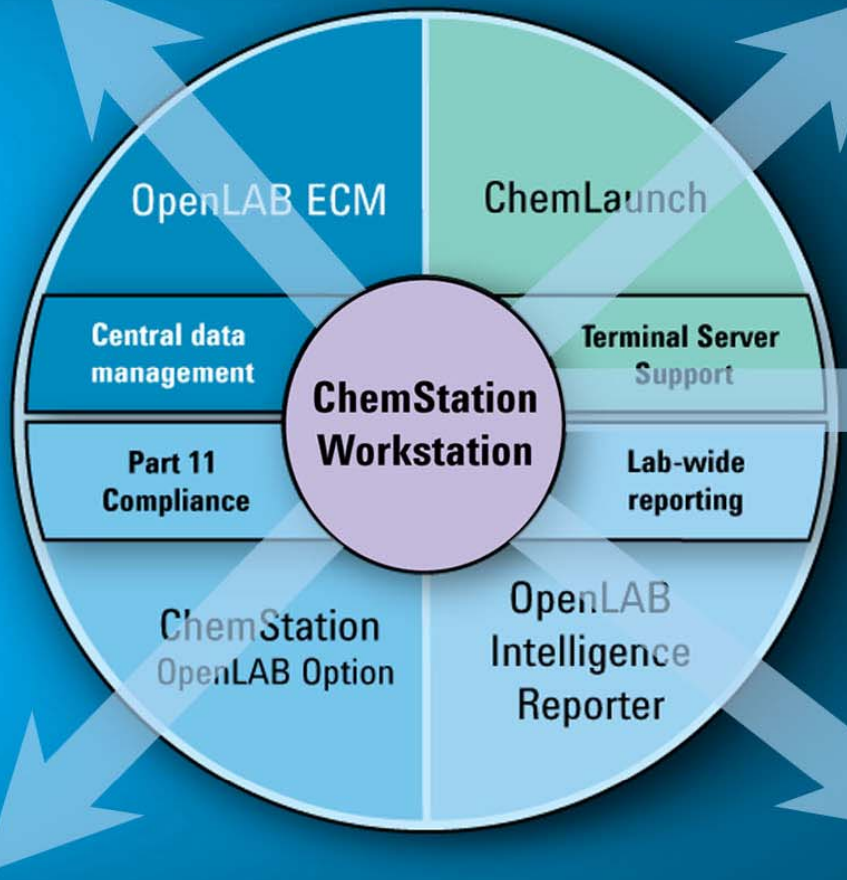
ChemStation E-Seminars

ChemStation Data Storage Concept.
October 15, 2008

Integrating my results.
December 10, 2008



How to set up a calibration table in ChemStation.
January 14, 2009

ChemStation Navigation Table – How to improve Review and Reprocess.
November 12, 2008

Various Reporting in Chemstation.
February 04, 2009

ChemStation E-Seminar Agenda

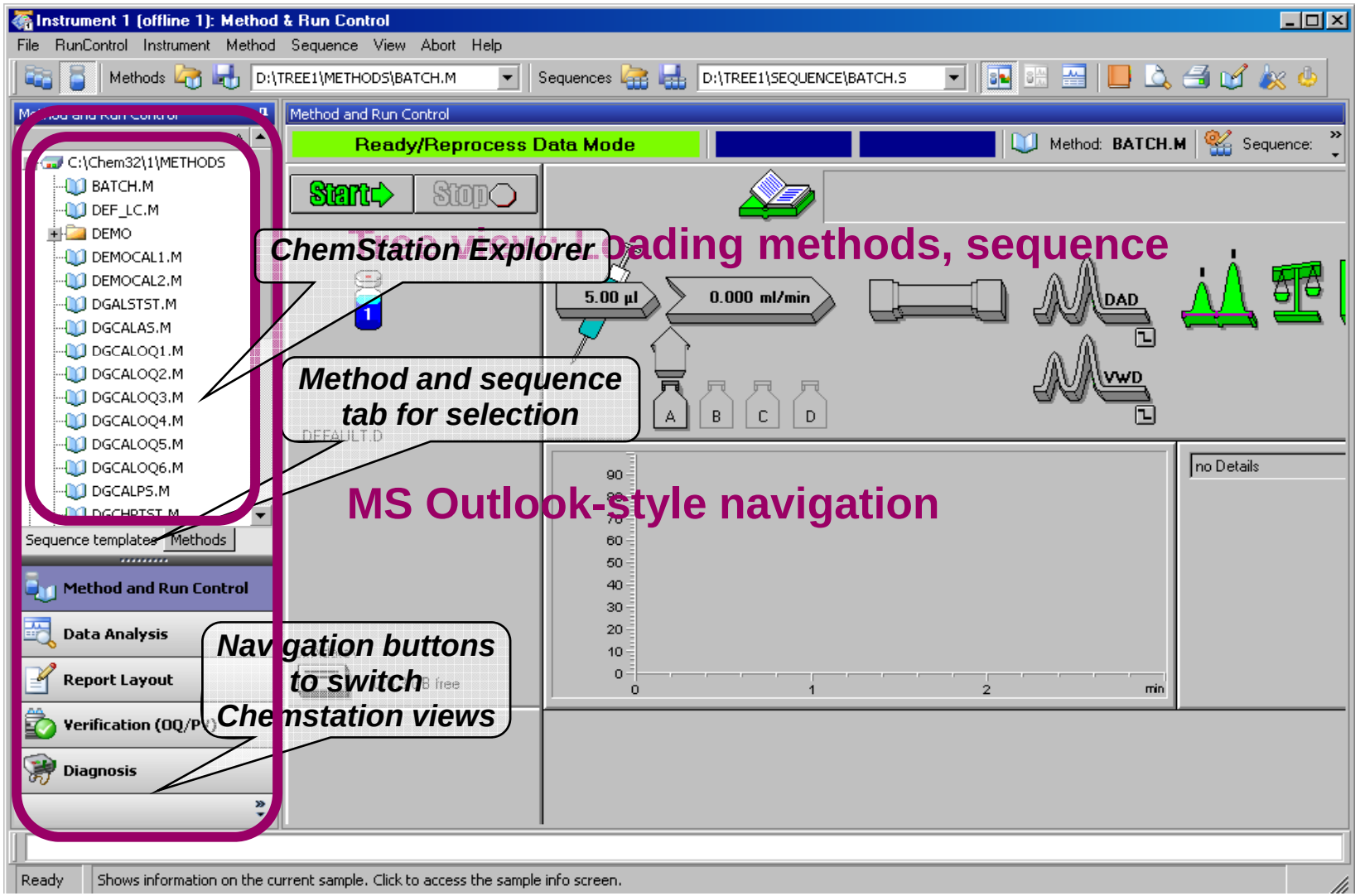
Schedule	Short description	Agilent Speaker
15 Oct 2008	ChemStation Data Storage Concept	Steven Brown Ortrud Emde
12 Nov 2008	ChemStation Navigation Table How to improve Review and Reprocess	Steven Brown Ortrud Emde
10 Dec 2008	Operational Functions for Data Generation, Data Analysis and Instrument Configuration	Steven Brown Ortrud Emde
14 Jan 2009	How to set up a calibration table in ChemStation	Steven Brown
04 Feb 2009	Various Reporting in Chemstation	Steven Brown Ortrud Emde

