

GC SOLUTION SOFTWARE

USER BASICS

Craig S Young

Sr. Technical Support

Shimadzu Scientific Instruments

GC SOLUTION – Two Modules

GC Real Time Analysis & GC PostRun

Use Real Time Analysis to set the instrument configuration.

Use Real Time Analysis to set run methods and acquire data.

Use PostRun to process data, integrate peaks, and perform quantitation.

Real Time Analysis

Initialize the instrument

Turn on your GC and establish gas flow for the carrier and any detector gases. Refer to the end of this document for the information about the gases to be used for GC. Open the GC Solution Real Time Analysis module. From the **View** menu, choose **Instrument Monitor**. The Monitor appears on the right hand margin of the screen. Click on **System Start**. Also click **ON** any modules that are currently OFF (detector, injector, column oven). The GC will attempt to reach temperature and flow set points for any devices on all analytical lines according to the method last used. Analytical lines (separate physical analysis paths made up of at least one injector and one detector) are distinguished by separate tabs on this Instrument Monitor screen. The Monitor will indicate when your instrument is ready to analyze samples by producing the ready-state signals shown below:

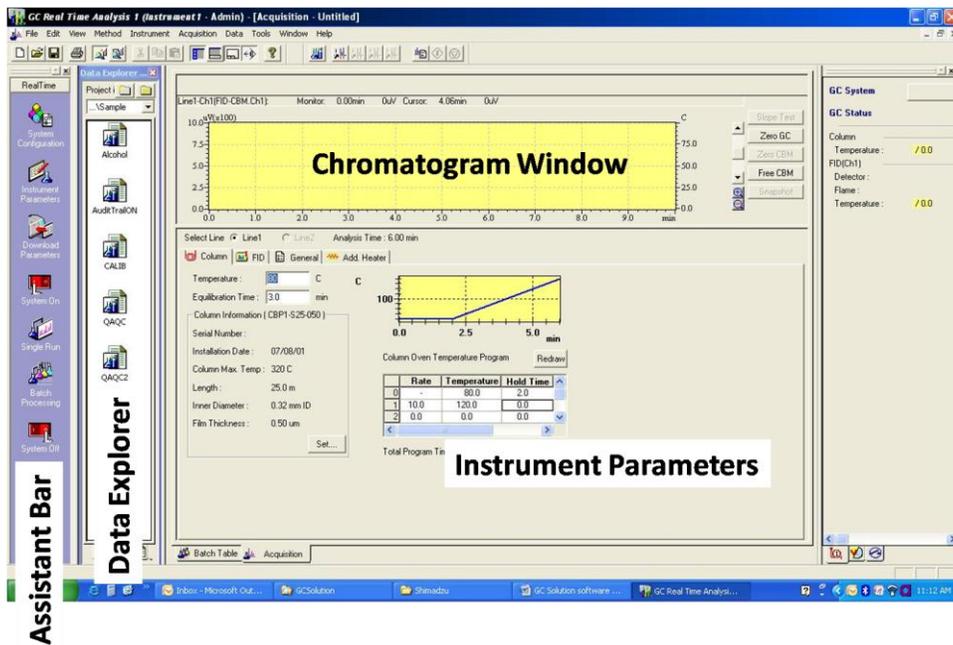
```
~~~~~  
GC SYSTEM   O N  
GC STATUS   R E A D Y  
...  
...  
~~~~~
```

You cannot run samples until a READY condition has been reached.

Set the Instrument Parameters (the analysis method)

The middle of the screen comprises the Acquisition Window and Instrument Parameters. Right above it, the Acquisition Window shows a real time detector trace. From the **Assistant Bar**, open **Instrument Parameters**—the GC method appears in tabular form in the middle of the screen. Here, set conditions for the column oven (starting temp., isothermal or gradient, etc.), the detector and general chromatograph run time. When you are finished with the method, save it by choosing **File/Save Method File As...** and give it a name. To immediately download the starting run conditions to the GC, press the **Download** button from the Instrument Parameters window.

