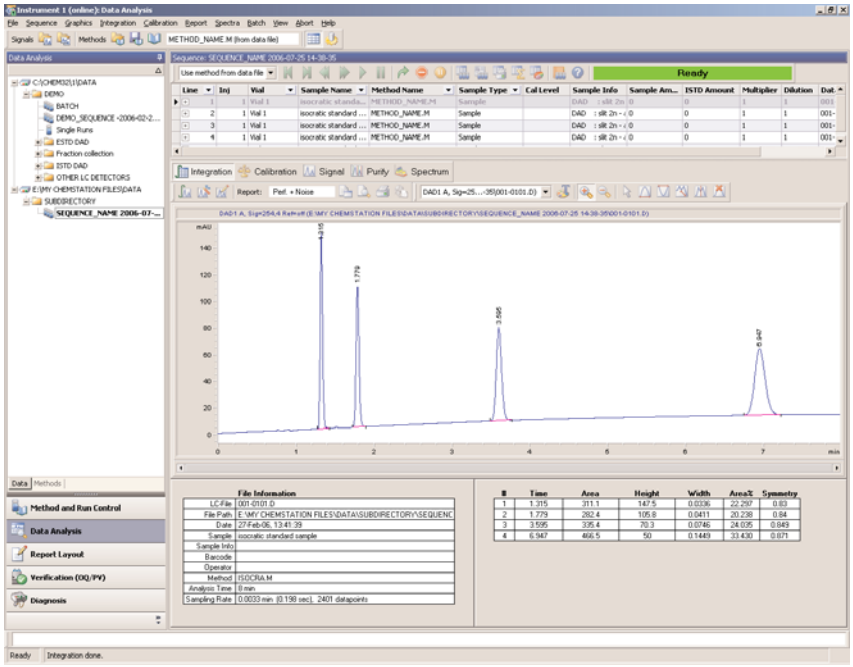
# Agilent ChemStation B.02.01 / B.03.01: New Concepts of Data Organization

## Technical Note



## Introduction

In analytical laboratories, chromatography data need to be acquired efficiently in a short time. Clarifying ambiguous results can be time-consuming, and may result in high administrative costs. Starting with ChemStation revision B.02.01, data storage and data browsing capabilities have been improved to enable fast review and reprocessing of result data. In this Technical Note, we describe the efficient use of the new data storage and retrieval functions in ChemStation B.02.01/B.02.01 B.03.01 to boost your lab's productivity. In revision B.03.01 users can choose to keep their established workflows in ChemStation. For both scenarios a typical workflow is described.

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## Overview

This Technical Note describes the efficient use of data storage and retrieval functions in ChemStation B.02.01/B.03.01.

# 1. ChemStation Data Structure

**ChemStation prior to B.02.01**
In ChemStation revisions prior to B.02.01, sequences, method and the generated data files and results were stored in fixed specified and separated paths. For example, methods were referenced by name in a sequence and it was the user's responsibility to maintain the integrity of methods, sequences, and data files. Because of this, the long-term archiving of data, and reproduction of results was a tedious task. Users had to document the chromatogram, results, and associated method; this was the case not only for regulated labs, but also for some areas of unregulated labs (such as environmental labs). In ChemStation prior to B.02.01, this could be achieved only by printing everything on a report.

**ChemStation B.02.01/B.03.01**
In order to strengthen the association between data files and methods, the following new data organization scheme has been implemented with ChemStation B.02.01/ B.02.01 SR1. When used with the ChemStation, the Agilent Enterprise Content Manager (ECM) also makes use of the new data concept, since the complete data set (sequence/methods/data files) can now be transferred (archived) to ECM as one entity (figure 1).

The methods in the folder Chem32\1\methods serve as master methods, i.e. during acquisition and data analysis, they remain unchanged once method development has been completed.

Similarly, the sequences in the folder Chem32\1\sequence serve as sequence templates that can

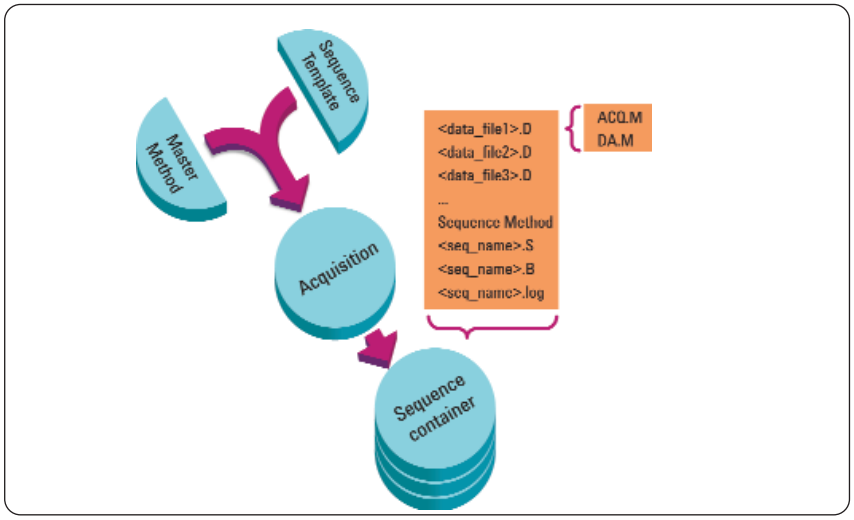


**Figure 1**
**Sequence acquisition.**

be used to rerun (but not reprocess) a sequence several times.

The data storage pattern varies depending on whether single run data or sequence data is acquired:
1. When a sequence is executed, a new folder is automatically created ("sequence container") with a unique name in the specified subdirectory. When a single sample is run, the data file (*.d) is written to the specified subdirectory.

2. For sequence data, the executed sequence template (*.s) and all the methods (*.m) involved are copied into the sequence container. The copies of the methods are called the "sequence methods" in order to distinguish them from the original master methods. All sequence-related tasks (e.g. acquisition and data analysis) are performed on the copies of the sequence and the methods. Therefore, the sequence template and the master methods remain unchanged for future sequence execution.

While executing the sequence, all generated data files (*.d) are stored in the sequence data folder, along with the corresponding batch file (*.b) and sequence log file (*.log).

3. Each data file contains two copies of the method used to create the run.
- The first one, called ACQ.M, is saved directly after the acquisition part of the method is completed.
- The second copy, called DA.M, is saved after completion of the data analysis part.

The preservation of the state of the method at acquisition of the specific data file is thus ensured. The DA.M can be modified during data analysis. In this case, these two methods may differ if, for example, the calibration table is updated.

## 2. Data Acquisition

The following sections explain the impact of this structure on typical workflows in more detail.