Seminar 1: ChemStation Data Storage Concept

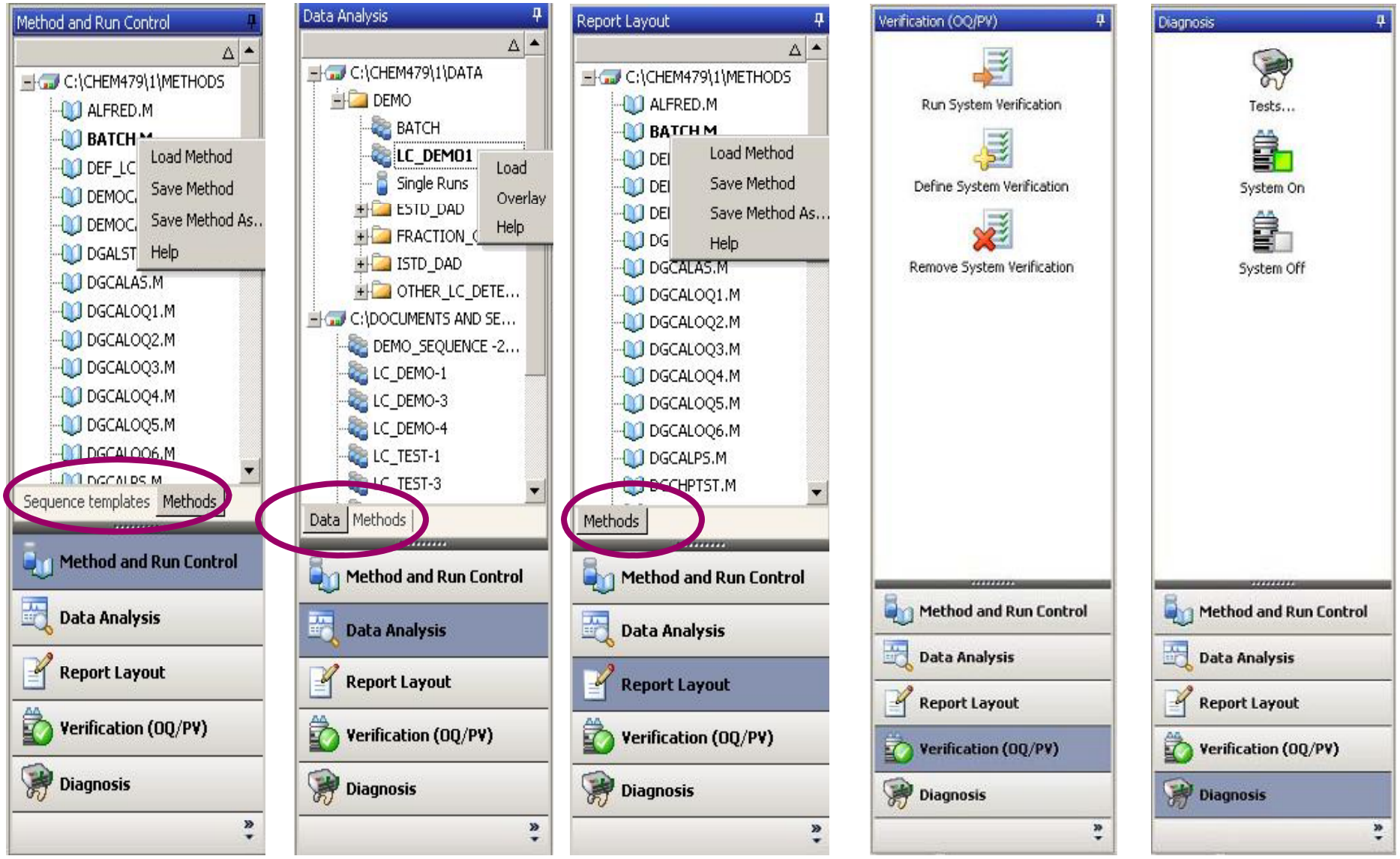
Topics
ChemStation User Interface Enhancements Rev. B.02.01 or higher
The ChemStation „Preferences“
ChemStation Data Structure using Preference settings „Unique Folder Creation ON/OFF“
Advantages of the Sequence Container Concept „Unique Folder Creation ON“
Partial Acquisition Sequence in ChemStation B.04.01
Benefiz of OpenLAB with ChemStation