If you have changed parameters, a **NOT READY** message will appear as the GC warms or cools to the new set points for the method. Do not attempt to do a run until the **READY** status appears.



Perform a single run

With the method set and the GC in a ready state, submit a single run by clicking on the **Assistant Bar, Single Run/Sample Login**. Here, the minimum amount you need to define is a **Data File** name and, if you have an autosampler, a Vial# and injection volume. The **Data File** name is the file that gets written to the hard drive. Note: Vial number and volume do not apply for manual injections. You can also define **Sample ID** and **Auto Increment**—with **Auto Increment** each run in turn has a base name augmented by a new digit (e.g. demorun001, demorun002,...).

AUTOSAMPLERS –

Click **OK** and then choose **START** from the **Assistant Bar**. The GC run will occur, triggered by the autosampler injection event. During the run, the top-screen message will read **ACQUIRE**.

MANUAL INJECTIONS –

Choose **START** from the **Assistant Bar**. The top-screen message will read **ACQUIRE(Standby)** as the GC is waiting for a trigger. Inject the sample manually and immediately hit the green **START** key on the face of the GC to start the run. During the run, the top-screen message will read **Analysis**.

The Chromatogram Window (the real detector trace)

At center-screen is the chromatogram window showing the real time detector trace. When the run proceeds, the top of this window says **ACQUIRE** and data is collected. To enlarge the x-axis time window to equal that of the method, right click on the chromatogram and choose **Chromatogram Display Settings...**, then choose, for example, **Channel1/Time/25** minutes or so if the method is time frame is 25 minutes. Use the scroll bars and zoom tool to focus in on the detector trace.

At any time, you may **Autozero** the detector trace using the **AUTOZERO** button to the right of the chromatogram window. Further, choosing **SNAPSHOT** will grab the current picture of the

data and launch it into **GC PostRun** so that it can be examined (zoomed, peaks integrated, etc.). This is very useful to evaluate the baseline or analyte peaks without affecting the outcome of the current chromatography run.

Perform a batch run

A **Batch Table** is a series of runs laid out like a spreadsheet. Batches are best utilized with an autosampler for unattended operation of up to several hundred injections, but a batch may be used with manual injections also. When doing manual injections, the next injection is done by the operator (and **START** is depressed on the GC) after the previous run ends and the **READY** state is once again shown on the software screen. Thus, batches with manual injections require the operator to be present.

Create a batch by clicking on the **Assistant Bar/Batch Run** and then choose the **Wizard**. The **Wizard** will ask you to define whether to run unknowns or standards or both, the method to use, the number of sample vials and replicates, Sample ID and Sample Data File Name (autoincremented?). You can ignore references to calibrations and levels. The wizard can define hundreds of runs in just a few seconds. Click **Finish**.

After the **Batch Table** is created, you can click on any given cell and change it. For example, maybe every 10th run you want to use a different method. The minimum fields necessary in the **Batch Table** are: Vial #, Volume, Method File, Data File. Once the **Batch Table** is created, you can right-click on the margin next to it and choose **Table Style...** to change which columns are displayed in the table. For example, Vial # and Volume are meaningful only if you have an autosampler, or you might want to add Report Output to print a report with each run.

A **Batch Table** is a file itself and must be saved to be reused. Choose **File/Save Batch File As...** and give it a name for later use.

Data Explorer

In both **Real Time** and **PostRun**, you can enable a very useful **Data Explorer** view by choosing **View Menu/Data Explorer...**. This opens a column next to the **Assistant Bar** that is a file browser for data, methods, and batches and reports. In **Real Time Analysis**, any method or batch file can be chosen and dragged to screen center to be viewed. In **PostRun Analysis**, any GC data file may be chosen and dragged to screen center to be viewed.

PostRun Analysis

PostRun Analysis is reserved for manipulating data—integrating peaks, defining Compound Tables, quantitation, etc. PostRun cannot operate the hardware.