Starting with ChemStation B.02.01, flexible data storage for single runs and sequences allows you to specify various saving locations without reconfiguration. The Path Tab in the newly introduced Preferences dialog box in the View menu gives you the opportunity to add multiple paths in addition to the default path C:\chem32\x\DATA (where x is the instrument number). Using the Add and Remove buttons, existing paths can be simply deleted, or you can navigate to a selected location and add the path to the new location into the Preferences. The default path cannot be removed from the list, but can be changed in the Configuration Editor (figure 2). All newly specified Data Paths are then available for selection in the Sample Info/ Sequence Parameters dialog box when performing runs (figure 3).

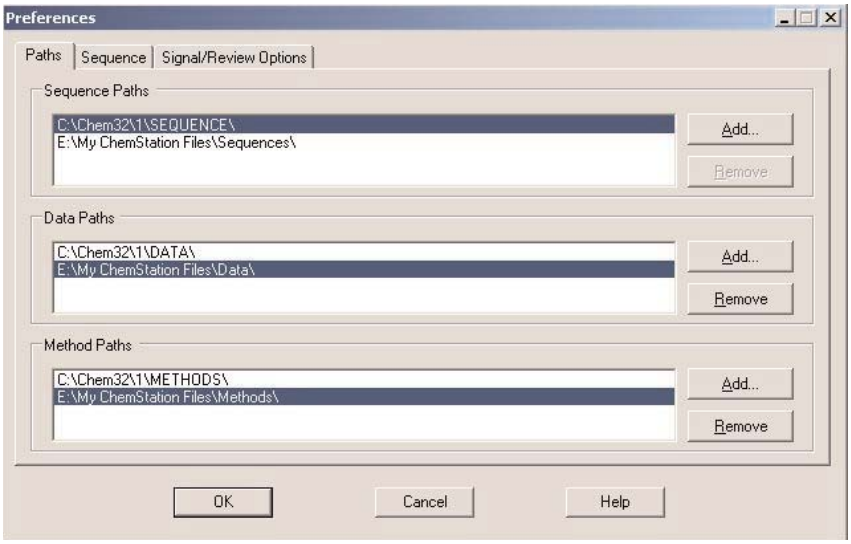


**Figure 2**
**Preferences dialog / Paths tab.**

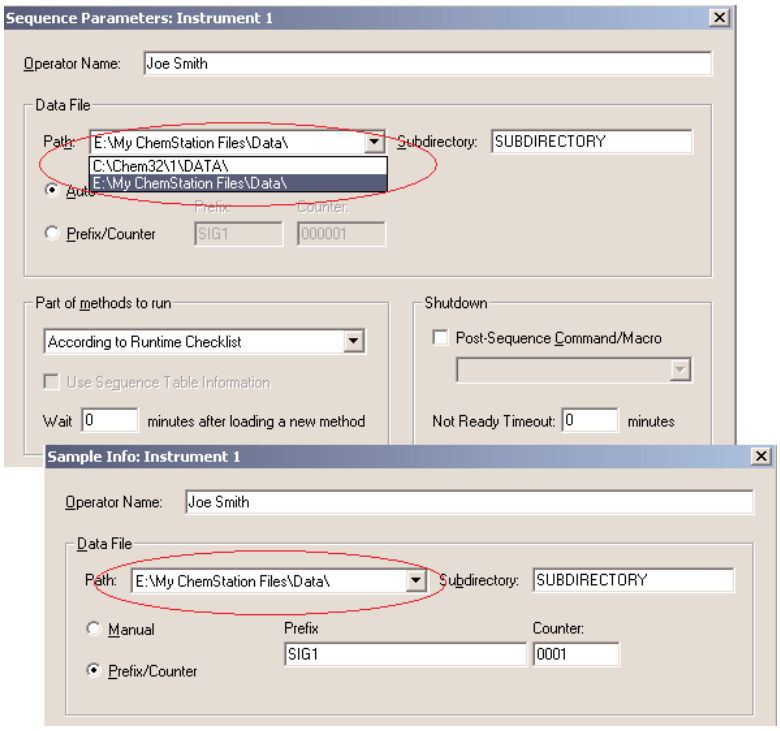


**Figure 3**
**Data path selection.**

### Data Acquisition in a Sequence

In order to run a sequence, appropriate pre-defined methods must be available. These are the master methods as outlined above. Typically, master methods and sequence templates are worked on in the Method and Run Control view of the ChemStation. For this reason, in Method and Run Control view, the ChemStation Explorer provides access to master methods and sequence templates.
The sequence template references these methods in the

sequence table.

As explained previously, when a sequence is run with sequence template <sequence_name>.S and the master method <method _name>.M is used, a new folder is created containing all resulting files from the sequence run ("sequence container"). The location of this folder is determined by the settings in the Sequence Parameters dialog box and the naming is determined by the Sequence tab of the Preferences dialog box. By default, the name is <sequence _name> <acquisition _date> <acquisition_time>, but it can be configured by using the tokens Operator, Instrument, Counter, and PC Name, or you can manually enter any name (figure 4).

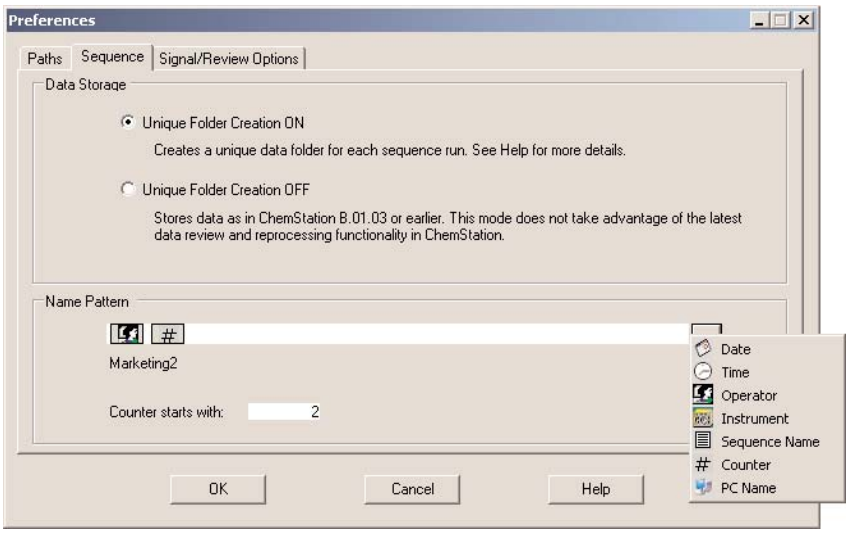


**Figure 4**
**Preferences dialog / Sequence tab.**

At the start of an acquisition sequence, the method specified in the sequence table is copied from the master methods folder into the sequence container. In addition, a copy of the sequence is created and placed with the sequence log and the batch (*.b) file in the sequence container. All updates of the method (e.g. updates of the calibration table) are written to this sequence method in the container. All necessary files are now available for future data review and reprocessing, without changes that were applied to the master method or sequence template for other sequence runs.
During acquisition, the data files are stored to the sequence container. Within each data file (*.D), two additional methods, ACQ.M and DA.M, are saved for this specific run. These two methods are copies of the sequence method, preserving the state of the method as it was at the time of acquisition of the specific data file. In the case of e.g. calibration table updates the DA.M methods differ for each of the runs.
The individual acquisition method ACQ.M is intended to preserve the acquisition parameters, therefore it is recommended that you do not change this method during future data review activities.