User Interface Enhancements
ChemStation Rev. B.02.01 or higher

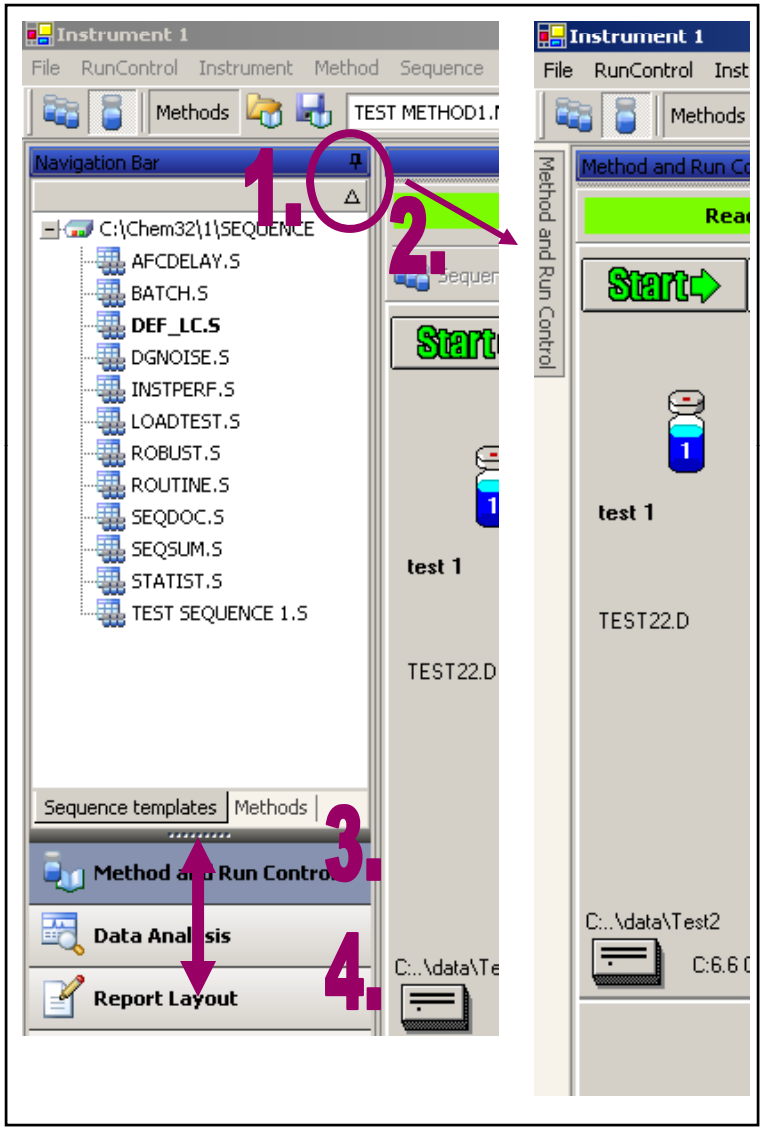
Method and Run Control - User Interface

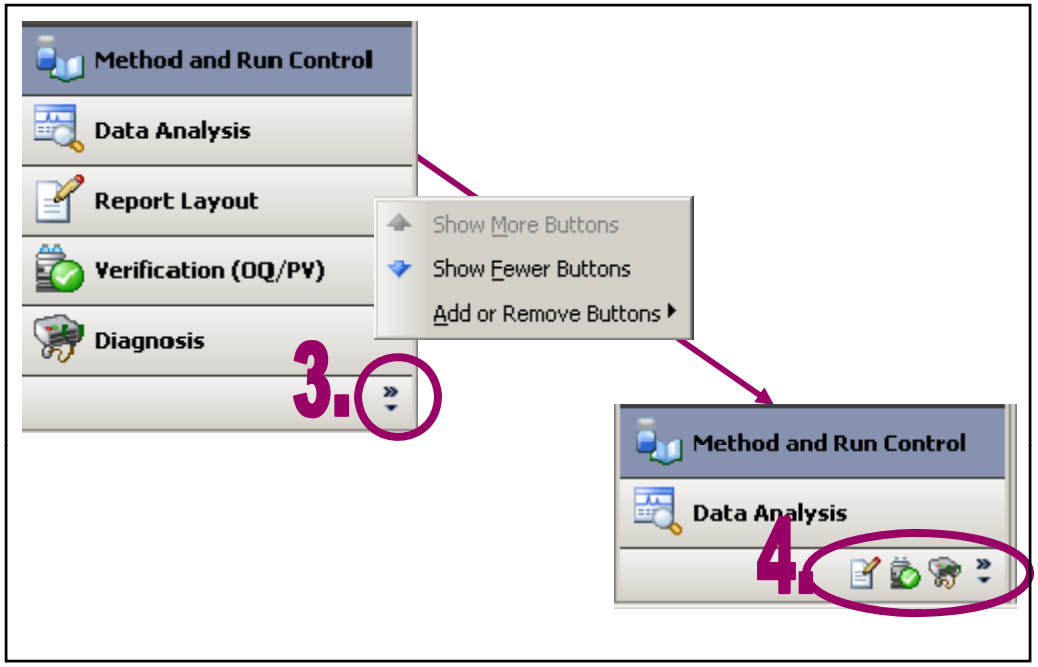


ChemStation Explorer - Views

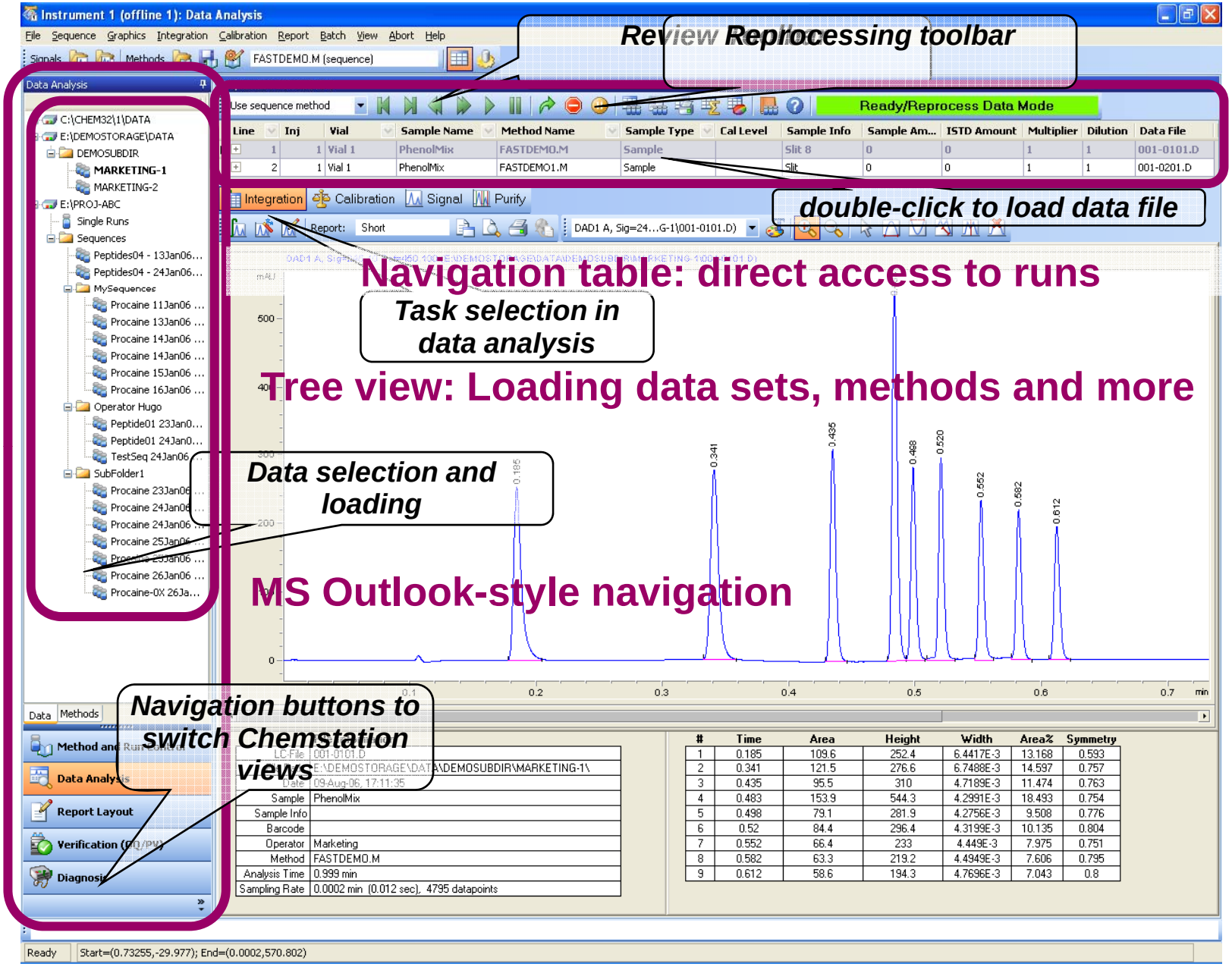


Navigation Pane – Customization

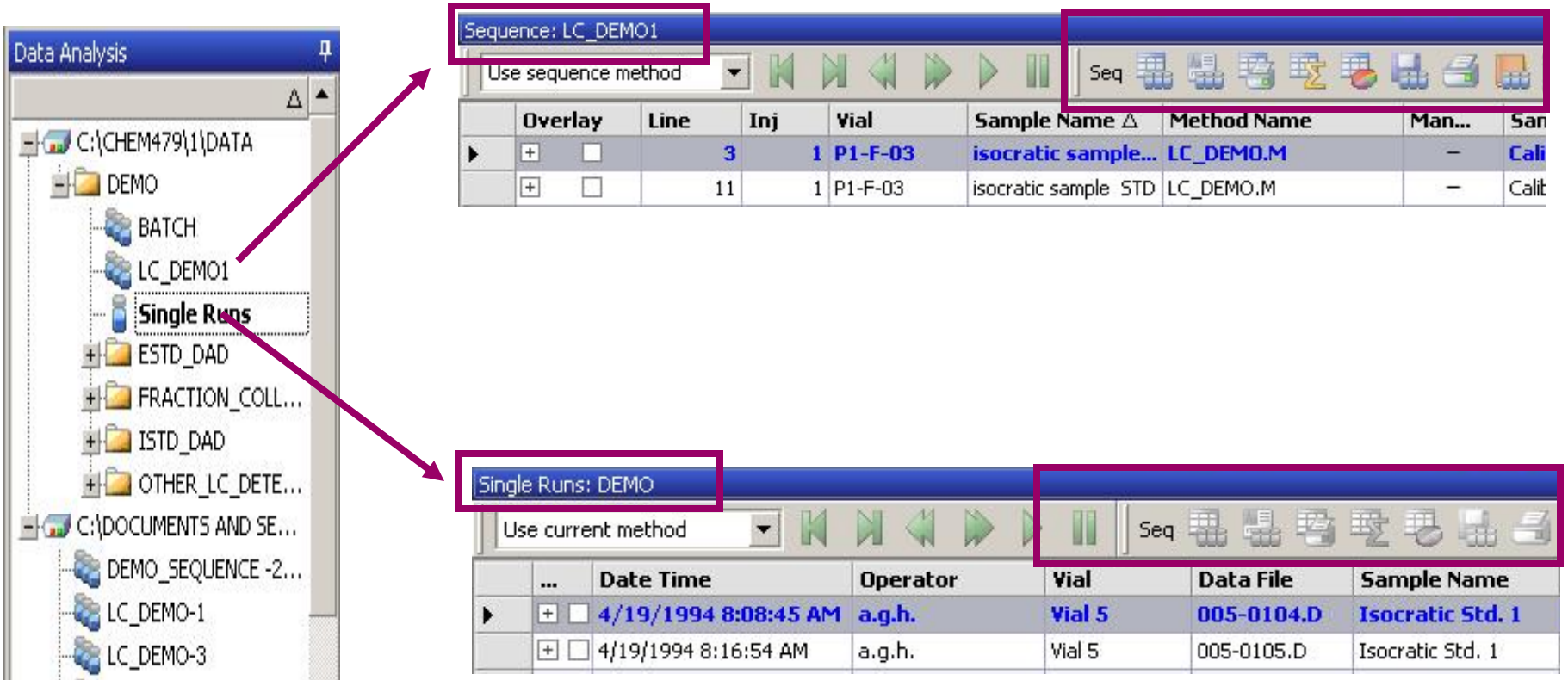




- Recommended Screen resolution: 1280x1024
- Customization features
- Sorting features

