PeakSimple is SRI's software that allows a GC to communicate and interface with a Windows computer through an A/D (analog to digital) converter. The latest version can be downloaded for free from www.srigc.com.

Download the validation data package from www.srigc.com. Place the three files (Validation components.cpt, Reproducibility.chr, and Linearity.chr) into a folder on your C: drive named "Validation" (C:\Validation).



In order to validate the PeakSimple software the user will employ either **Hardware loopback** or **Software loopback**, which can be selected from the "Overall controls" menu accessible from the "Edit" Menu on PeakSimple's main screen. Make sure that the "Sample rate" is set to 5Hz.



Initiate communications between PeakSimple and the GC or datasystem. In the "Channels" Menu, make sure that Channel 1 is active, displayed, and integrated by checking the appropriate boxes. Ensure that Channel 6 is displayed and integrated.

From the main PeakSimple screen, right-click on Channel 1 and select "Components". From the Components screen select "Load" and open the "Validation components.cpt" file from the C:\Validation file folder. Do the same thing for Channel 6.

Load the "Reproducibility.chr" chromatogram into Channel 6 by selecting "Open" from the File menu, selecting the "6" Channel button, and selecting the Reproducibility.chr file from the C:\Validation folder. Hit the Open button.



a Load component file								
COO → Computer → OS (C:) → Validation → 4 Search								
Nganize 🔻 🏢 Views 💌 📑 New Folder 🕐 🕐								
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and chromatogram file						
Look in: 🚺 Validation				← 🔁	<u>r 🗄 🕆</u>	
Name	Date modif	Туре	Size			
≣ Linearity ≣ Reproducibility						
File name:	Reproducibility				Open	
Files of type: Binary files(*,CHR)  Cancel						
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Include time & date (ascill only)						



Retention 0.510 1.010 1.510

2.010 2.510

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3,510

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5.013

Update

Close

Copy results log

Height 898.162 898.633 899.073

899.420

899.552 899.352

898.950 898.491

898 180

898.65

Results

Component

Peak 1 Peak 2 Peak 3 Peak 4 Peak 5 Peak 6 Peak 7 Peak 8 Peak 9 Peak 10

Channel: 6 👻

Recognized peaks only

Undetected components

Area 5002.1034 5002.1086 5002.2028

5002.1536 5002.2016 5002.3356

5002.3356 5002.2496 5002.0976 5002.0056 5002.3102 50021.7686

Save.

Calibrate.

Clear results log Show

Results

Component Peak 1 Peak 2 Peak 3 Peak 4 Peak 5 Peak 6 Peak 7 Peak 8 Peak 9 Peak 10

Channel: 🚺 👻

Recognized peaks only

Undetected components

Once the run is completed compare the results of Channel 1 to Channel 6 in order to see how faithfully the data was reproduced. In this instance, the area counts of all the peaks are identical.

In order to calculate statistically meaningful measurements (i.e. standard deviation), several validation runs may be required. To simply the process, the user can automate the validation runs by opening up the "Postrun" menu from the Channels menu. In the Postrun menu ensure that the "Save file as" box is checked and given a name and the "Auto-increment" box is checked. Check the "Add to results log" box and give it a name. Finally, check "Restart run after" and enter a time and the number of runs that you would like to have it perform. The data from the runs will be saved to the .LOG file where it can be viewed or easily exported to a data management program like Excel.

Channel 1 post-run actions					
Save file as: Gaussian03.chr	Auto-increment				
Cruse list of filer	names: List				
Save results 🔽 Add to results log: CH1.LOG					
🗖 Print results 🔲 Update DDE link 🔲 Save picture					
Execute:					
Restart run after: 0.50 minutes 10 times total (9 remaining)					
Recalibrate at level:     Save results file to FTP site					
🗖 Smooth first	Save data file to FTP site				
Copy data to channel: 1	Email No				
Add to 3D display	On alarm condition				
	() Always				
ОК	Cancel				

X

Retention

0.510 1.010 2.010 2.510 3.010 3.510 4.010

4.513 5.013

Update

Close

Copy results log

Area 5002.1034

5002.1086 5002.2028

5002.2028 5002.1536 5002.2016 5002.3356 5002.2496 5002.0976 5002.0056

5002.3102 50021.7686

Save...

Calibrate.

Clear results log

Height

898.16

898.633 899.073

899.073 899.420 899.552 899.352 898.950 898.491

898.180 898.654

Integration...

Calibrate all...

Show results log...

Format...

Сору

Add to results log

To test for linearity rather than reproducibility, simply perform the same process as previously outlined, except this time load the "Linearity.chr" file into Channel 6. For this chromatogram each succeeding peak has half the area counts of the one before it. When you do this the PeakSimple screen will look something like this.

To perform Hardware loopback validation select "Hardware loopback" from the "Overall controls" menu. In general, Hardware Loopback will have more deviation than Software loopback due to a difference in resolution (14 bits for Hardware, 24 bits for Software). With Hardware loopback the chromatogram in Channel 6 is played back as an analog voltage which Channel 1 re-acquires just like a real chromatogram.

If you have a 333 single channel data system (or board inside your GC) connect a wire from ground to the negative signal input terminal, and another wire from the TP 1 terminal to the positive signal input terminal. It should look like the picture to the right.



If you have a six-channel 302 data system (or board inside your GC) connect a wire from ground to the negative channel one and another wire from the 1 analog out terminal to the positive channel one terminal. It should look like the picture to the right.

With the Validation components file loaded into Channels 1 and 6 and either the Reproducibility or Linearity chromatogram loaded in channel 6 (in this case Linearity is loaded) start the run.

When the run is completed compare the area counts between the two channels. As discussed previously, you can automate a number of validation runs in order to collect statistical information.





The Reproducibility.chr and Linearity.chr chromatograms are very clean and easy for the software to integrate. It may be beneficial and more realistic to use your own chromatogram in order to obtain your validation data. In this instance, load a chromatogram of your choosing into Channel 6 and perform Software loopback or Hardware loopback as discussed previously.

Make sure to add retention windows over the peaks (see the PeakSimple tutorial for adding retention windows), save the resulting component file, and load it in channel 1. This will allow you to quantify the area counts of your peaks after each validation run.

For any validation runs, print the chromatograms in order to have a hard copy of your data.

