97-0953

on-line

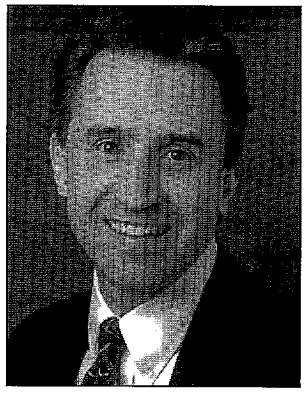
FOR MILLENNIUM SYSTEM USERS

VOLUME 5 NUMBER 1

WINTER 1997 • $250 per year

Getting the Most from Your Millennium Database

By Guy Verrastro



A fundamental aspect of Millennium Chromatography Manager Software, is that it is based on an underlying relational database. Many Millennium software users may not be aware of this fact, or may not understand the significance of a relational database in terms of the day to day use of the system. In this article we will describe how the experimenter can use the predefined relationships in Millennium software to manage and sort data.

What is a Relational Database?

To begin we will start by defining exactly what a relational database is. On the most basic level, a database is a collection of data related to a specific topic, function or purpose. By this definition, a file cabinet, the yellow pages, or a three-ring binder full of chromatograms qualify as a database.

Millennium software uses Oracle, a relational database management system which stores and retrieves information using a computer. What makes this a relational database, as opposed to just a database, is that this information is stored electronically as separate data fields. These fields are all interlinked according to rules (relationships) which are defined either by the user, or by the original designer of the software. This ability to link any combination of fields, and define the rules governing a specific link, is what makes relational databases such a powerful tool.

In Millennium software there are four types of custom fields available to the experimenter, three of which are most likely to be used: Sample Identifiers, Peak Calculations, and Result Calculations (Figure 1). (Please see the most recent issue of OnLine, and the article entitled "Millennium Chromatography Manager: Advanced Features of Custom Fields" in this issue, for a more in-depth discussion.)

The fourth type of custom field is an External Field, whereby Millennium software can be programmed to accept data from an outside source and incorporate it into calculations in the Millennium database. Data in an External Field can be linked to Millennium software from a spreadsheet, an external database, or a table from a word processor. All four of these options make it easier to track data related to specific samples and perform calculations on this data.

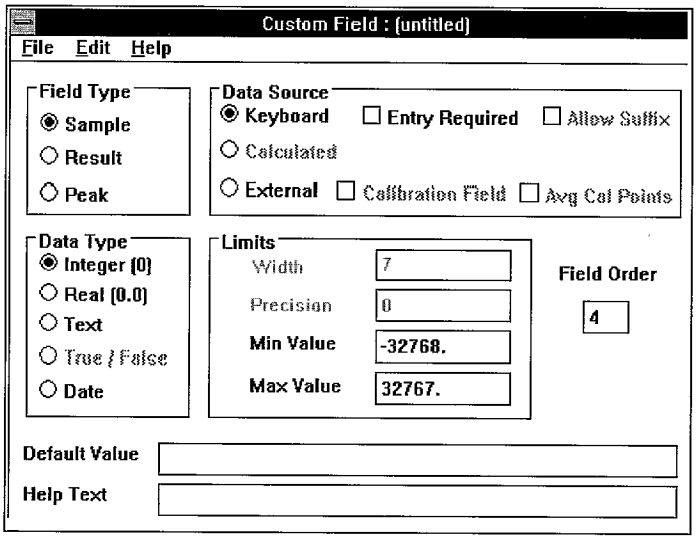


Figure 1: Custom Field editor

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Using View Filters to Locate Specific Chromatograms

Once data has been generated using a Millennium system it becomes crucial to be able to view the data in a meaningful form. The most basic way of extracting certain data is by using the View Filters to organize the information in the database. These filters allow you to selectively retrieve samples or channels in Millennium's Project Window, and Results Window. The View Filter also allows you to sort any data by date, sample name, or the name of the experimenter in either ascending or descending numeric or alphabetic order (Figure 2).