With these files saved in the sequence folder, all data review and reprocess activities can be performed without altering the master method or the sequence template. If needed, method changes can also be saved to the master method again.

**Data Acquisition of Single Runs**
The new data concept is also introduced for single runs starting with ChemStation B.02.01 SR1. In this case the data file is saved directly into the respective subdirectory. Since only one method is employed for a single run, this method does not need to be copied into the subdirecto-

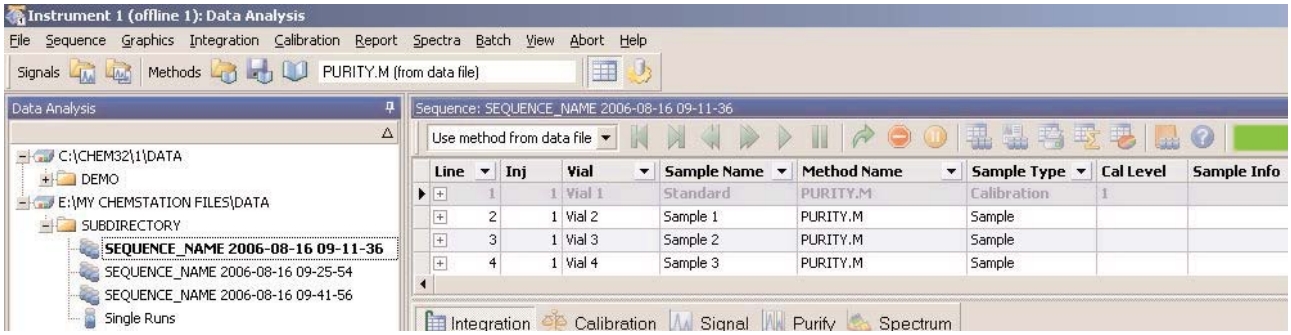


**Figure 5**
**Loading a sequence from the ChemStation Explorer into Navigation Table.**

ry.
All actions are performed directly with the master method. After the acquisition part of the method is completed a copy of the master method is saved into the data file directory (ACQ.M). Another copy (DA.M) is saved after the data analysis part of the master method has been executed.

Once the data have been acquired, they can be analyzed in

**Figure 6**
**Data review toolset of the navigation table.**

ChemStation Data Analysis view. When selecting the Data tab of the ChemStation Explorer, you can load all the runs of a sequence or all single runs in a specific folder by double-clicking the corresponding symbol. The corresponding data set is then available in the Navigation Table (figure 5).

The main body of the Navigation Table consists of a list of all runs of the set. Instead of loading a run via the File / Load Signal menu, a run can now be loaded into ChemStation memory by double-clicking the relevant line in the Navigation Table. Once the run is loaded, you can review it, i.e. adjust data analysis parameters, integrate the signals and finally print a report. In this case you analyze the run as a single run without taking the sequence context into account. This way of data analysis is called “Data Review”. The Navigation Table provides the tool set shown in figure 6, which makes data review more convenient.With this toolset, you can jump to the beginning or end of the Navigation Table, step on to next or previous run, automatically step through the runs, and stop automatic stepping.

**Figure 7**
**Sequence Reprocessing toolset of the Navigation Table.**

A different way to analyze your data is to “Reprocess” a complete sequence. During this process, all runs are reanalyzed in the

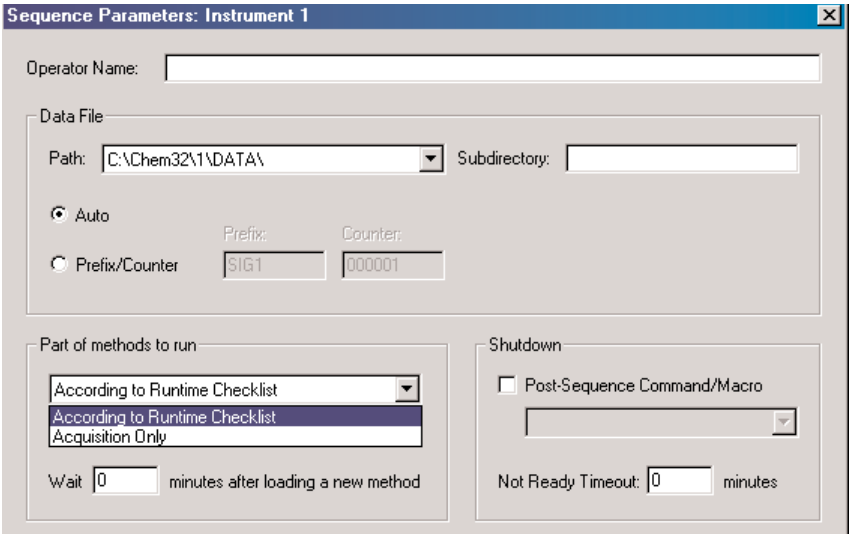


**Figure 8**
**ChemStation B.02.01 Method and Run Control Sequence Parameters**

sequence context, i.e. the calibration tables of the sequence methods are updated in the case of calibration runs, multipliers, amounts etc. can be changed in the sequence table, new methods can be added to the sequence container, etc. For reprocessing, the Navigation Table provides the toolset in figure 7.
Please note, the reprocessing icons in the Navigation Table are available only for sequence data generate starting with ChemStation B.02.01 and higher. For Single Run data, as well for data generated prior to B.02.01 reprocessing in Data Analysis is not accessible. Sequence aquired prior to B.02.01 need to be reprocessed in "Method and Run Control", defining the sequence parameter "parts of method to run" to "reprocess only". For B.02.01 and higher generated sequence, the reprocessing option in Method and Run Control has been removed, and the Navigation Table offers reprocessing as an Data Analysis Task. (figure 8).

### Data Analysis Data Review

Data Review means analyzing on a run-per-run base. ChemStation allows you to specify default actions that are performed automatically when a data file is loaded from the Navigation Table. These include data analysis tasks like integrating the chromatogram directly after loading, and also to specify the method that is to be loaded. The corresponding options for reviewing (not used for reprocessing) are set up on the "Review/Signal Options" tab of the Preferences dialog (figure 9).

The first section, "Load Signal Options", specifies which of the signals in a run are loaded, and if the chromatograms are to be integrated and the results reported directly after loading. In the second section,"Data Review Options", you have the possibility to configure the interval for stepping through the runs in the Navigation Table automatically. The remainder of this section specifies which method is loaded during data review when a run is loaded from the Navigation Table.
Table 1 shows the separate option sets that are available for sequence runs and single runs.

The following sections describe how to use these options in different workflows.

