

# Inserting Sample-Identifying Information into ChromGraph Data Files

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*New versions of ChromGraph data processing software (version 1.5x and above) allow you to import sample-identifying information during automated operation. The information is permanently saved with the data and will appear on final reports, providing an additional level of assurance to the results.*

ChromGraph software has always allowed the user to attach information identifying samples to the data file for each chromatographic run (**F1**). This had to be done manually at the start of the run. (GLP requirements preclude entering the information at a later time—data sets must be inviolate once collected.)

New ChromGraph versions (1.5x and higher) allow the incorporation of sample identifying information even when using an autosampler for unattended operation. This is accomplished by means of a table containing all the identifying information for all the runs. ChromGraph automatically imports the relevant information from the table at the start of each run, then saves the information with the data when the run is complete. We call this table a RAN file, after the 3-letter extension (.ran) of its DOS-format name. RAN stands for random, because the entries in the table can be in any order.

## Structure Of The RAN File

The RAN file is written in text format with fixed spacing. This means that all characters have the same width, so columns line up perfectly (**F2**). This is important, as ChromGraph uses the line number and column number to find the correct information to import. Tab characters are not allowed— all white

space on a line must be filled in using the spacebar.

The first ten lines of the RAN file are totally ignored by ChromGraph. These can be used to enter information about the project. If you find an old RAN file on your disk, you need only open it up and read the header to find out what it was used for and whether it is still needed.

ChromGraph begins looking for information to import at line 11 column 16. Columns 16-25 contain the run number. The numbers here and in the other fields must be left-justified (they must start in the first column of the field and extend to the right as many columns as necessary). When ChromGraph prepares to start a new run, it will examine the first field for a number that matches the run number. If it finds a match it will import the entire line.

Columns 26-35 contain the autosampler vial position in which the sample resides. When using the BAS Sample Sentinel Autosampler with the BCD vial position option, the vial number received from the autosampler is compared to the numbers in these columns. If a match is found, the entire line is imported.

Columns 36-45 contain the volume or weight of a sample. Volumes or weights are used only when the final numbers must be corrected for differences among samples (for example, the weight of a sample before

homogenization and extraction). This advanced feature, which is off topic for this article, is discussed fully in the ChromGraph manuals. Most users should put a zero in column 36 to disable this feature.

Columns 46-80 contain sample identifying information such as patient name or number. These sections will be imported into the Run Notes section of the data (**F1**).

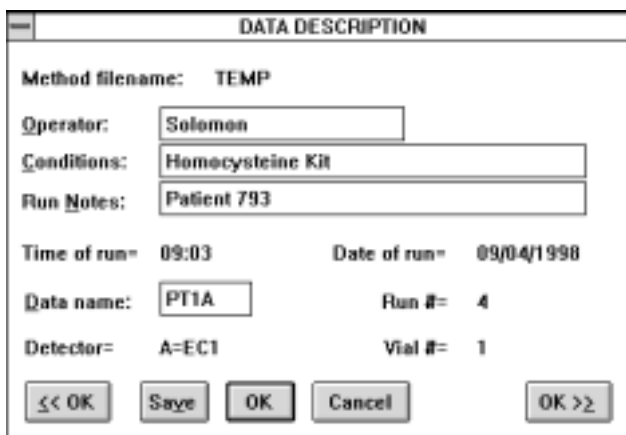
## Entering Information Into The RAN File

We have provided a template for the RAN file (template.ran) for convenience in entering data into the correct columns. It can be found in the c:\bas\data directory. If it has been accidentally erased or moved you can load a fresh copy from the original ChromGraph installation disks. Or you can create one yourself, following the column and line restrictions detailed above.

The RAN file can be edited with any text editor. Or you can use the Notepad text editor that comes with Windows. You can do this from within ChromGraph— simply take the option to edit the RAN file from ChromGraph's Data menu (**F3**). It's a good idea to rename the RAN file when you have finished making entries, so the original template is not overwritten (use the "Save As . . ." option in Notepad).