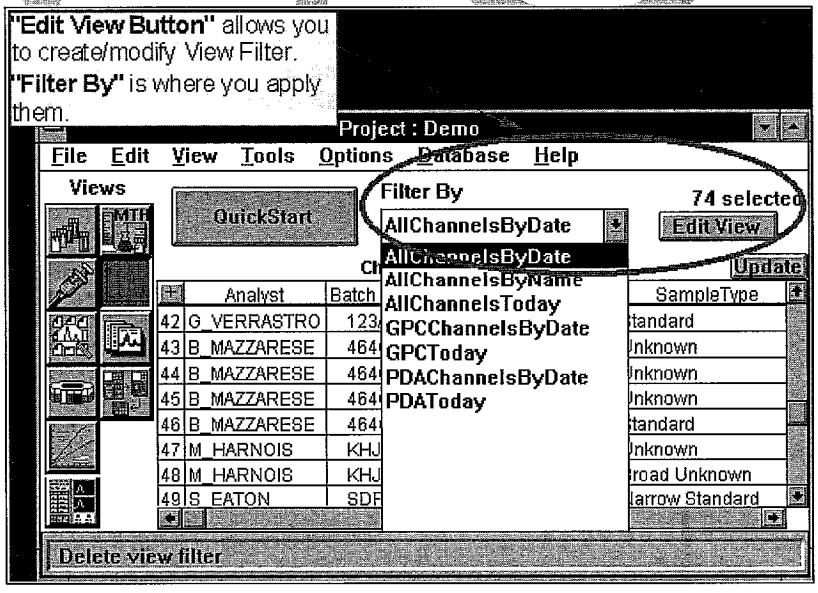

Figure 2: Millennium software makes it easy to create and sort by view filters

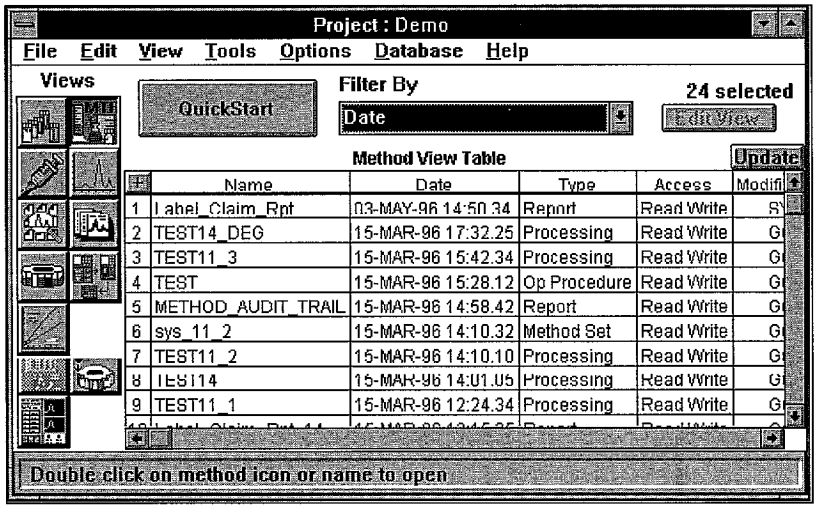

Figure 3: Method View table sorted by date

View Filters and Time Stamps Aid in Data Management

The View Filter sorts are possible because each field in the database is unique, and you can organize data based on any one field, or combination of fields. A sort of data by time and date is also possible because Millennium software applies a date and time stamp to every "transaction" that is performed. Examples of transactions include: acquiring a chromatogram, creating or editing methods, calculating results from a process chromatogram, etc. Likewise the system also records which experimenter is responsible for a given transaction.

Because these transactions are unique, old samples, sample sets, and previous methods cannot be overwritten, a feature which many Millennium users are not aware of. The system in essence saves each revision, using a transaction-triggered time stamp to differentiate between versions. Thus if you have revised a particular method, but wish to revert to the original version, it is possible to do so.

The Time Stamp function highlights the strengths of a relational database. With a relational database, data reside separately in tables, the system keeps track of all links between the individual data fields. Thus, there is a link uniting user name, operating conditions during sample acquisition, method description, and the name of the user who wrote the method as just one possible scenario.

Now if you are dealing with just a few chromatograms, and you can remember all of the significant data pertaining to them, these functionalities will not have that much significance. But if you are dealing with several years worth of work, and you are trying to identify one particular experiment which was performed in a three- or four-month timeframe, suddenly it becomes apparent that the more you know about the experiment that you are trying to dig up, and the more tools you have to narrow down the possibilities, the less time you will spend digging for the data you need.

Instead of having to remember all of the specifics about when data were acquired, and on which system, you only need to know a few basic particulars to do a search. The View Filter (Figure 3) is the tool which facilitates this type of search. You can access the View Filter in the Project Window in the Edit View drop down menu. In fact, once you create a particular View Filter, you can save the Filter for future use.

Using View Filters

In a real world example, lets say that you have 74 chromatograms. As the analysts, I will use John Smith, Brenda Thomas, and Guy Verrastro. I can then query the database on experiments performed by a particular analyst. Let's say that I want to see all runs performed by Steve Bates on raw material batch numbers 1-3 with the sample name "STD." I set up the View Filter, using the column and row View Edit screen (Figure 4) specifying Steve as the analyst, and STD as the sample name, and that I want runs numbered 1 through 3.

To digress for a moment, in this particular case I am using Boolean logic or the use of "and statements" to narrow my search. For example I could search for any chromatograms which were either generated by Guy Verrastro, or were named STD but perhaps generated by someone else for batch numbers 1-3.

When I run our original query on our 74 existing chromatograms (and it could just as readily by 740 or 7,400,) the view filter reduces the list to just 15 possible chromatograms (Figure 5). Now the task of identifying the chromatogram that I am after is much easier, rather than reviewing all 74 chromatograms individually.

Though this is a fairly straight forward example, depending on the number of custom fields and how selective you wish to be, a search could get quite involved. And though it might take a few minutes to develop the appropriate search, the time spent is minimal in comparison to reviewing the data without the relational database to narrow your search.

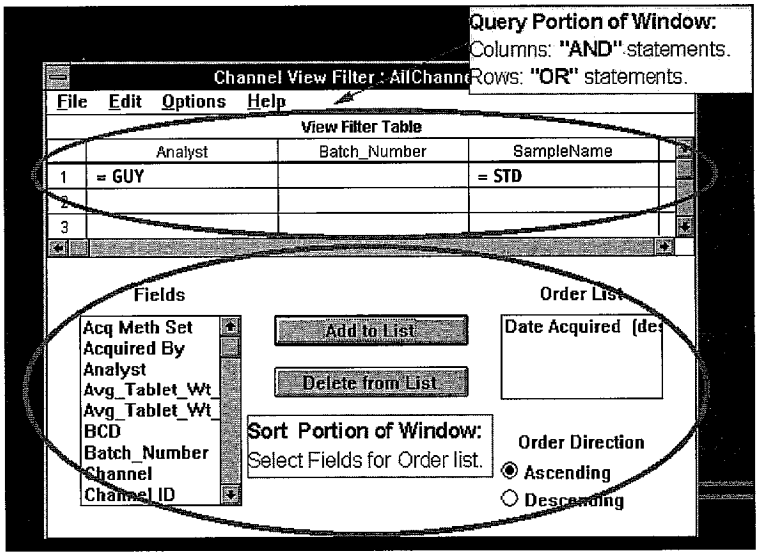

Figure 4: Millennium software allows you to create specific view filters based on your needs

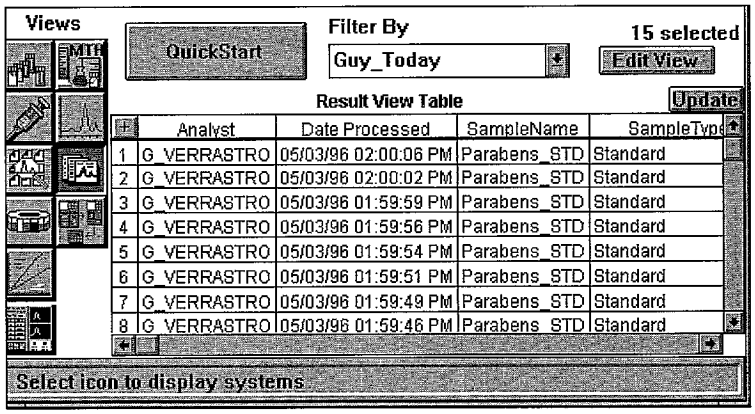

Figure 5: View filters make the task of locating specific chromatograms fast and easy

Report Publisher

While the View Filter allows you to locate individual chromatograms, sorting by various criteria, the Report Publisher goes a step further and allows you to both identify experiments which meet specific criteria, and to perform calculations on the specified chromatograms.