*Keep "Current Method"*
The review setting "Current Method" should always be used when you want to use the method that is currently loaded. In this respect, for data review the current method remains irrespective of which single run data file or sequence container file is loaded. This setting should be used for method development, to

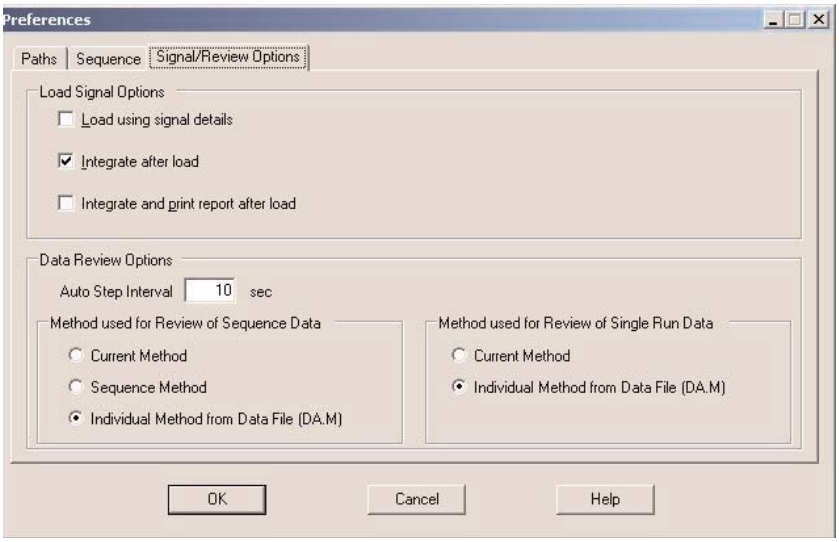


**Figure 9**
**Preferences dialog / Signal/Review Options tab.**

| Method used for review of sequence data | Method used for review of single run data |
|---|---|
| Current method | Current |
| Sequence method | Individual method from data file (DA.M) |
| Individual method from data file (DA.M) | |

**Table 1**
**Data Review options for Sequence and Single Run data.**

create a calibration table or other updates. For example, you run a sequence with runs of different concentrations in order to optimize integration parameters, and afterwards build the calibration table. As these changes in data analysis parameters must be available for all future acquisition runs, you have to apply them to the master method. In order to do this, you select the option “Current Method” in the Preferences dialog, (figure 10). This ensures that, for each run loaded, the same method is always kept in memory.

You load the master method, most conveniently from the Method tab of the ChemStation Explorer.
Now, you optimize the integration parameters and use the runs to construct the calibration table. All future acquisitions using this method will apply these optimized data analysis parameters.

*Load “Sequence Method”*
It may also occur that sequence-specific events require changes in all the methods employed with the sequence. Once every run has been reviewed and the sequence methods have been improved, the complete sequence can be reprocessed with the updated methods. In this scenario, you review the data using the option “Sequence Method” (figure 11).

This means that each time you load a run from the Navigation Table, the sequence method corresponding to the run's sequence line is loaded. Once the data review has been completed, it may be necessary to reprocess

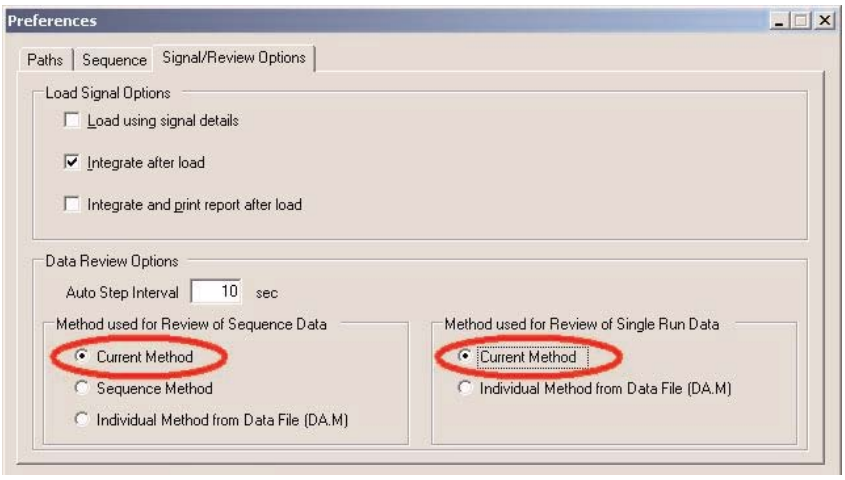


**Figure 10**
**Keep the current method for data review.**

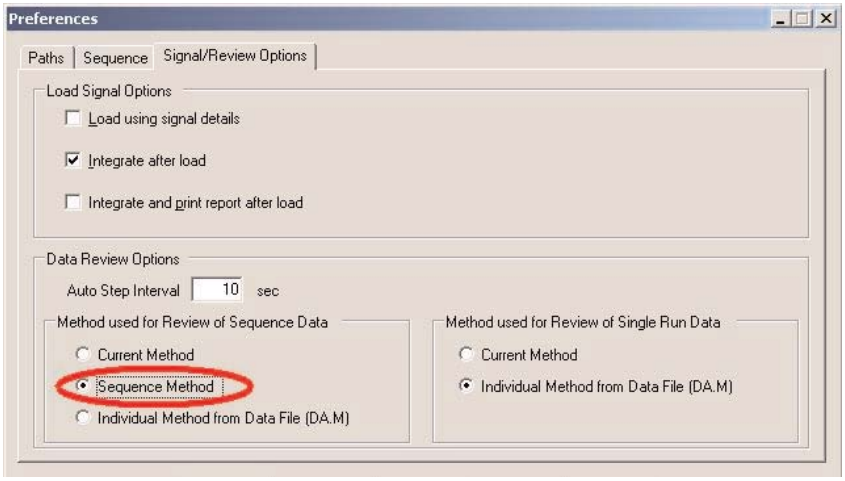


**Figure 11**
**Load Sequence Method for data review.**

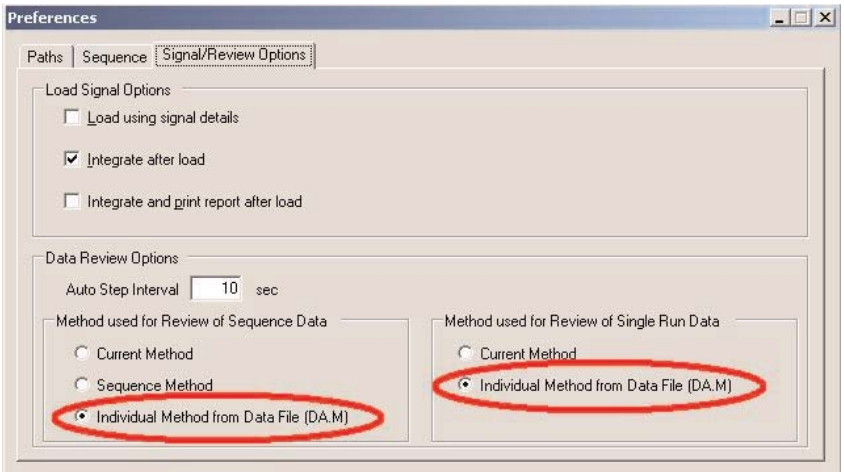


**Figure 12**
**Load Individual Method from Data File for data review.**

the complete sequence in order to apply the method changes not only on a run-per-run base, but also in the complete sequence context (including calibration table updates etc.).