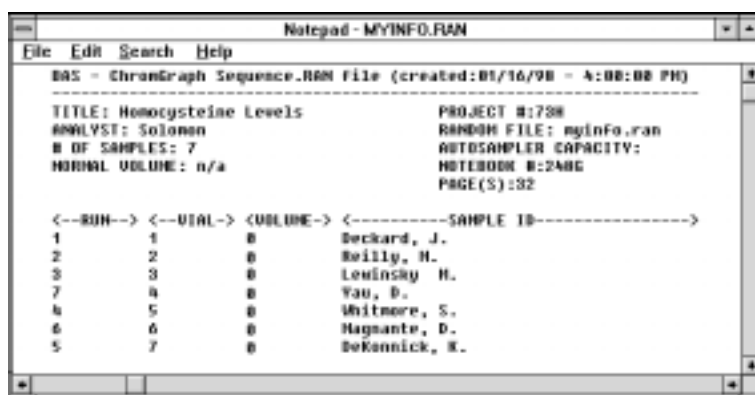
**F1**

The Data Description section of the Method, showing the three fields available for comments.



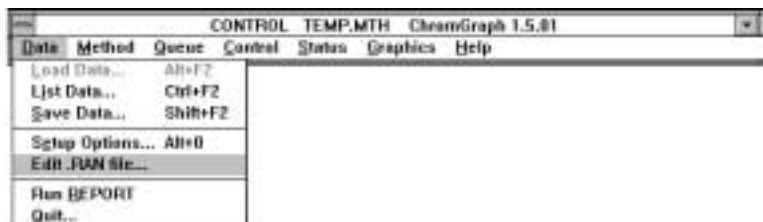
**F2**

A typical RAN file. Note the alignment of columns.



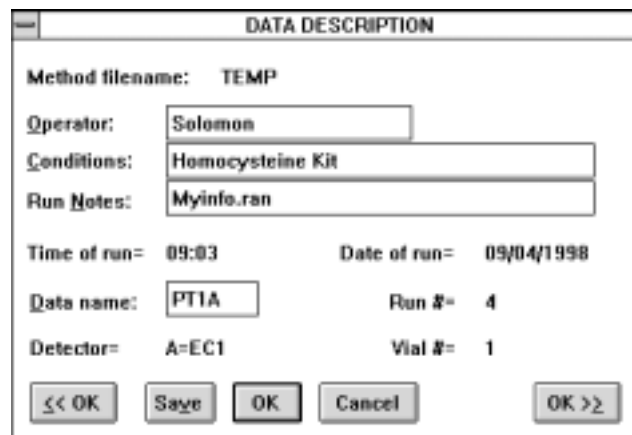
**F3**

Opening a RAN file for editing from within ChromGraph.



**F4**

Telling ChromGraph to use the RAN file.



It is not necessary to enter the lines in any particular order. ChromGraph will scan the RAN file at the start of each run, going down the list until it finds a match or reaches the end of the file. By the same logic, if there are two lines starting with the same line number, ChromGraph will import the data from the first line only. You can add lines to the RAN file at any time during a run, but avoid opening the file at the start of a run when ChromGraph will be trying to read it.

**Putting It All Together**

The RAN file must reside in the same directory as the data files. Once it is in place you must tell ChromGraph to use it. This is easily accomplished by writing the name of the RAN file in the Run Notes section of the Method (**F4**). Then simply start the runs.

**Other Features**

ChromGraph version 1.5x is a major revision that includes many improvements. For those users controlling a BAS-200 or LC-4C Amperometric Detector, the range settings used during the run are saved, so the chromatograms always show appropriate detector units, even when zoomed. And for those users whose calibration standards contain an endogenous analyte, the standard addition method of calibration is now supported. Finally, version 1.5x is year-2000 compliant.

**Conclusion**

GLP requires a certain level of assurance that results attributed to a particular sample actually are from that sample. The new version of ChromGraph software increases that assurance by automatically importing sample identifying information and saving it permanently with the data.

ChromGraph version 1.5x is available as an upgrade to registered users as part number MF-4712.