All report generation is done through the Report Publisher Window (Figure 6). There are various Report Method templates which are part of the Demo project on Millennium. The "Default" Report Method is one of these pre-existing reports, and a good place to begin to learn about Report Methods.

In the Default Method (or any Report Method) there is a list of available Reporting Groups located in the upper left of the Report Method Window. This list includes: Table Groups, Header/Footer Groups, Chromatogram Groups, PDA Groups, System Suitability Groups, etc.

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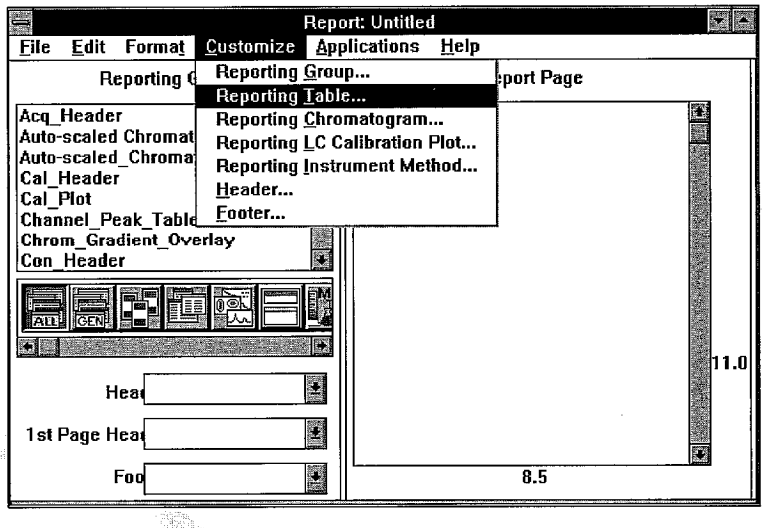

Figure 6: Report Publisher window

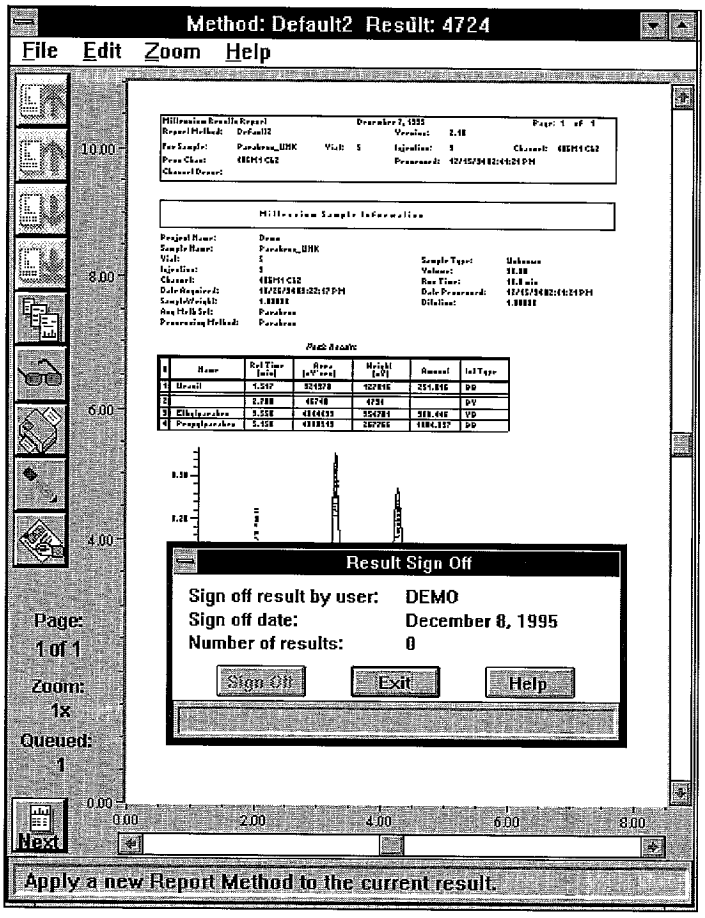

Figure 7: Report Preview window

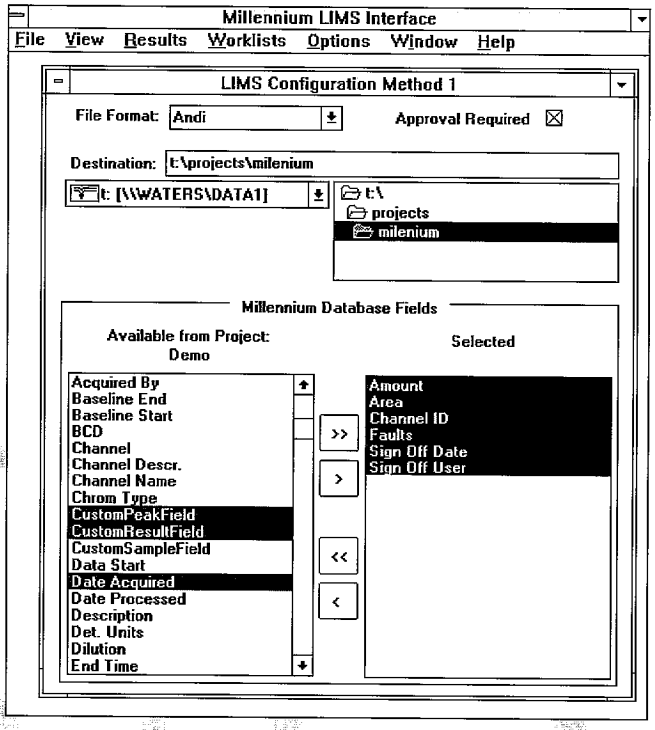

Figure 8: LIMS Interface configuration screen

Getting the most from your Millennium Database (continued from previous page)

It is rather straightforward to either modify an existing report to meet your needs, or to generate a totally new report. By selecting specific Report Groups and sorting these groups by various criteria, or even performing calculations on the groups, you are able to generate meaningful analyses of your Millennium data.