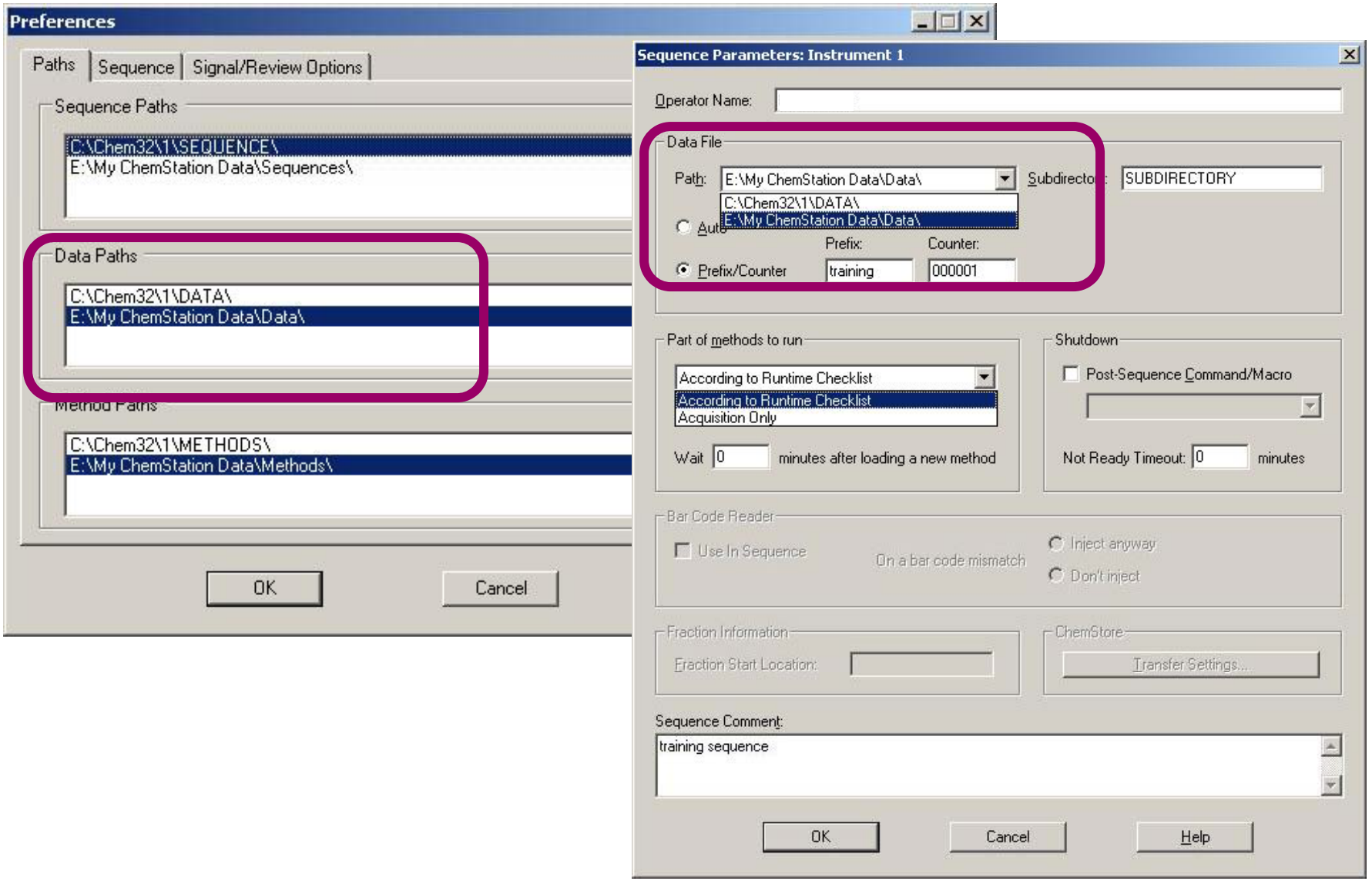

Review Reprocessing toolbar
double-click to load data file
Navigation table: direct access to runs
Task selection in data analysis
Tree view: Loading data sets, methods and more
Data selection and loading
MS Outlook-style navigation
Navigation buttons to switch Chemstation views
Instrument 1 (offline 1): Data Analysis
Ready/Reprocess Data Mode
Data Analysis
Method and Run Control
Data Analysis
Report Layout
Verification (OQ/PV)
Diagnosis

Loading Sequences and Single Runs from ChemStation Explorer

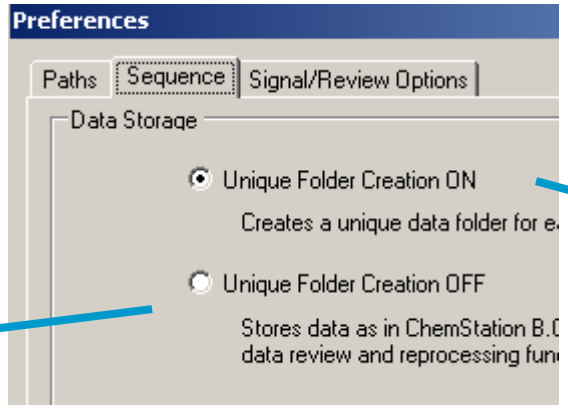


The ChemStation “Preferences”

Preferences Dialog – Flexible Path Settings



Choose your Data Storage Model



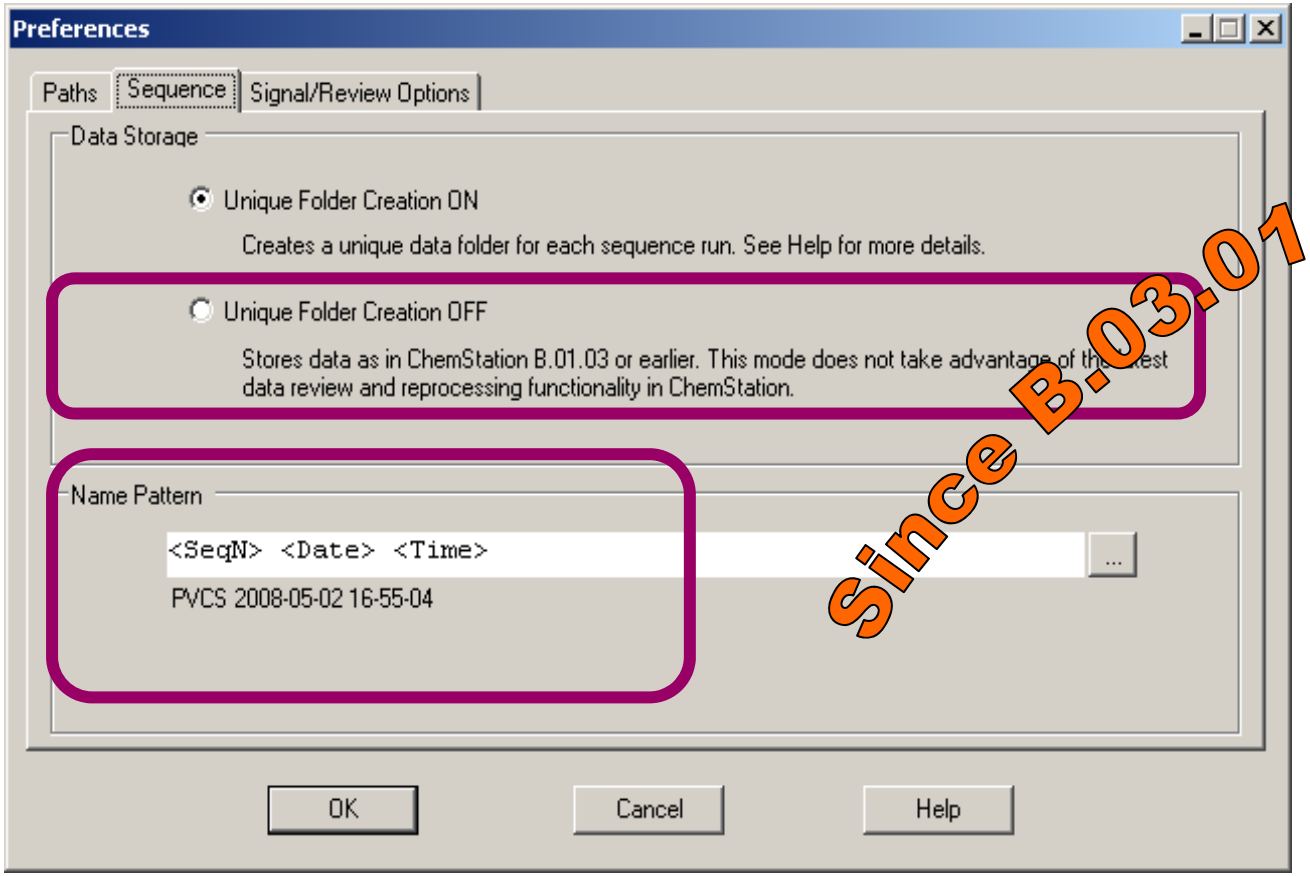
Unique Folder Creation OFF:

- ChemStation only
- Data are stored at a defined directory, the methods and sequence used to generate the data remain at their original location
- Possible to overwrite data
- Easy data review sequence possible
- Reprocessing of a complete sequence needs to be performed in Method and Run Control

Unique Folder Creation ON :

- With ECM integration or ChemStore
  - Ensure data integrity: store related methods and sequence templates with sequence data
  - Each sequence creates a uniquely named sequence container
  - Not possible to overwrite data
  - Easy data review or reprocessing of a complete sequence possible