*Load "Individual method from data file"*
The review setting "Individual Method from Data File (DA.M)" (figure 12) should be used, if you want to load the individual DA.M automatically along with the corresponding datafile, when this file is loaded using the navigation table. When you change a method and then load the next run, you will be asked to save your method changes, because you load a new method: the DA.M of the next run.

Various workflows may require that you always review data with the individual data analysis method (DA.M) loaded. For example, when all runs are loaded with DA.M, the analysis results are the same as during acquisition or last reprocessing. Additionally, it is possible to perform run-specific changes and save them in the individual data analysis method of the run. This is especially useful for manual integration events.

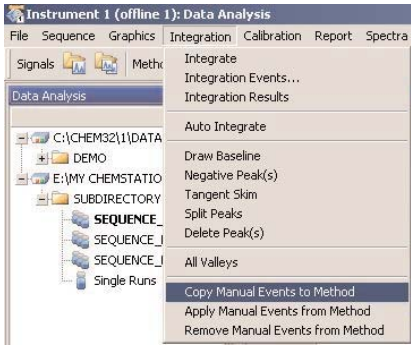


**Figure 13**
**Copy Manual Integration Events to a Method.**

Using the individual data analysis method (DA.M) a convenient means is available to store manual integration events to a specific data file only. So, when you use the automatic review and print the reports, the specific manual integratios are reported in one shot. Use the following steps to copy manual integration events to a method (figure 13).
1. Perform manual integration until the results are satisfactory.

2. Select Integration -> Copy Manual Events to Method. When the manual events have been saved to the individual method (instead of e.g. the corresponding master method), it is probably most useful to always apply those events when the chromatogram is integrated.

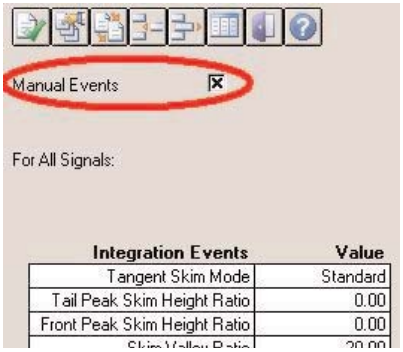


**Figure 14**
**Apply the Manual Integration Events each time the chromatogram is integrated.**

3. Check the "Manual Events" option in the Integration Events dialog (figure 14).

4. Save the method.

*Note: When a sequence is reprocessed, all actions are performed on the sequence methods and the DA.M of each data file is overwritten, including the manual integration events!*

### ChemStation user interface during data review

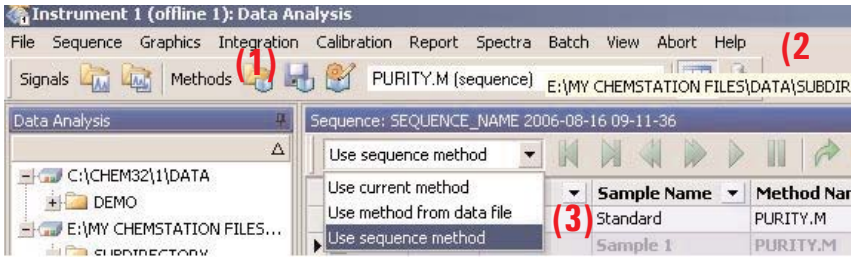


**Figure 15**
**User Interface in Data Analysis.**

The ChemStation user interface provides a number of features to facilitate working with the different methods available for data analysis (figure 15).

1. The method modification status is displayed in Data Analysis view, so you can easily follow if there are unsaved method changes. The user interface always displays the name of the currently loaded method (together with the information whether it is an individual data analysis method of a data file or a sequence method).

2. When you move the mouse pointer over this field, a tool tip additionally displays the complete path and name of the method.

3. A dropdown box provides a "shortcut" to the method options of the Preferences dialog. You can directly enable any of the available options and it will be applied the next time you load a run from the Navigation Table. Moreover, it is also very convenient to see which option is currently active.

*Update master method feature*
During working on the individual data analysis method, you may decide that you want to have the data analysis parameters you developed for the individual method available for the sequence or master method. A right-click in the Navigation Table on the corresponding run allows you to update your sequence or master method with the data analysis parameters. (figure 16)

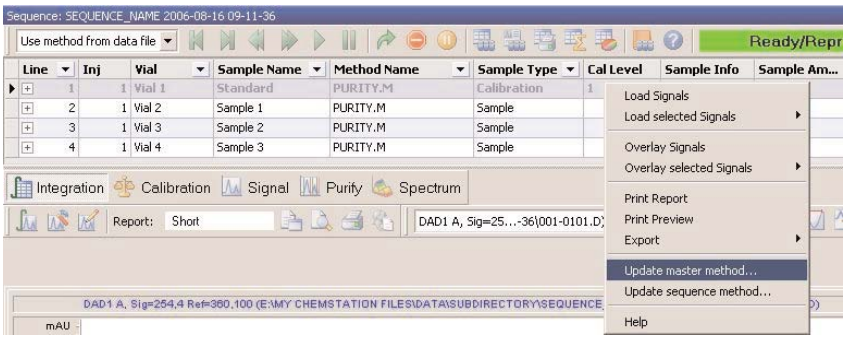


**Figure 16**
**Update Master or Sequence Method.**

| Loaded method | Available options |
|---|---|
| Individual data analysis method (DA.M) | Update Master Method |
| | Update Sequence Method |
| Sequence Method | Update Master Method |
| Master Method | – |

**Table 2**
**Availability of the Update ... Method functionality.**

This feature is available in the situations listed in table 2. It is important to note that this feature only updates data analysis parameters of the target method, and that it overwrites all data analysis parameters.