The reports that are generated can pull data from one result, or a summary report can draw data from a range of reports, collect the data, and present the results of your search in a report.

In addition to the ability to draw data from any field captured by Millennium software, the Reporting function also has the ability to format the resulting information in a variety of ways. It is possible to align the results of various calculations flush (left, right, or center) with each other, change the font size or style to differentiate various areas in the report, and even setup headers and footers which will print repeatedly on the top/bottom of every page of a report.

In short, with all of the significant data that is generated using Millennium software, the Millennium reporting tools allow the user to manipulate large volumes of existing data, and present it in a meaningful and compelling format.

Electronic Results Sign-Off

One final feature of the Millennium database is the ability to electronically sign-off on results generated. This function gives you the ability to have an auditor or reviewer approve experimental results. If a particular data set is within your acceptable limits, this reviewer can indicate that a given experiment is complete. This reviewer signs off on a particular set of results by typing in a password, which also generates a time/date stamp (Figure 7).

Using the Millennium Laboratory Information Management System (LIMS) Interface, it is possible to set up the Millennium system so that only results that have been signed-off are sent over the LIMS Interface. For example if you are doing sample life cycle tracking in LIMS, it is not necessary to deposit every result on the LIMS. With the electronic sign-off function it is possible to designate that only results which have been signed-off are sent to the LIMS thus ensuring that only quality-approved finished results are stored in the LIMS.

During sign-off it is possible to zoom in on the results of a particular chromatogram, or view a summary report and sign off on 50 results with the click of a button and the entry of the reviewer's name. To backtrack just for a moment, it would then be possible to use the View Filter to query the database, showing only signed-off results. These results could then be sent via the Millennium LIMS Interface to my LIMS system (Figure 8).

Conclusion

So now we have highlighted some of the most powerful features of the Millennium database in order to give you an idea of how to best take advantage of the system. We have seen that custom fields allow you to adapt the system to the particular needs of your laboratory, and that the inherent flexibility and data structure of a relational database allows you to track and manage your data efficiently.

Likewise the time stamping of the Oracle database provides an effective index of all "events" occurring on a Millennium system while the View Filter allows you to sort using the time stamp, or a variety of other criteria, in order to recall past results for examination at any time.

For more in-depth manipulation of data, the report generator is a powerful tool for both performing calculations on either individual results, or the data from a range of experiments, and presenting this information in well-formatted, easy to understand manner. And finally when a particular set of results has been reviewed and completed, through electronic sign-off, Millennium software allows a project manager to determine, by entering a password, that results are to be released to a wider audience.

Hopefully this overview will help you to get the most out of your Millennium software. In future articles we will explore the Report Generator in more detail and discuss, in-depth, other functions of the Millennium software.

For questions or comments, email either Dave Levy at levy_david@waters.com or Tom Hall at hallt@waters.com.

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Millennium Chromatography Manager: Advanced Features of Custom Fields

By Lauren Angus

The last issue of *Millennium On-Line* featured an article entitled "Millennium Software's Custom Fields Feature Simplifies Tracking and Management of Results." This article described the basic use of custom fields in Millennium software. This article builds on the first article and goes on to discuss the advanced use of Custom Fields in the Millennium software. These advanced features include: calibration fields, fields that build upon each other as well as inter- and intra-peak calculations.

Calibration Fields

Any Peak type field can be designated as a Calibration Field by selecting the Calibration Field check box found in the Data Source area of the Custom Field dialog box. Please refer to Figure 1.

By definition, a Calibration Field is only calculated for Standard type samples. The result generated by this field is associated with the processing method used to calibrate the data, much as the calibration curve is linked to the processing method. And as the calibration curve is used to quantitate unknown samples, calibration type custom fields can also be used to quantitate unknowns. Normally, the result of the calibration field for the last standard that was processed is linked to the processing method. If *Avg Cal Points* is chosen, the average result for all standards processed would be tied to the processing method. (Avg Cal Points does not take differing amounts, or levels, of standards into consideration and therefore should not be used for standards of varying amounts or levels.) In effect, when using a Calibration Field, you are creating a single-level calibration curve using a single point or one averaged point. The Clear Calibration feature can be used to remove this result preventing it from being linked to the processing method.

For example, if you are interested in quantitating unknowns based on response factors, you would need to create a series of custom peak fields. The first field would calculate the response factor itself. It would need to be a peak type field with a formula of $Amount_{std}/Response_{std}$. Let's name this field 'RF.' This field would be defined as a calibration field and would therefore be calculated only for standard type samples. The next field would be a regular (i.e. not a calibration field) peak field and would calculate adjusted amounts based on the response factor of the standards. Its formula would be $(Response_{unk})(RF)$. Let's call this field CorrectedArea. Bear in mind that $RF=Amount_{std}/Response_{std}$ and therefore $CorrectedArea = (Response_{unk})(Amount_{std}/Response_{std})$. The Response units cancel and you are left with the amount of the unknown which has been corrected for by the response factor of the standards. Custom Fields for RF and CorrectedArea are shown in Figures 2 and 3, respectively.

Notice that the field 'Corrected Area' incorporates the field 'RF'. This can be thought of as fields building upon each other. When this is done, the Field Order parameter becomes important. Field Order defines the order in which fields are calculated by the Millennium software. In the example above, RF needs to be calculated prior to Corrected Area and should be a lower Field Order. The Field Order will automatically escalate as new Custom Fields are created. However, the Field Order value can be changed simply by entering in the desired value.