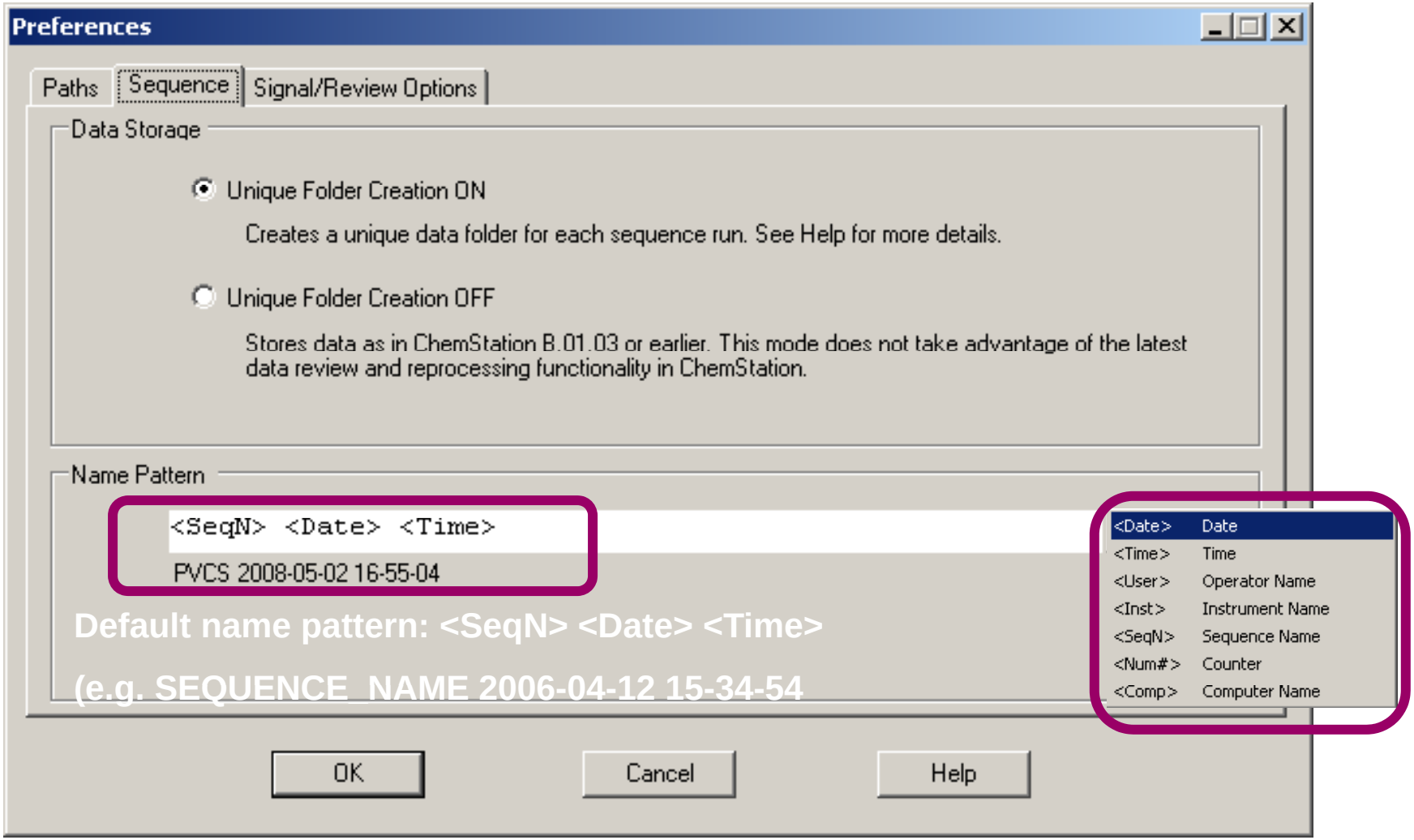
Preferences Dialog: Sequence Tab



- Present in On-line ChemStation only
- This setting influences only future data acquisition.

- Sequence Name Pattern is grayed out when Unique Folder Creation is off.

Preferences Dialog: Sequence Tab



ChemStation Data Structure using Preferences Setting „Unique Folder Creation ON/OFF‘

Comparison Start Prerequisites

ChemStation Rev. A – B.01.03	ChemStation Rev. B.02.01
Methods: C:\Chem32\1methods*.M	Master Methods: C:\Chem32\1methods*.M
Sequence : C:\Chem32\1\sequence*.S	Sequence Templates: C:\Chem32\1\sequence*.S
Data Structure: C:\Chem32\1\data*subdirectory*\	Data Structure: C:\Chem32\1\data*subdirectory*\

Press “Start Sequence” – What happens now?

Comparison - Single Run Acquisition

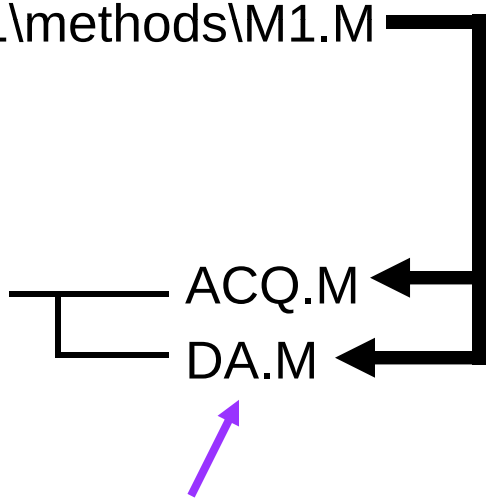
ChemStation Rev. A – B.01.03

ChemStation Rev. B.02.01

Master Method: C:\Chem32\1\methods\M1.M

Location of the data file:

C:\Chem32\1\data\subdirectory\D1.D



Run Method

Individual Method of the data file

Start the sequence – impact of the Data Storage chosen

Master Methods: C:\Chem32\1methods\Method1.M
\Method2.M

Sequence Template: C:\Chem32\1\sequence\Sequence1.S

Data Structure: C:\ Chem32\1\data*subdirectory*\

Data1.D
Data2.D
Data3.D
Data4.D
Data5.D

ChemStation Rev. A - B.01.03

Sequence1.log ← Sequence Logbook
Sequence1.b ← Sequence Batch File

Unique Seq. Data Container - Counter

Sequence1.S Sequence

Method1.M ← **Sequence Methods**
Method2.M ← **Sequence Methods**

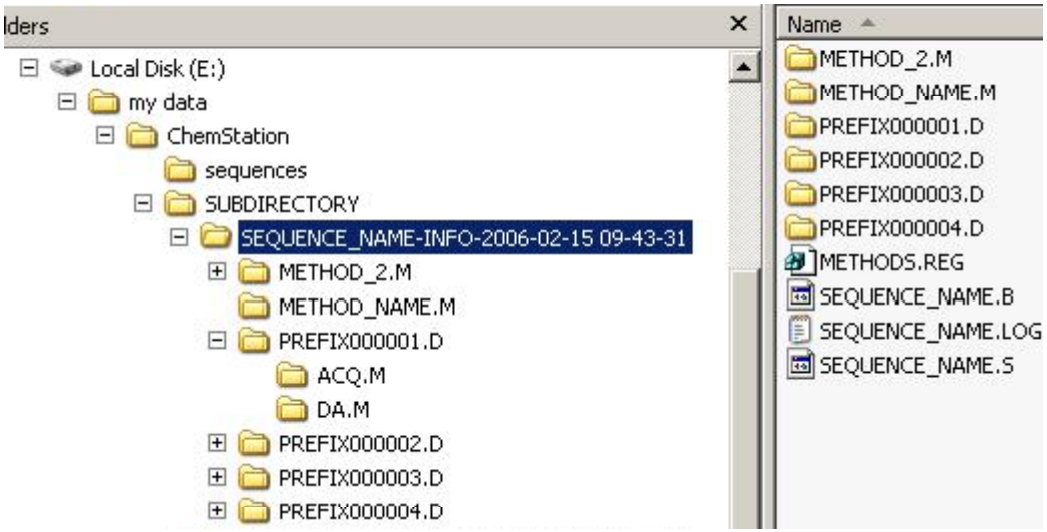
Data1.D
Data2.D ← ACQ.M, DA.M — Individual Methods of the data file
Data3.D
Data4.D
Data5.D