*Note: For technical reasons, in addition to the data analysis parameters, the Method Change*

**Figure 17**
**Toolset for Sequence Reprocessing.**

*History of the target method is also overwritten with History of the source method.*

**Data Analysis: Reprocess your Data**

In contrast to data review, sequence reprocessing means that all the runs of a sequence are reanalyzed in the sequence context, i.e. including calibration table updates, parameters changes in the sequence table, additions of new methods to the sequence, etc.With the new data organization concept, the sequence container includes all files needed for reprocessing: the data files, a copy of the sequence file, and all the sequence methods originally employed with the acquisition. Thus, in order to reprocess a sequence you simply have to load it into the Navigation Table and the required tool set is available (figure 17).
Please note the following rules with regard to reprocessing:

- All actions are performed on the sequence methods. If changed data analysis parameters are to be applied, you have to change the sequence methods.
- The method loading settings of the Preferences dialog have no influence on reprocessing; it always works on the sequence methods. This feature set is valid for reviewing only.
- During reprocessing, the Batch (*.b) file, the sequence/single run log (*.log), the Navigation Table, and the individual data analysis

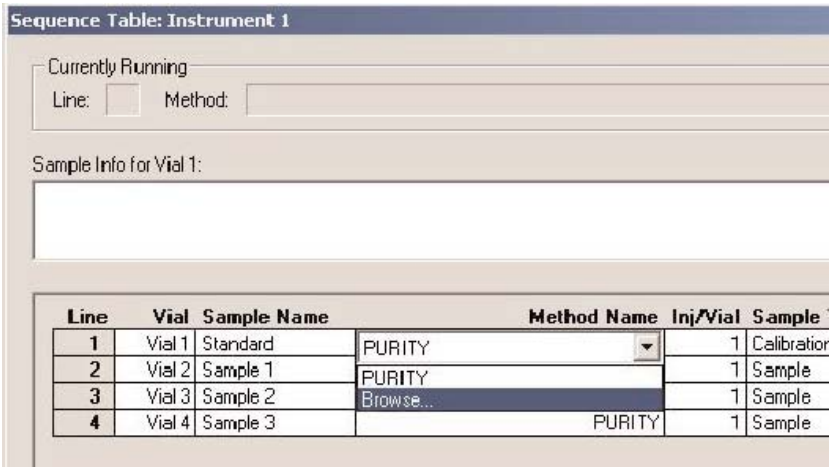


**Figure 18**
**Browse to the Master Methods Directory in the Sequence Table.**

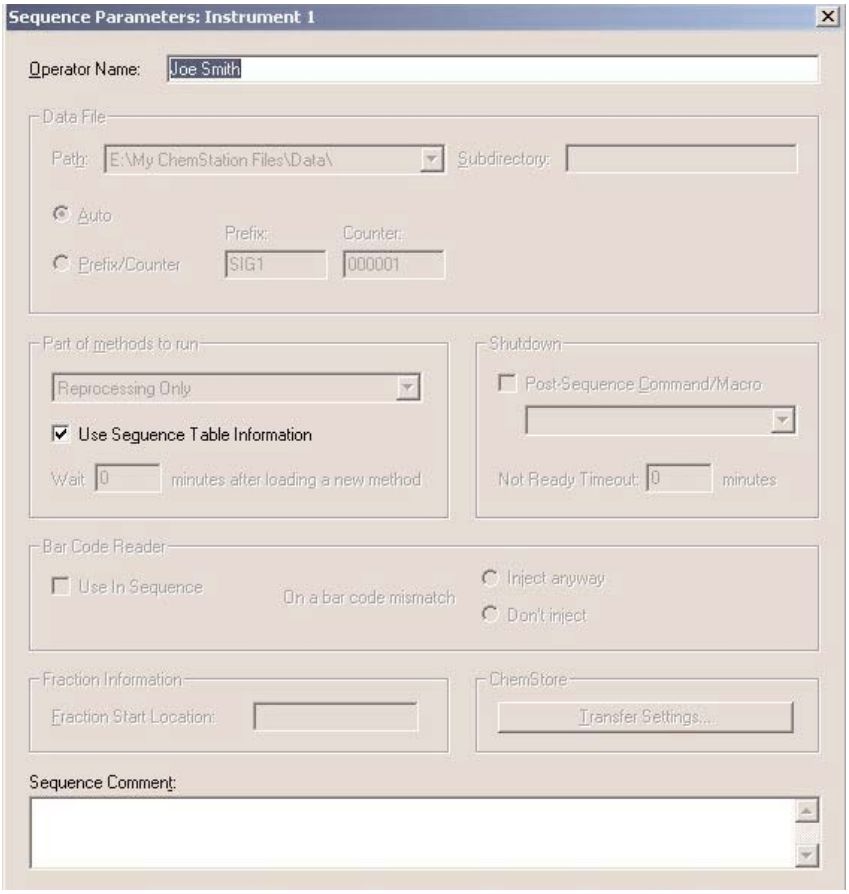


**Figure 19**
**Sequence Table in Data Analysis.**

method (DA.M) of each processed data file are updated.

• If you want to add new methods from one of the master method directories to the sequence table, you have to use the Browse item in the list of methods to browse to any specified method directory. The new method is also copied to the sequence container during reprocessing. This implies that you cannot select a method with the same name as a method already present in the container (figure 18).

5) In the sequence table, it is not possible to add or remove lines.

6) In the Sequence Parameters dialog, only a limited set of fields can be changed, e.g. Dilution, Sample Amount. All other fields have been set during data aquisition (figure 19).

### How to configure back to earlier ChemStation UI

If you prefer the ChemStation UI of previous revisions, perform the following steps:

1) Collapse the ChemStation Explorer with its tree view and navigation buttons by clicking the push pin at its upper right corner; the side bar collapses and frees more screen estate for the customary ChemStation user interface. Now, when you move the mouse over the side tab, it