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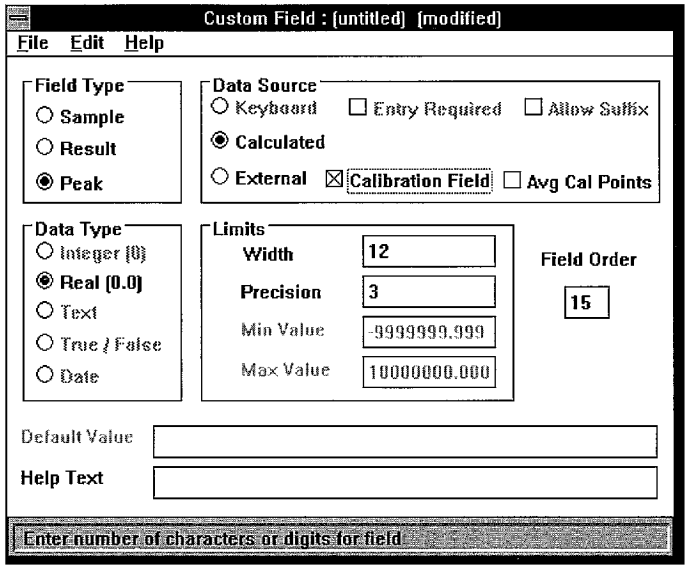


Figure 1: Custom Field editor

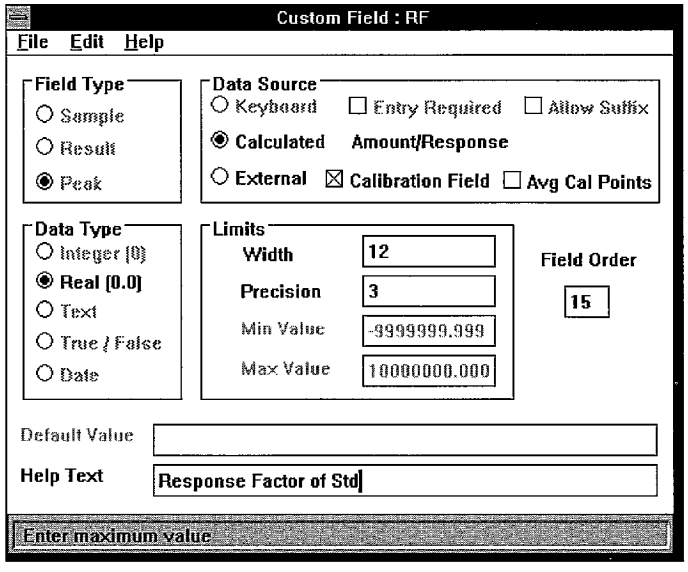


Figure 2: Custom Field editor with Help Text entered for Response Factor

Reference Peaks

Reference peaks are used to identify a known peak in the chromatogram on which calculations can be performed. In Millennium, these peaks can be referred to as CCalRef or CCompRef (with numerical identifiers ie: CCompRef1, CCompRef2 or CCompRef3). CCalRef1 is a global reference, indicating that one peak is used as the reference throughout the chromatogram. CCompRef1 through 3 are not global and can be defined differently for each peak.

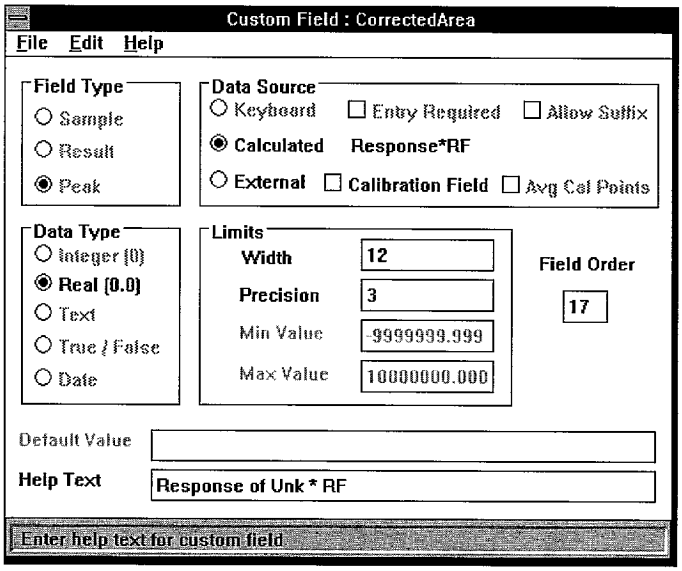


Figure 3: Custom Field editor with Help Text for Response of Unk* Response Factor

For example, in dealing with response factors, as in the previous examples, it is sometimes necessary to calculate a response ratio. This response ratio normalizes the response factor (RF) for each component by dividing it by the response factor of a reference peak. The mathematical formula is $RF_{component}/RF_{reference\ peak}$. The reference peak in this case is the same for every component in the chromatogram. Therefore, a global reference, CCalRef1, is used. The formula used in this custom field is as follows Response Ratio=RF/CCalRef1[RF]. Note that 'CCalRef1' defines the component acting as the reference peak and the value in square brackets is the parameter used in the calculation. This calculation takes the RF value of each peak and divides it by the RF value of the peak that is defined as the reference peak. Reference peaks are defined in the processing method's component table as shown in Figure 4.

CCompRef1, CCompRef2 and CCompRef3 are used in a manner similar to that of CCalRef1, however a CCalRef can be defined differently for each component, thus making the custom field calculation different for each peak.