ChemStation Rev. B.02.01

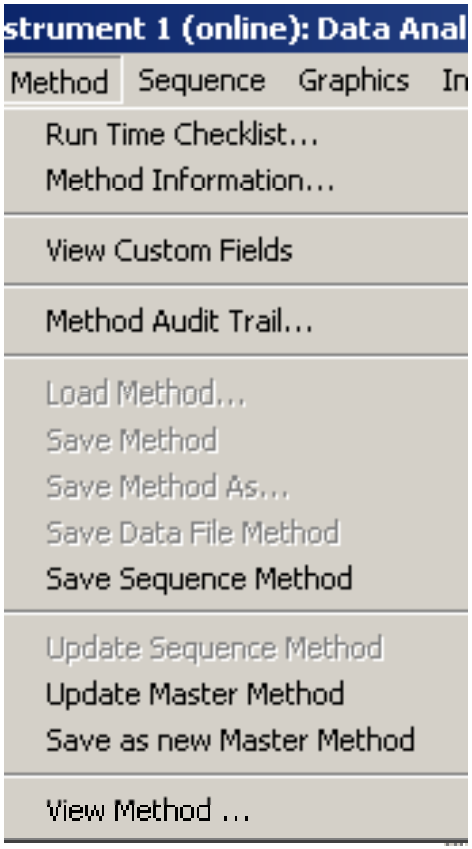
Sequence1.log ← Seq. Logbook
Sequence1.b ← Sequence Batch

ChemStation - Data Integrity

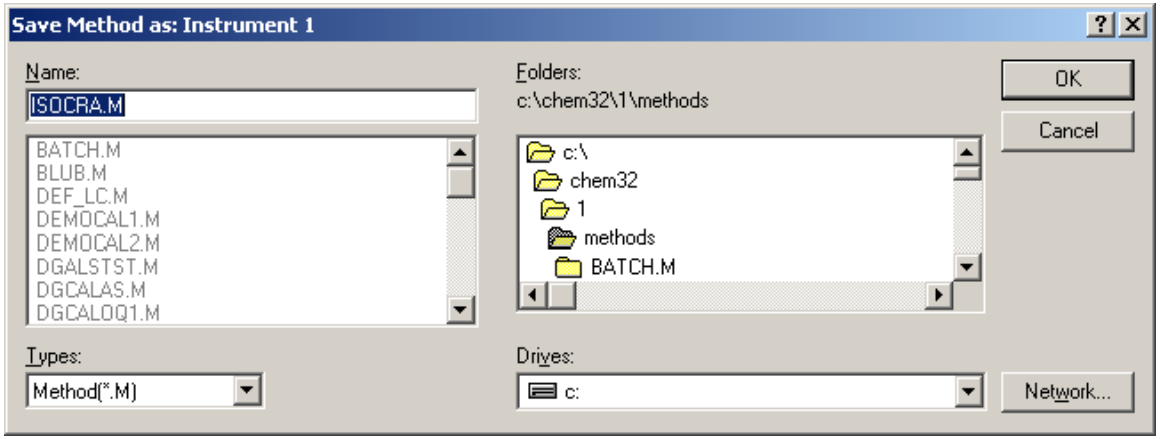
- Unique Sequence Data Container
- No data is ever overwritten
- Data are filed along with relevant methods and sequence template
- Container includes sequence logbooks
- Each data file contains its own run logbook



Saving the Method

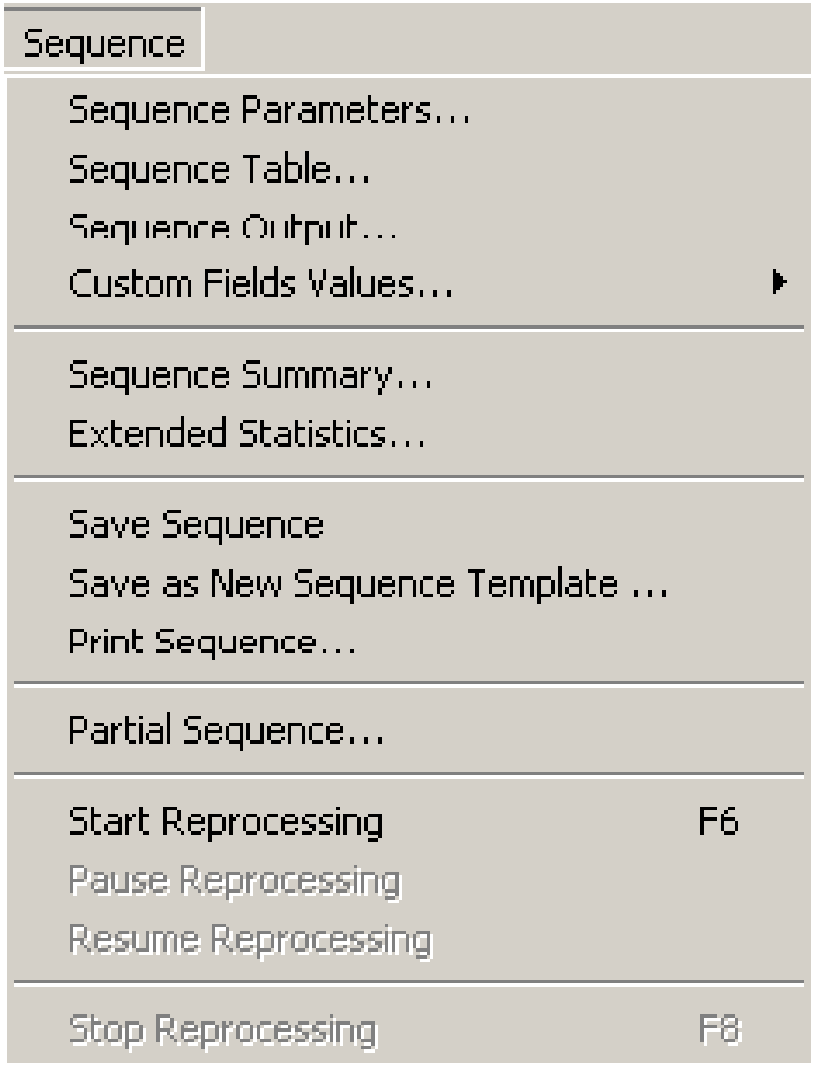


- Save Sequence Method:
  - Save the method with the same name, overwrite the previous parameters.
- Save as new Master Method:
  - Allows saving the method with a different name and to a different location; default target location is the master methods folder.



Agilent Technologies

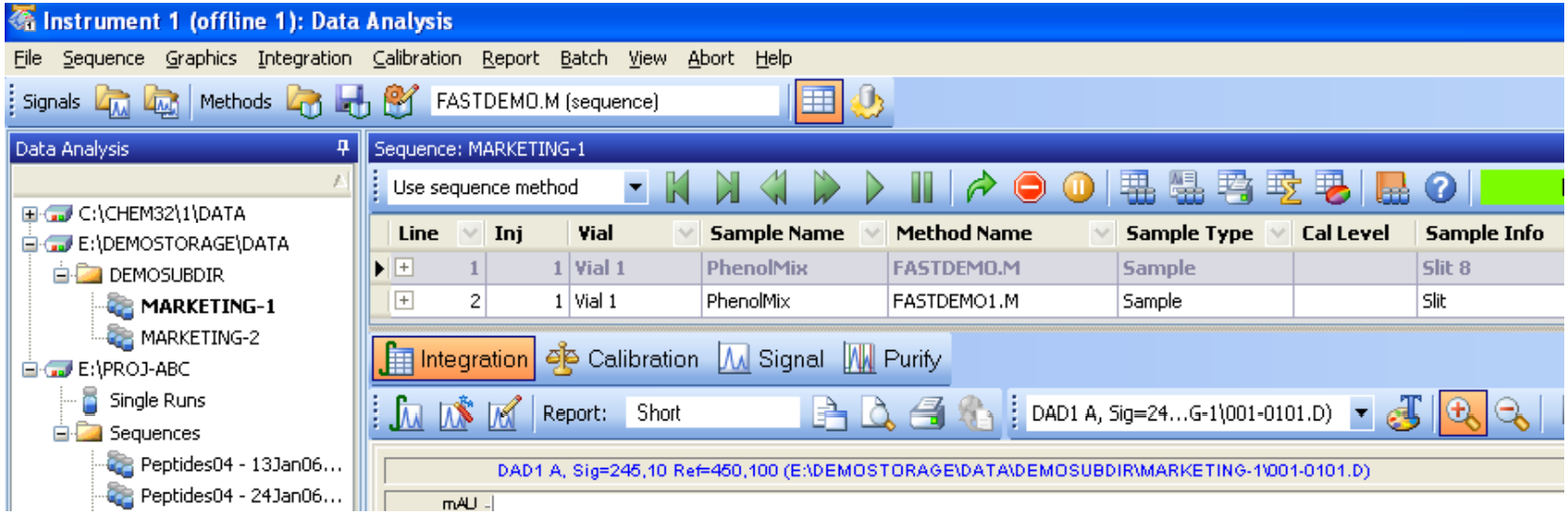
Saving the Sequence File



- Save Current Sequence:
  - Save the sequence file with the same name, overwrite the previous parameters.
- Save as New Sequence Template:
  - Allows saving the sequence file as a sequence template; converts the file to enable acquisition and editing of acquisition parameters.