Integrating Peaks

From the **Data Explorer**, select a data file and drag it to the chromatogram view at screen center. GC Solution will automatically attempt to integrate the peaks it finds according to the method which loads with that data file. To change the peak integration parameters, use the **Method-Peak Integration Parameters** window in the lower right hand quadrant of the screen. Place this window in **Edit** mode by clicking the **Edit** button next to the View button. Also, select the **Time Program** button to change peak integration parameters.

Use the icons to move graphically the baseline ticks. You can also directly edit the Integration Time Program. For example, entering Time 0.00 – Integration OFF and then Time 4.20 – Integration ON will cause the program to begin integrating peaks at 4.20minutes. For each change you make, hit the **Simulate** button to see the result. When finished, choose **OK**. Finally, select the **View** button on the **Method-Peak Integration Parameters** window to update the screen-center chromatogram with your integration changes. If you like the result, save the updated Method or Data File by choosing **File/Save Method/Data File As...**

Calculating Peak Areas and Peak Labeling

Right-click on the chromatogram view and choose **Display Properties**. A dialogue will open in which you can choose to apply a peak-top-label of Peak #, Peak Area, etc. Peak Names may only be applied after you create a **Compound Table**, presented next.

Calibration Curves and Quantitation—Creating The Compound Table

The **Compound Table**, once created, is held within the method and contains information necessary to identify peaks by name and assign concentration level values to peak areas for standards. The **Compound Table** is necessary for the creation of a calibration curve from a set of standards.

To create a **Compound Table**, choose the **Wizard** from the **Assistant Bar**. After reading the initial alert, click **Next**. Enter Quantitative Method settings such as those below:

Quantitation

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External Standards  
 Calculated by – Area  
 # of Calibration Levels –5  
 Curve Fit Type –Linear  
 Zero –Not Forced  
 Weighting Method –None  
 Unit –ppm  
 X Axis of Calib. Curve –Concentration

#### **Identification**

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Window/Band –Window, 5%
 Identification Method –Absolute Rt
 Peak Select –All Peaks
 Grouping –Not Used

...click **Next**. The next step allows you to “Select all necessary peak by putting check marks next to the identified peaks on the Compound Table”. In other words, choose which of the identified peaks to use as standards or peaks to be labeled:

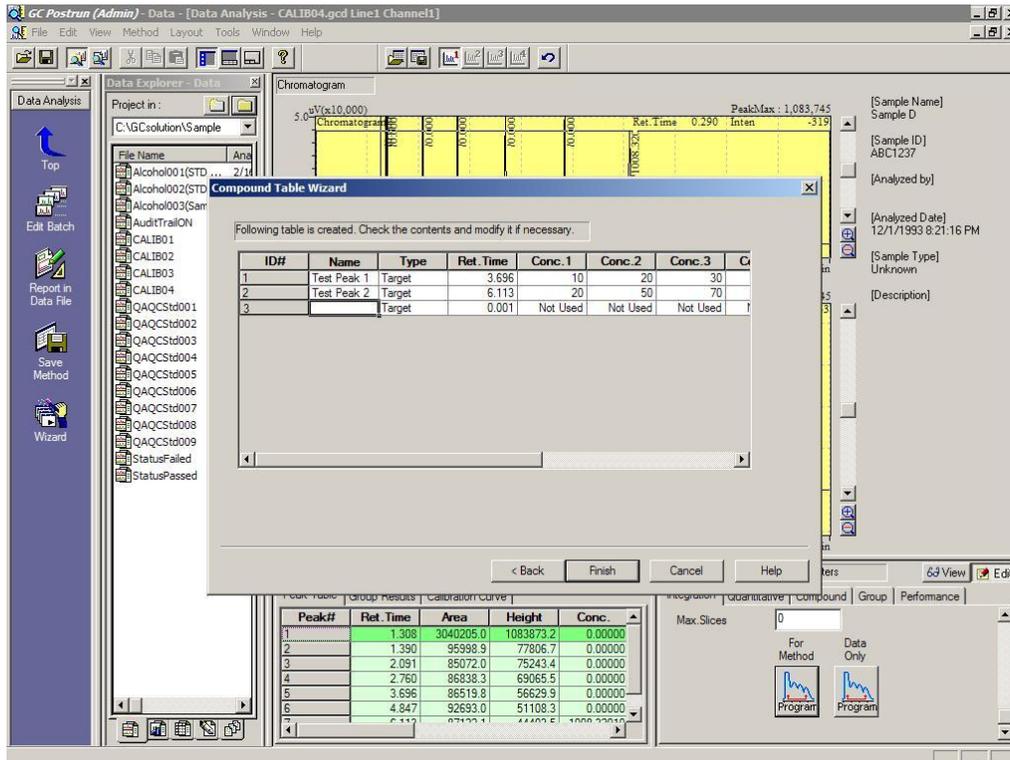
<u>Process</u>	<u>Type</u>	<u>Ret. Time</u>	<u>Area</u>	<u>Height</u>
√	Target	2.234	59797	11335.2
√	Target	3.170	71328	15726

