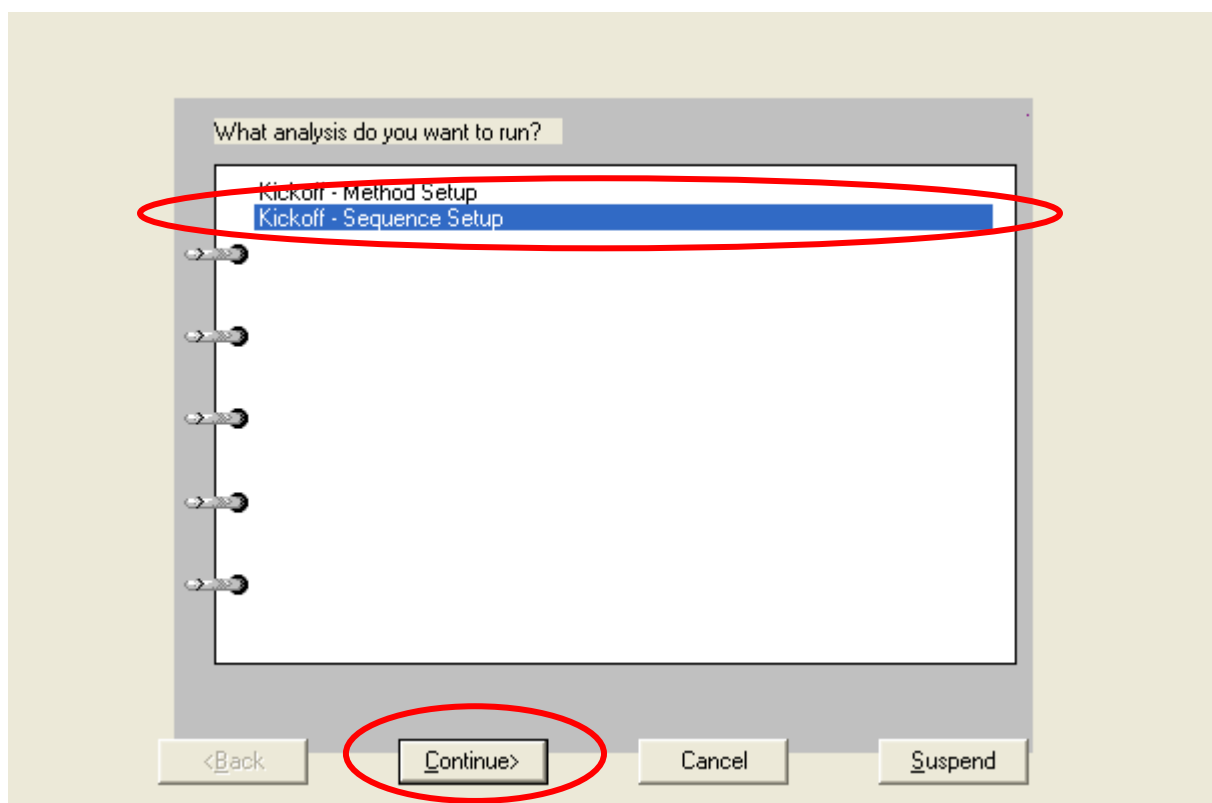
4. Kickoff – Simplified User Interface - continued

The TotalChrom **Kickoff** application configured for a Sequence setup uses a previously generated sequence. This allows the user to pre-define the data file names and the set the data path in advance.

4. Using Kickoff – Sequence Setup.

- a. Select the **Kickoff – Sequence** analysis to be setup.

Note: When using Kickoff – Sequence setup the **data file name** is pre-defined in the sequence for each injection. However, for all subsequent Kickoff analysis the data file name is appended with a date and time stamp. The data file is automatically stored in the data directory defined in the sequence.



Kickoff Sequence setup - Simplified Use Interface Application.

[ChromLab](#) - On-Site TotalChrom Training Programs

On-site TotalChrom™ operator training programs can be scheduled at your laboratory location.

These hands-on training programs are designed to assist your personnel to utilize the software features described herein to generate, optimize and calibrate quantitative methods for your GC or HPLC applications.

If you would like information of these customized, on-site training programs please contact *ChromLab* at 610-644-2260 or online at www.FastGCChromLab.com.

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