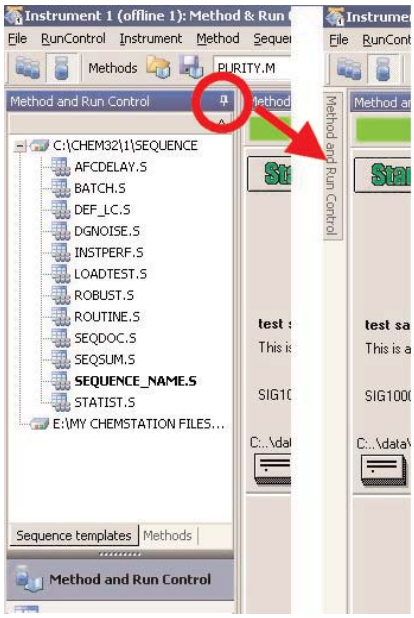


**Figure 20**
**Collapse and expand the ChemStation Explorer.**

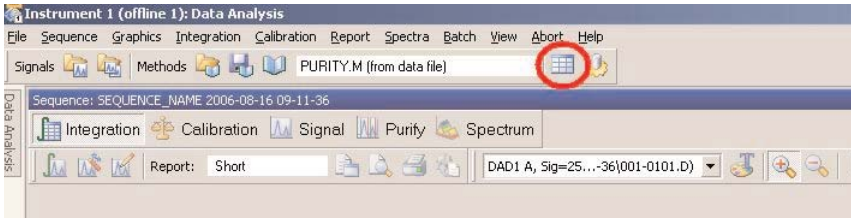


**Figure 21**
**Hide the Navigation Table.**

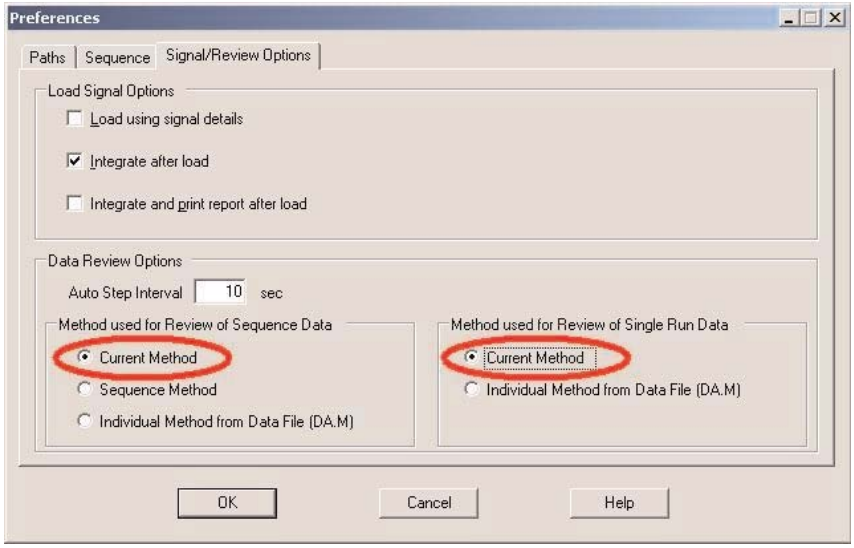


**Figure 22**
**Keep Current Method for data review.**

# 4. Workflow with *Unique Folder Creation* switched off

This section provides information on working with *Unique Folder Creation* switched off which allows you to store data as in ChemStation revisions B.01.03 or earlier. This mode does not take full advantage of the latest data review and reprocessing functionality in ChemStation.

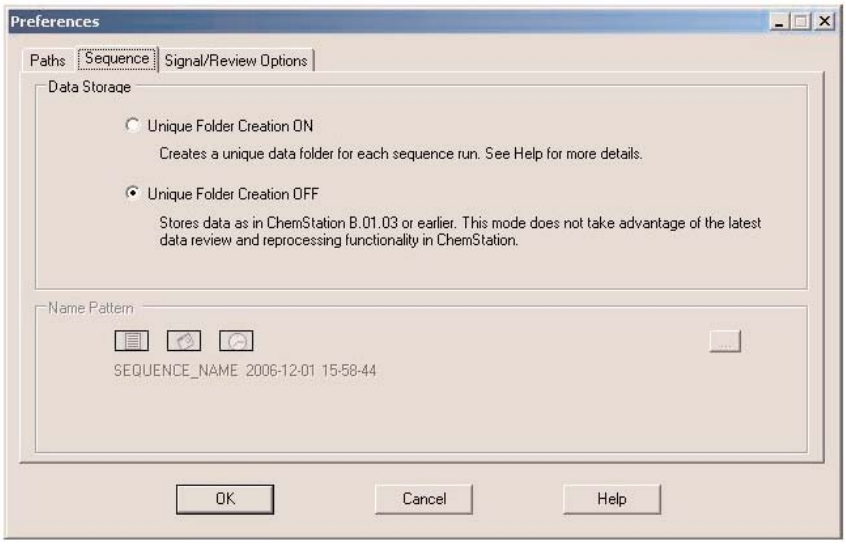


**Figure 23**
**Preferences Dialog/Sequence Tab**

### Working with *Unique Folder Creation* on or off?

The new data concept as outlined in the previous chapters provides a number of advantages:

- Sequence data are not overwritten. Each sequence acquisition stores the resulting data files in its own sequence container with unique name.
- With the sequence container concept, the data are stored with all necessary information needed for data analysis, i.e. copies of the sequence file and of all methods employed with the sequence. These methods can be changed with sequence specific input and do not influence the original master method. The container concept thus strengthens the meaning of a sequence as a set of data files and methods belonging together for result creation.
- Data review and reprocessing are both available in *Data Analysis* view via the *Navigation Table*.
- The data container concept provides the optimal preconditions for the ChemStation Integration with the Agilent Enterprise Content Manager (ECM). However, there may be situations where users may want to store their data as in ChemStation B.01.03 or earlier and work according to the corresponding workflows:
- During method development it may be more convenient to have only one method for both acquisition and data analysis to automatically have changes available for future acquisition and reanalysis of already acquired data.
- Data from several acquisitions have to be in one folder, e.g. in case of partial acquisition.
- Customized macro solutions on a ChemStation system that have been designed for older revisions may require the data, methods, or sequence to be stored according to the old data organization scheme.
- When ChemStation B.03.01 runs in a lab where there are also system still running on ChemStation revisions B.01.03 or earlier, it may be more convenient to use the same data organization mode on all systems.

### Working with *Unique Folder Creation* switched off

In order to allow working with a data storage concept as in ChemStation revisions before B.02.01, the *Sequence* tab of the *Preferences* dialog box a *Data Storage* section. Here you can choose between *Unique Folder Creation ON* and *Unique Folder Creation OFF* (figure 23). Per default, *Unique Folder Creation ON* is selected. *Unique Folder Creation ON* enables the data storage concept as outlined before.

*Note:*
*Switching Unique Folder Creation on or off only affects*

*future acquisitions, but does not change the data organization of already acquired data. We recommend to decide between the two modes at the beginning of your work and not to switch between them. Switching Unique Folder Creation off is not supported with the ChemStation ECM Integration or ChemStore/Security Pack installed.*

Selecting *Unique Folder Creation OFF* has the following impact on data storage:

- Sequence data are not acquired into a sequence container, but directly into the subdirectory as specified in the *Sequence Parameters*. Therefore, the sequence name pattern is grayed out on the *Sequence* tab of the *Preferences* dialog (figure 23).
- This means that for two or more sequence acquisitions the data may be acquired into the same subdirectory. This implies the risk to overwrite existing data, but on the other hand allows to split sequences using partial sequence execution and still combine the results in one folder (which would not be possible with *Unique Folder Creation* switched on).
- No sequence methods (.M) or copies of the sequence file (.S) are stored with the data, but only the sequence logfile and the batch file (.B). This means only the methods and sequences in the paths specified in the *Preferences* dialog are available. They have to be used for acquisition as well as for data review and reprocessing. Sequence or data file specific method changes can only be stored by saving the method with different name. Otherwise these changes are also applied to the acquisition method. On the other hand, this may be desired behavior during method development.