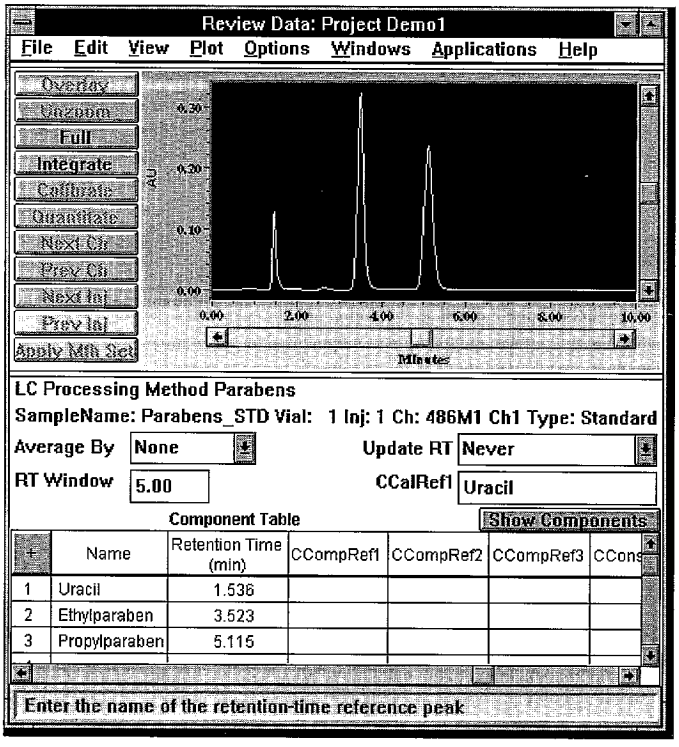


Figure 4: Reference peaks are defined using the component table

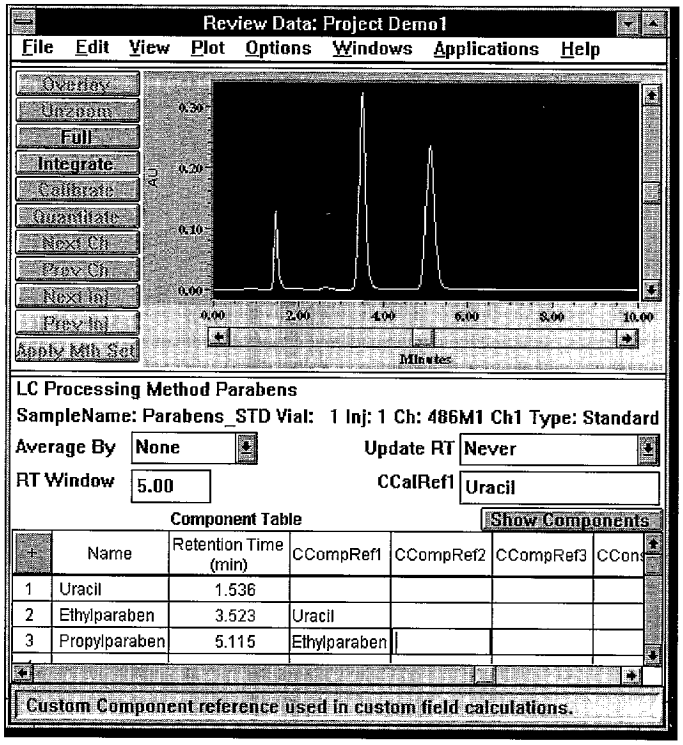


Figure 5: Millennium software allows you a different calibration peak for each component

In addition, different reference peaks are needed in order to calculate resolution; the formula for resolution is as follows:

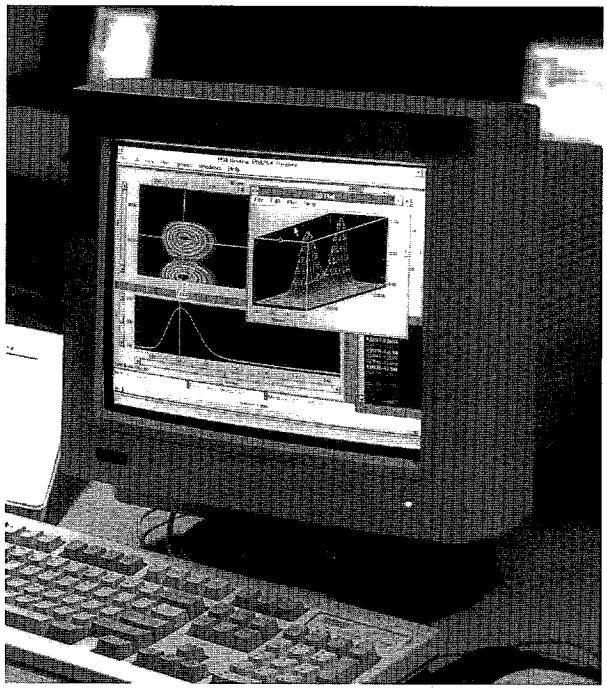
Resolution = $2(Rt_{current\ peak} - Rt_{previous\ peak})/Width_{current\ peak}$.

In this case, CCompRef1, CCompRef2 or CCompRef3 would be used to refer to the reference peak as shown in Figure 5.

The formula, as entered into the Custom Field formula window, reads:

Resolution = 2 (Retention Time – CCompRef1[Retention Time])/Width.

As Figure 5 indicates, resolution will not be for the Uracil peak as no component is defined as CCompRef1 since there is no component eluting prior to Uracil. The peak prior to Ethylparaben is Uracil, which will therefore be used to calculate resolution for Ethylparaben. Likewise, Ethylparaben will be used to calculate resolution for Propylparaben.



Conclusion

So we see that the use of custom fields in the Millennium Chromatography Manager Software goes beyond the basic tracking of data, and allows the experimenter to perform complex calculations on experimental data in real-time. The two examples above elegantly describe how custom fields can be built at several levels, with one user-defined custom field relying upon another custom field, previously defined by the user, in order to obtain the final, desired result.

This article presents just two examples of the advanced usage of custom fields. With experience, you should be able to develop your own unique uses for this powerful, flexible feature of Millennium software. If you have any particularly interesting examples of ways in which custom fields have been used in your laboratory, please contact us at Waters to discuss possible publication in a future issue of OnLine.