Note: Type=Target is for unknowns; Type=ISTD is for Internal Standards; Type=Ref is for reference peaks.

...click **Next**. The next step allows you to give the identified peaks names and site any concentration values for the standards used:

ID#	Name	Ret. Time	Conc. 1	Conc. 2	Conc. 3	Conc. 4....
1	uracil	2.234	5	10	25	50
2	toluene	3.170	10	20	50	100

...click **Finish**. In the lower right quadrant of the screen, the **Compound Table** will appear under the tabbed view called **Method-Compound Table**. Notice your Named Peaks with their Standard Concentration Levels.

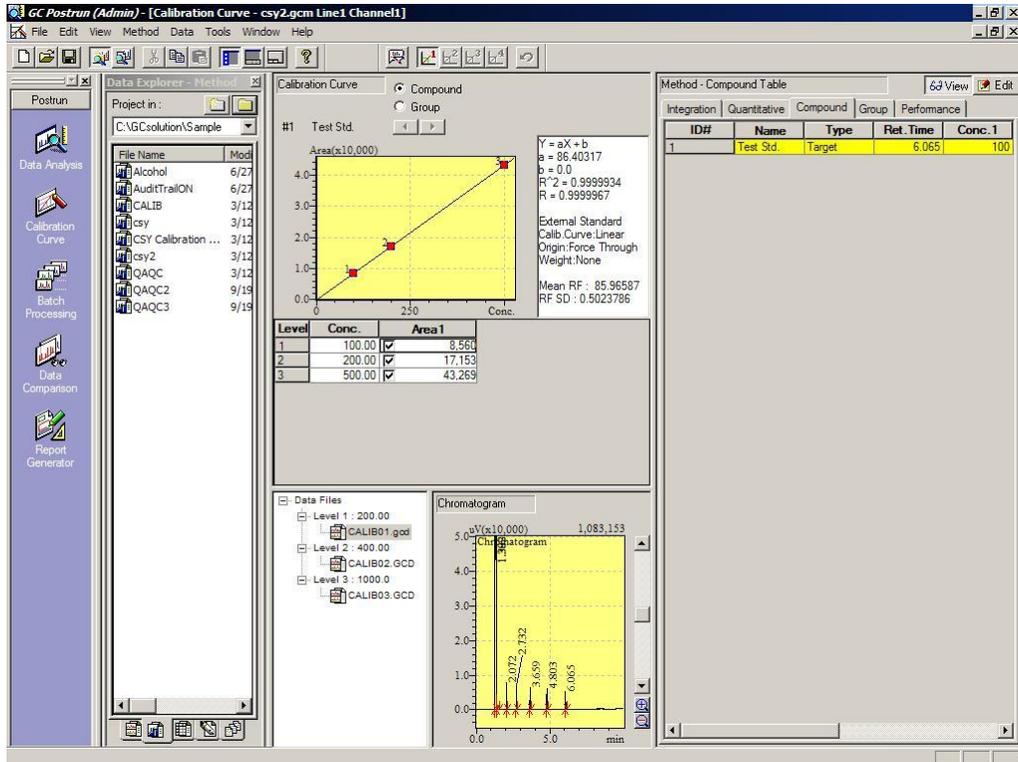


Creating the Calibration Curve

From the **Assistant Bar**, choose **Top** to go to the top set of icons, then choose **Calibration**. The screen changes to reflect a calibration curve. Use the **File** menu to **Open** the **Method** containing your **Compound Table**, or drag-over the **Method** using the **File Browser**. A **Calibration Curve** graphic appears and, right below it, a Calibration Tree representing Data File levels.

To build the **Calibration Curve**, browse to the Data Files representing the standards of different concentration levels specified in the Compound Table. Click on each file and drag it to the appropriate **Level #** on the tree. As you do so, the **Calibration Curve** will be populated as concentration levels are associated with peak areas. To the right of the **Calibration Curve**, the best fit equation is presented along with the correlation coefficient. From the example parameters used above, a calibration of 5 levels would be built along with a linear trend line not forced through zero.

Once finished, resave the Method File by choosing **File/Save Method/Data File As...** . Any data file analyzed with this method will contain a reference to the curve to estimate unknown concentrations.



Data Comparison