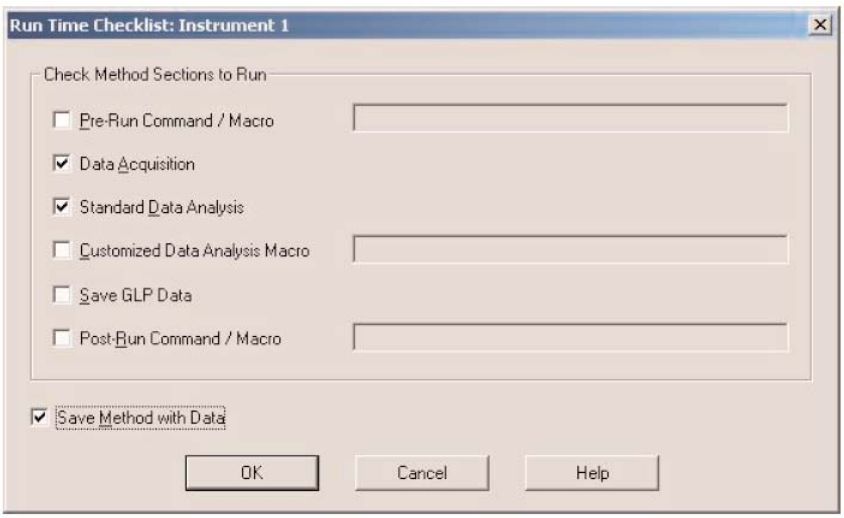


**Figure 24**
**Runtime Checklist: Save Method with Data.**

There are no data file specific methods ACQ.M and DA.M stored. Saving information about the original acquisition is only possible by including this information in the report or by selecting *Save Method with Data* from the method's runtime checklist (figure 24).
With this option the acquisition method will be stored as RUN.M in each data file.

The enhanced ChemStation user interface as introduced with ChemStation B.02.01 is also available when *Unique Folder Creation* is switched off.

However, there are functions you can not take advantage of in this mode. The same limitations also apply to any run acquired with ChemStation prior to B.02.01.

- When a sequence is loaded into the Navigation Table, the reprocessing toolset is grayed out (figure 25). Sequences that have been acquired in this data storage mode can only be reprocessed in *Method and Run Control* view using the *Reprocessing only* option in the *Sequence Parameters*

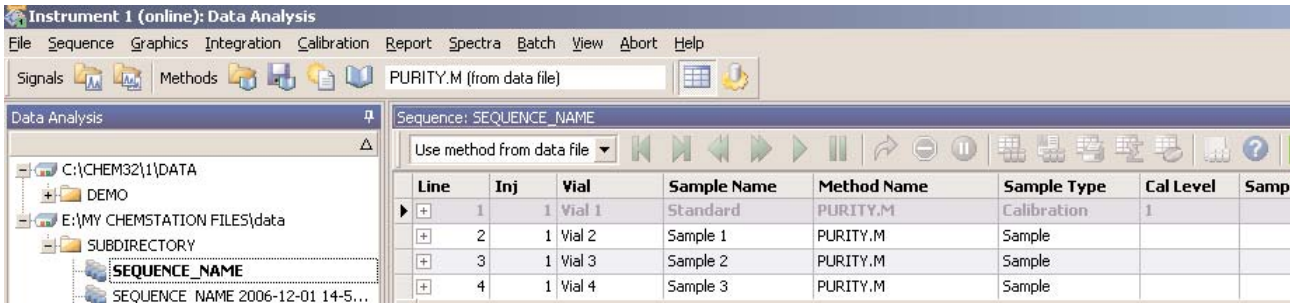


**Figure 25**
**Naviagation Table for Seqeunces aquired with *Unique Folder Creation* switched off**

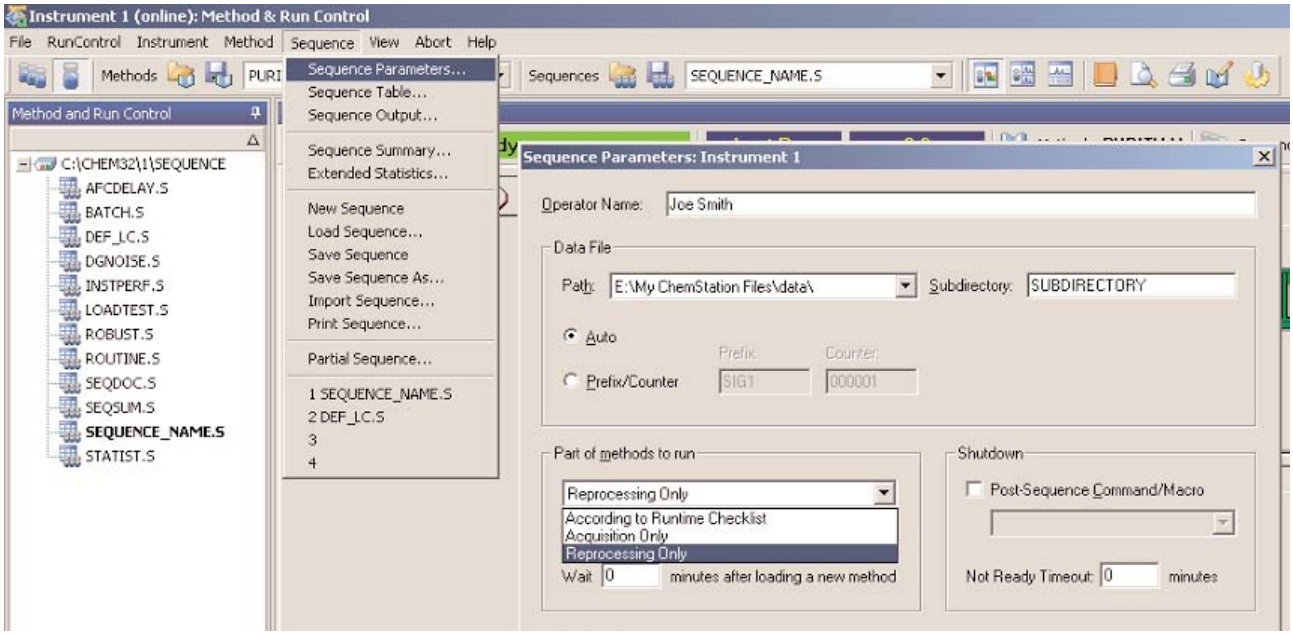


**Figure 26**
**Reprocessing of sequence data acquired with *Unique Folder Creation* switched off.**

(figure 26).

- With the method usage options *Use method from data file* and *Use sequence method*, a warning message will be displayed each time a run is double-clicked in the *Navigation Table* that the individual method/ sequence method does not exist. As outlined above, these methods are not stored with the data. In this case, the only meaningful option for data review is *Use current method*.

## Conclusion

With revision B.02.01/B.02.01 SR1 of ChemStation, data review and data reprocessing capabilities have been significantly improved to enable fast review of result data.

The new data storage functions in ChemStation help to efficiently organize sequence data and methods. This provides also easier connectivity with the Agilent

expands temporarily to allow you to use it until the mouse leaves that region (figure 20). Of course, when you click the push pin again, the side bar reverts to its fixed state.

2) In Data Analysis View, hide the Navigation Table by pressing the Hide/Show-button on the toolbar indicated in figure 21.

3) Change the method loading settings to “Current Method” in the Preferences. This allows you to work always only on the master methods or on any manually selected method as in previous ChemStation revisions (figure 22).

Please note, that with these changes the ChemStation will look more familiar, but many of the new features and their benefits are no longer available.

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