For questions or comments regarding this article, email me at lauren_angus@waters.com

ON TARGET

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Alternatives to "Norton Compatible" Devices for Back-Up of Millennium Data

By The Technical Service Group

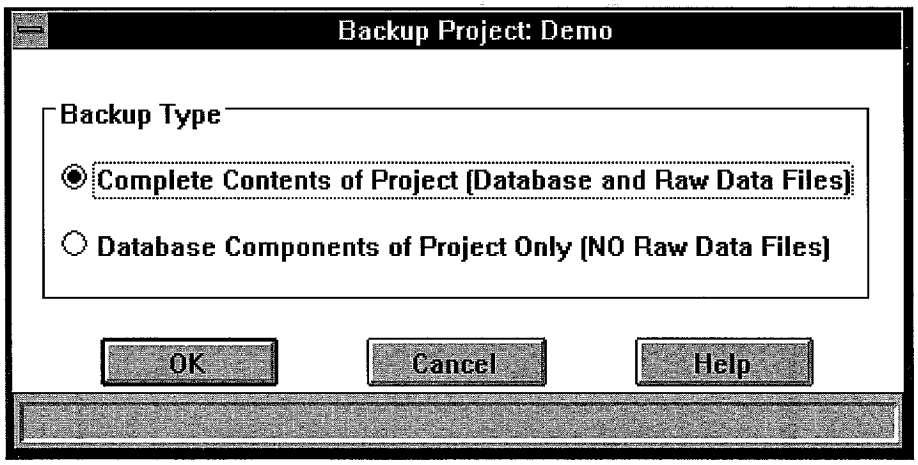

Figure 1: Backup Project Selection dialog box

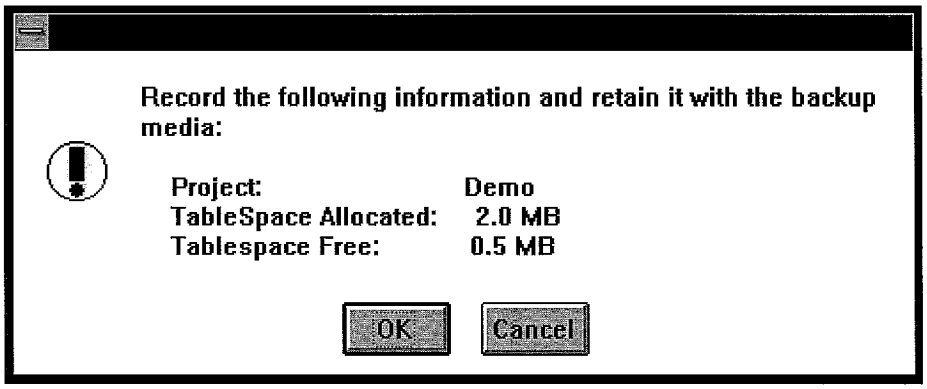

Figure 2: Backup information dialog box

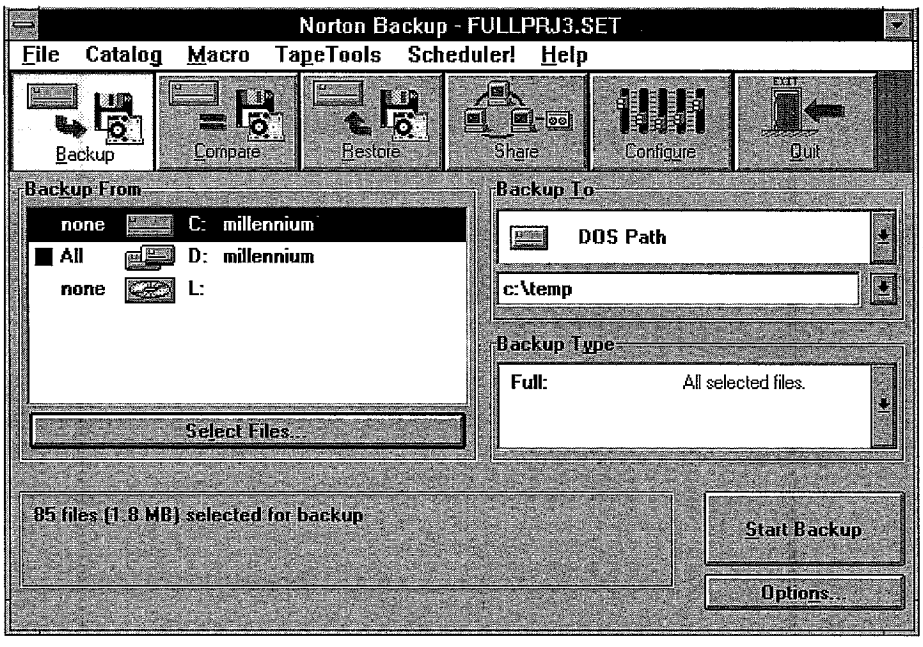

Figure 3: Norton Backup Utility

Millennium software includes Norton® Back-up 3.0 from Symantec Corporation to provide a robust and secure method for long term data storage. Millennium files saved to a data storage device are commonly referred to as "back-up" files. Norton's Back-up 3.0 has been integrated into the project and database procedures in the Session Manager screen of the Millennium software.

Norton supports serial tape drives as well as SCSI tape drives. Recently however many new back-up devices from multiple vendors have been introduced, (magnetic tape, DAT tape, and newer serial drives etc.) which are not supported by Norton Back-up 3.0. Initially one might assume that Millennium can take advantage of these newer devices, but this article will provide a simple back-up procedure using Norton and virtually any back-up devices.

This procedure will be accomplished in two steps. The first is to establish a temporary DOS path on a local hard drive or on a network drive. The second is to do the back-up.

The back-up begins in the Millennium session manager screen by highlighting the project in question and selecting Database from the menu bar. Select the type of back-up you wish to utilize. In this example we will use Back-up/Project from the pull-down menu. A screen appears with two options (Figure 1).

Generally, running a complete back-up is recommended. Click the OK button to continue to the next screen. The new screen informs you to write down the following information. Project name, tablespace allocated, tablespace free, and retain this information with the back-up (Figure 2).

When you click OK, the Windows screen will disappear and change to a DOS screen, at this time Millennium is exporting the data from the database to a temporary location to prepare the data for back-up. The Norton software will now be displayed on the screen (Figure 3). When entering Norton Back-up, a screen identical to that shown below is displayed. There are no selections to make except to select "DOS PATH" as the "back-up to" destination and to enter the actual DOS path back-up destination directly below. In our example it would be c:\temp.

After entering the "back-up to" destination, press the start button. The back-up will proceed very swiftly since only hard drive to hard drive communication is involved.