Data Comparison is a feature with which you can simultaneously display overlaid data files for visual comparison. To use the feature, choose **Data Comparison** from the **Assistant Bar**. A chromatogram window will appear. Browse to a folder containing data files you would like to overlay. Ctrl-Click on each data file and drag them together over to the chromatogram view. You can offset the baselines by right-clicking on the chromatogram and choosing Base Shift.

Generating Reports

From the **Assistant Bar**, choose **Report Generator**—a blank Report Editor screen will open. You can populate the editor page with objects by clicking and dragging from the object icons at the top. A better starting point is to open an existing Report Template—choose **File/Open Format File...** . To really see what this page will look like when it represents data, browse to a Data File and drag it over onto the Report Editor. Objects like headers, chromatograms, etc. will appear, depending on the report layout. To edit the objects, double-click on them. A dialogue will open allowing you to designate axes limits, scaling type, data channels to show, process parameters to include, etc. Choose **File/Print Preview** and then **Print** to generate the report. You can save the Report as its own custom Format file for use with other data by choosing **File/Save Format File As...** .

Types and Purities of Gases Used for GC

Detector (analyses type)	Carrier Gas (purity)	Combustion Gas (purity)	Support Gas (purity)	Make-up Gas (purity)	Note
TCD (General)	He, N ₂ , Ar 99.995% or greater	---	---	He, N ₂ , Ar 99.995% or greater	
TCD (High Sens)	He, N ₂ , Ar 99.999% or greater	---	---	He, N ₂ , Ar 99.999% or greater	
FID (General)	He, N ₂ 99.995% or greater	H ₂ 99.995% or greater	Air Compressed air	He, N ₂ 99.995% or greater	
FID (High Sens)	He*, N ₂ 99.999% or greater	H ₂ 99.999% or greater	Air Use air cylinder if possible (compressed air is acceptable)	He*, N ₂ 99.999% or greater	
ECD (all)	He, N ₂ 99.999% or greater (99.9999% recommended)	---	---	N ₂ 99.999% or greater (99.9999% recommended)	
FPD (all)	He, N ₂ 99.999% or greater	H ₂ 99.999% or greater	Air Use air cylinder if possible (compressed air is acceptable)	Not available	
FTD (all)	He 99.999% or greater	H ₂ 99.999% or greater	Air Use dry air cylinder.	He 99.999% or greater	