Advantages of the Sequence Container Concept

Impact on Data Analysis Tasks – Review and Reprocess



The data are stored with all necessary information needed for data analysis.

Your master method is now the sequence method of your newly acquired data container. All changes now are changes for the data set only, and remain only for this data set.

The sequence method used for the specific data file is automatically loaded.

Which Method is the Best to Use?

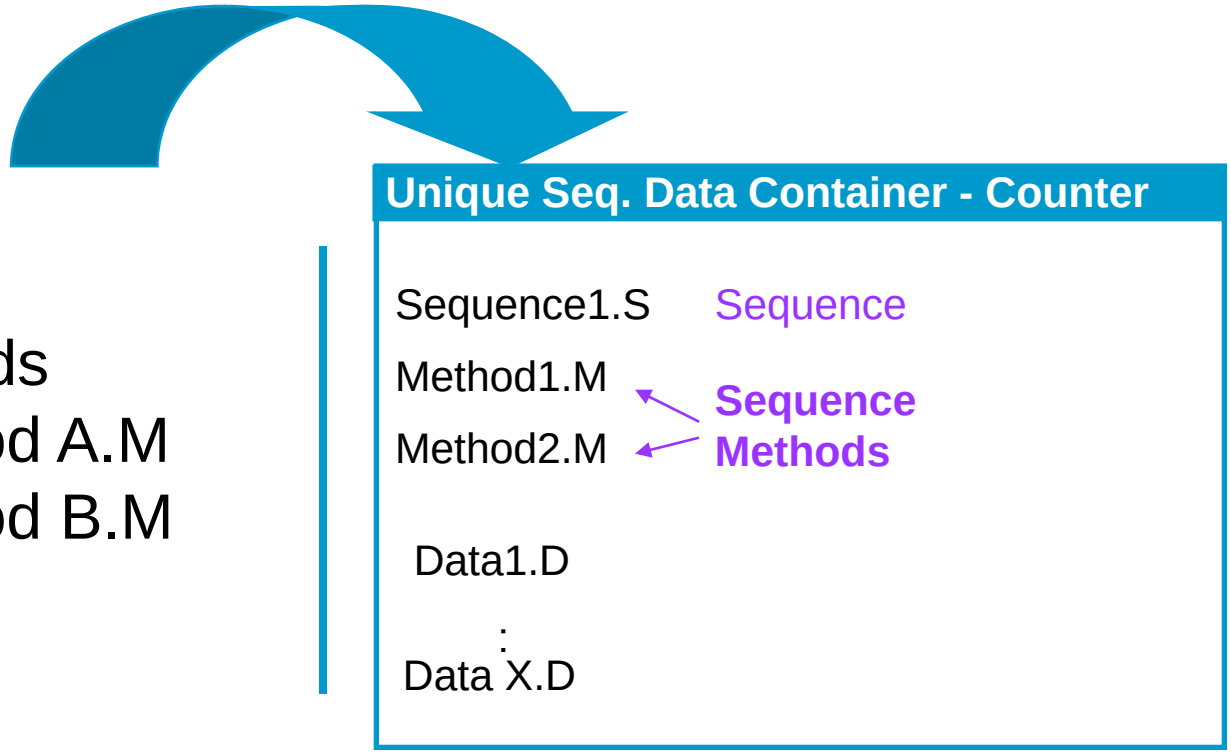
Working Methods:

For Data Acquisition – use the Master Method

For Data Analysis – use the Sequence Method

(which is a copy of your master method for the data set you are working on)

Master Methods:
C:\Chem32\1methods
\method A.M
\method B.M



Unique Folder Creation switched OFF: Summary

- Methods are saved to the C:\Chem32\x\Methods directory
- Sequences are saved to the C:\Chem\x\Sequence directory
- Data are saved to the C:\Chem32\x\Data directory
- Additional paths can be specified in the Preferences dialog
- Reprocessing is only possible from Method & Run Control – Sequence Parameters\Part of the methods to run – Reprocessing only
- Reprocessing is NOT possible from the Data Analysis view
- Data review IS possible from the Data Analysis view
- Possibility to perform partial acquisition into an existing folder
- Flexibility (for method development)
- Switching Unique Folder Creation off is not possible when ECM Integration or ChemStore are installed

New Data Organization - Key Advantages (Unique Folder Creation ON)

- All data is kept consistent, as related sets of data files, methods and sequences are kept together
- Data files created by the same sequence template are not accidentally overwritten, but automatically organized
- Results can be stored along with data files
- Easy data review and reprocessing of a complete sequence possible in Data Analysis
- Allows easier integration with data storage solutions such as Agilent ECM or ChemStore/Security Pack

History of Changes in the Sequence Container Concept

B.02.01	Introduction of sequence container concept
B.02.01 SR1	Enhancements of UI in Data Analysis view
B.02.01 SR2	Partial Sequence in Data Analysis view (Partial Reprocessing)
B.03.01	Option to switch Unique Folder Creation off
B.04.01	Partial acquisition into an existing sequence container Storage of manual integration results in the data file Introduction of a method menu in Data Analysis view Possibility to store a sequence file inside a sequence container as a sequence template

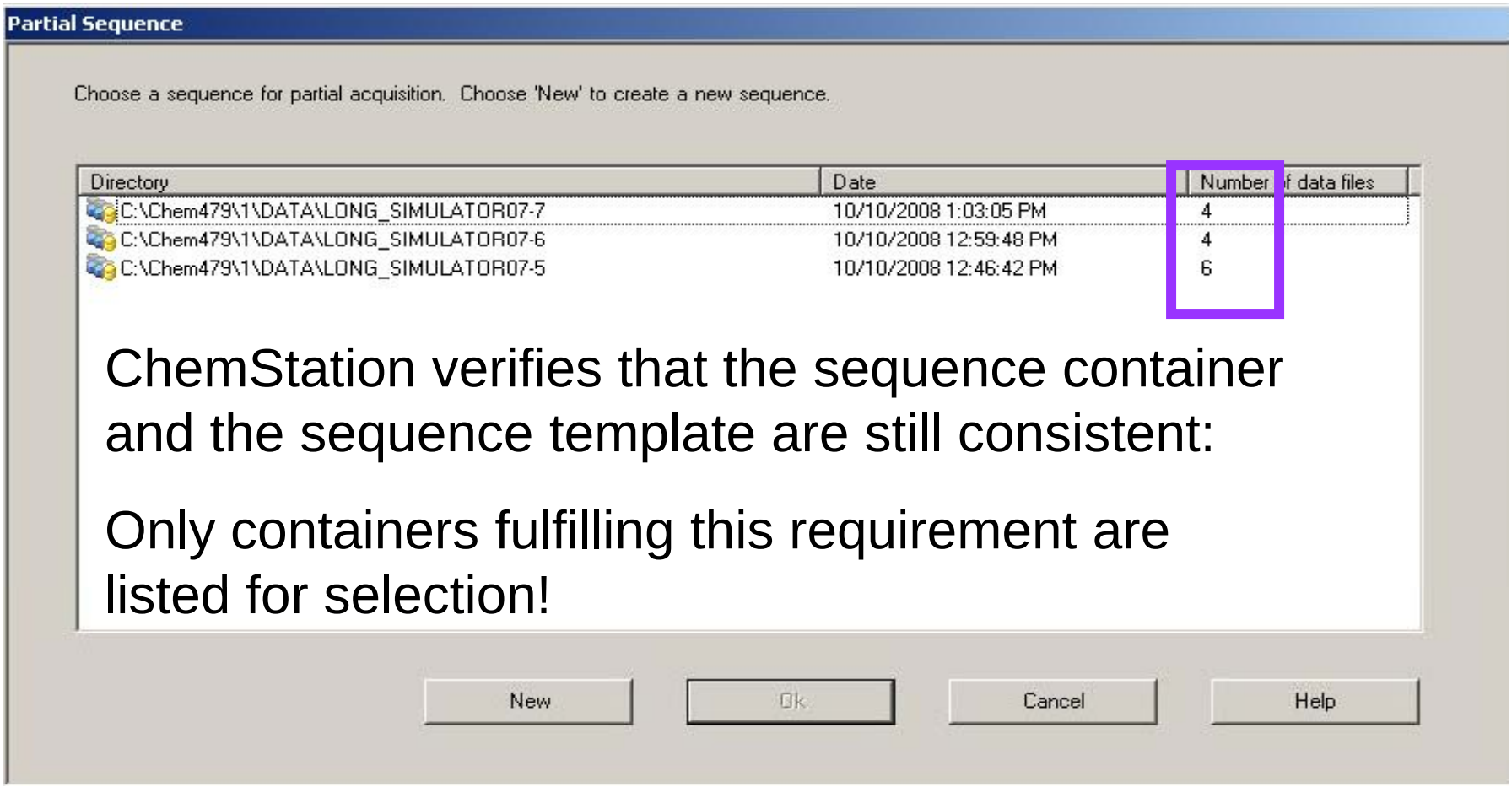
QUESTIONS?