When the back-up is complete, the file tree should look like the one below (Figure 4). The figure at the left shows the directory "C:\temp" as the recipient of one project back-up. The actual back-up files reside in the "dd61104a.ful" directory.

At this point, the DOS path phase of the back-up is finished. All that remains is to launch the software provided by the manufacturer of the new device, and back-up the DOS directory (and subdirectories) which contain the back-up.

If there is no network in place and the system in question has little remaining space on the hard drive, purchasing an additional hard drive is recommended. Today gigabyte drives are very reasonably priced.

Should it become necessary to restore projects which have been previously been backed-up, you simply reverse the process: First restore the files using the software for the device in use. Next, from the Millennium Session Manager select Database/ Restore Project. At this point the user will be prompted for a project name of the new project and its size (from the information saved with the project). Norton will display a prompt for the location of the catalog file of the back-up as shown below (Figure 5). Simply enter the DOS path containing the file.

Double-clicking the line will change the "None" to "All" (Figure 6). All the other fields should already be entered from information retrieved from the catalogue file. Press the Start Restore button. The restoration of the raw data files and the database import files will ensue. When these files are restored, the importation process will take place, thus completing the restore.

Using this procedure makes it possible to use the latest back-up hardware even if it is not compatible with Norton Back-up 3.0.

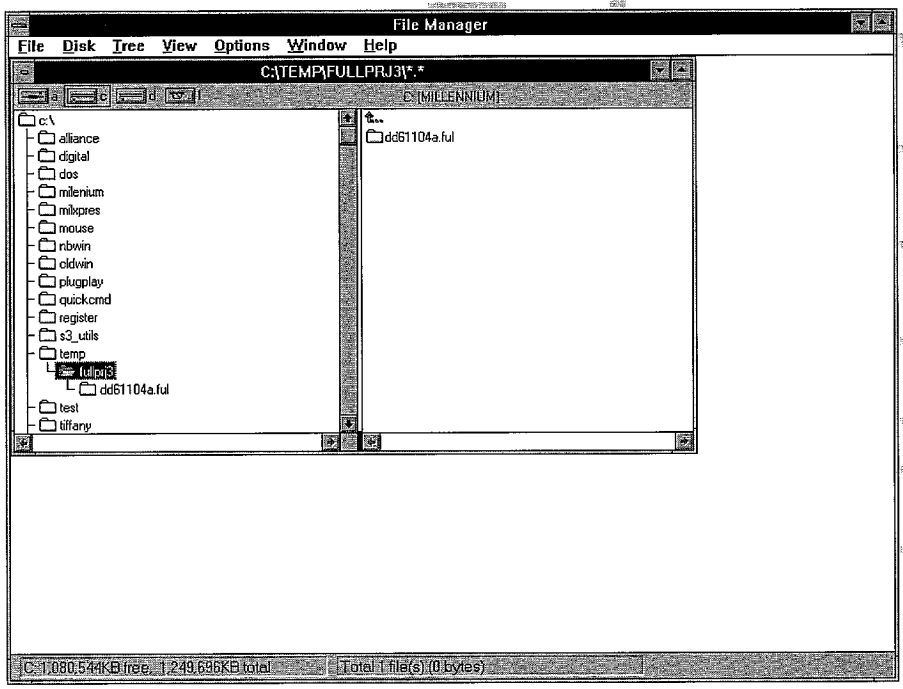

Figure 4: Windows file tree

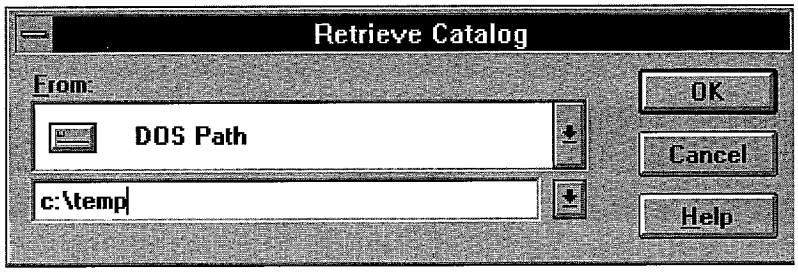

Figure 5: Backup catalog location

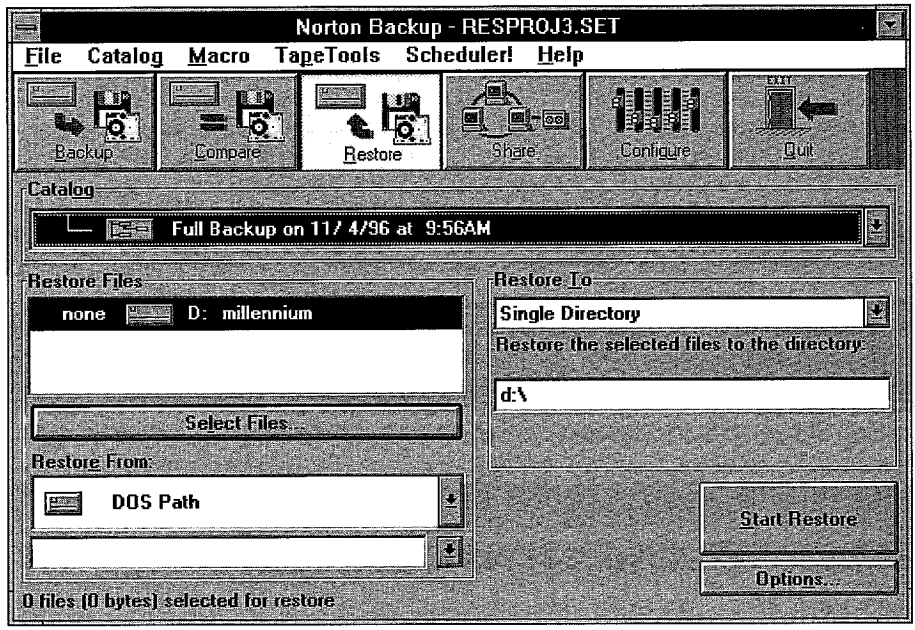

Figure 6: Norton backup utility

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