Partial Acquistion Sequence in ChemStation B.04.01

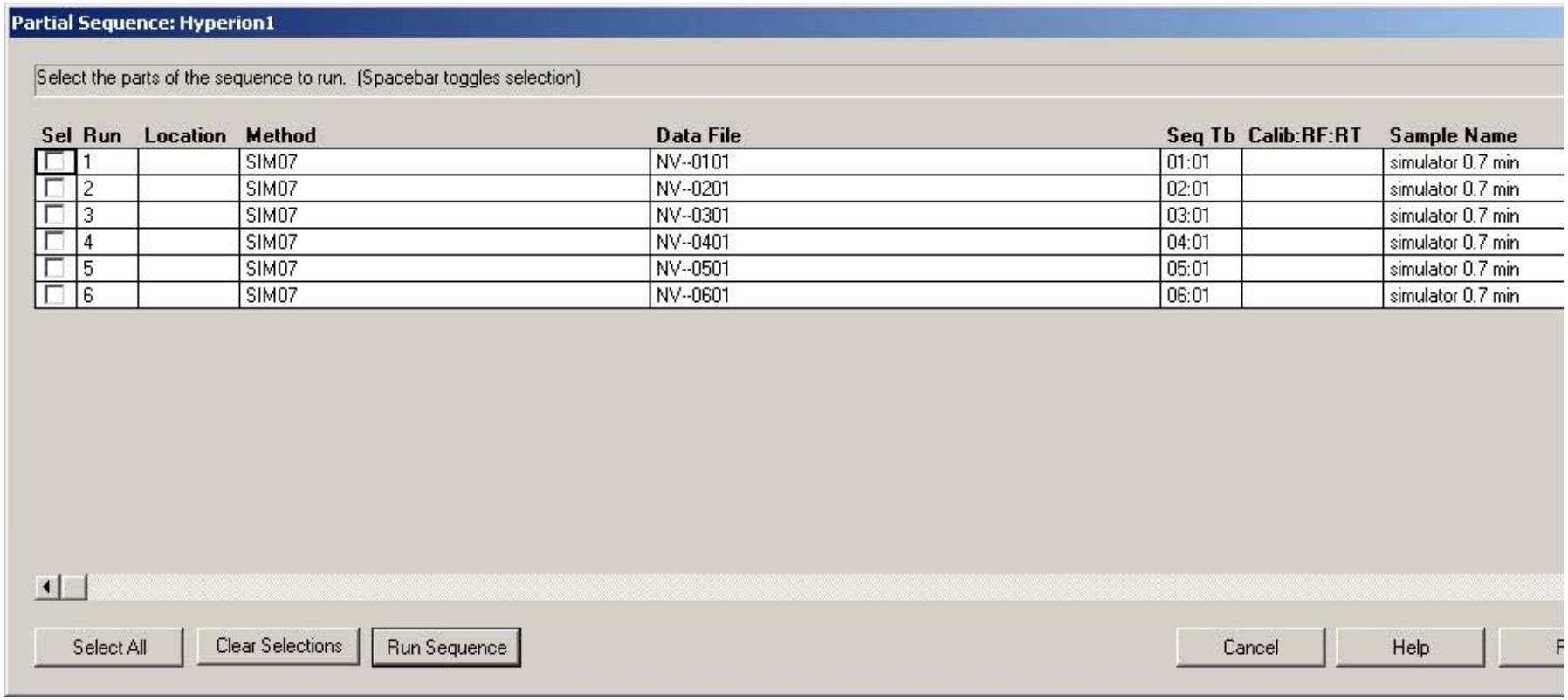
Acquiring Data into an Existing Sequence Container (1)

Select Sequence / Partial Sequence



Acquiring Data into an Existing Sequence Container (2)

After either selecting an existing container or pressing New, the familiar Partial Sequence dialog comes up:



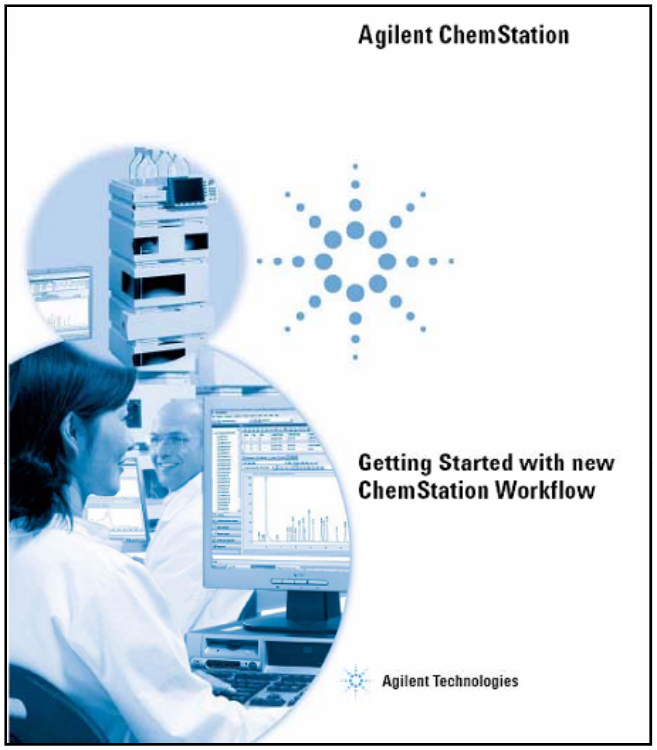
Information on ChemStation

Documentation can be found on the Agilent website
http://www.chem.agilent.com/Scripts/PDS.asp?lPage=61233

- Product Datasheet
- Specification
- Application Notes
- Manuals

Manuals can be found on your ChemStation Installation DVD

- Getting Started with New ChemStation Workflow
  Part No. G2170-90042
- OpenLAB Option
  Part No. G2170-90233
- Configure and Maintain Your Agilent ChemStation Computer
  Part No. G2170-9013



Software Status Bulletin
http://www.chem.agilent.com/en-US/Support/Downloads/Patches/Pages/default.aspx

Customer Trainings (NorthAmerica)

http://www.chem.agilent.com/cag/training/northam/index.asp

Learning Products – North America Course Catalog

Users needing to increase productivity in the lab by utilizing both standard and advanced features available in the Agilent GC/LC ChemStation may want to attend one of the following courses:

- H2606A - ChemStation for GC Data Analysis and Reporting (2 days)
- H5928A - Agilent HPLC (2D) Data Analysis and Reporting (2 days)
- H4039A - Agilent HPLC (3D) Data Analysis and Reporting (3 days)

Course Features

- Data acquisition and method creation
- Data analysis including integration and calibration
- Sequencing
- Reporting

For more information concerning course content, dates and locations, please visit:

http://www.chem.agilent.com/en-US/education/en-us/classroomtraining/Pages/Courselisting.aspx

Learning Products – European Course Catalog

Users needing to increase productivity in the lab by utilizing both standard and advanced features available in the Agilent GC/LC ChemStation may want to attend one of the following courses:

- H4033A – Agilent HPLC (3D) Method&Run Control, Data Analysis and Reporting (4 days)
- H8718A - Agilent HPLC (3D) Data Analysis and Reporting (2 days)
- H5928A – Advanced User Training, Quantification and Result Reporting (2 days)

Course Features

- Data acquisition and method creation
- Data analysis including integration and calibration
- Sequencing
- Reporting

For more information concerning course content, dates and locations, please visit:

http://www.chem.agilent.com/en-US/education/pages/homepage.aspx

QUESTIONS?

