## ChemStation E-Seminar Agenda

<table>
<thead>
<tr>
<th>Schedule</th>
<th>Short description</th>
<th>Speaker</th>
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<tr>
<td>15 Oct 2008</td>
<td>ChemStation Data Storage Concept</td>
<td>Steven Brown</td>
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<td></td>
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<td>Ortrud Emde</td>
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<tr>
<td>12 Nov 2008</td>
<td>ChemStation Navigation Table How to improve Review and Reprocess</td>
<td>Steven Brown</td>
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<td>Ortrud Emde</td>
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<tr>
<td>10 Dec 2008</td>
<td>Operational Functions for Data Generation, Data Analysis and Instrument Configuration</td>
<td>Steven Brown</td>
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<td>Ortrud Emde</td>
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<td>14 Jan 2009</td>
<td>How to set up a calibration table in ChemStation</td>
<td>Steven Brown</td>
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<tr>
<td>04 Feb 2009</td>
<td>Various Reporting in Chemstation</td>
<td>Steven Brown</td>
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<td>Ortrud Emde</td>
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</table>
# 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**: Loading methods, sequence
- **Method and sequence tab for selection**
- **MS Outlook-Style navigation**
- **Navigation buttons to switch Chemstation views**

[Image of the ChemStation Explorer interface showing method and sequence loading, navigation buttons, and a chemical measurement setup.]

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**Agilent Technologies**

ChemStation Tricks and Tips
March, 2008
ChemStation Explorer - Views
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
Loading Sequences and Single Runs from ChemStation Explorer
The ChemStation “Preferences”
Preferences Dialog – Flexible Path Settings

The image shows a software interface with various paths and settings configured for a ChemStation application. The paths include:

- **Data Paths**:
  - C:\Chem32\DATA
  - E:\My ChemStation Data\Data

- **Method Paths**:
  - C:\Chem32\METHODS
  - E:\My ChemStation Data\Methods

The interface also features a section for **Sequence Paths** and a **Sequence Parameters** dialog box, which is highlighted to emphasize the configuration of the current sequence. The highlighted sections include:

- **Data File**:
  - Path: E:\My ChemStation Data\Data\...
  - Subdirectory: SUBDIRECTORY
  - Prefix: training
  - Counter: 00001

The interface also includes options for **Part of methods to run**, **Shutdown** settings, and **Sequence Comment** fields.
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

Default name pattern: <SeqN> <Date> <Time>
(e.g. SEQUENCE_NAME 2006-04-12 15-34-54)
ChemStation Data Structure using Preferences Setting
„Unique Folder Creation ON/OFF“
## Comparison Start Prerequisites

<table>
<thead>
<tr>
<th>ChemStation Rev. A – B.01.03</th>
<th>ChemStation Rev. B.02.01</th>
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<tbody>
<tr>
<td><strong>Methods:</strong></td>
<td>Master Methods:</td>
</tr>
<tr>
<td>C:\Chem32\1methods*.M</td>
<td>C:\Chem32\1methods*.M</td>
</tr>
<tr>
<td><strong>Sequence:</strong></td>
<td>Sequence Templates:</td>
</tr>
<tr>
<td>C:\Chem32\1\sequence*.S</td>
<td>C:\Chem32\1\sequence*.S</td>
</tr>
<tr>
<td><strong>Data Structure:</strong></td>
<td>Data Structure:</td>
</tr>
<tr>
<td>C:\Chem32\1\data\subdirectory</td>
<td>C:\Chem32\1\data\subdirectory</td>
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</tbody>
</table>

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

Individual Method of the data file

Run Method

ACQ.M
DA.M
Start the sequence – impact of the Data Storage chosen

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

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

**Data Structure:** C:\Chem32\1\data\subdirectory\n
<table>
<thead>
<tr>
<th>Unique Seq. Data Container - Counter</th>
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</thead>
<tbody>
<tr>
<td>Sequence1.S</td>
</tr>
<tr>
<td>Method1.M</td>
</tr>
<tr>
<td>Method2.M</td>
</tr>
<tr>
<td>Data1.D</td>
</tr>
<tr>
<td>Data2.D</td>
</tr>
<tr>
<td>Data3.D</td>
</tr>
<tr>
<td>Data4.D</td>
</tr>
<tr>
<td>Data5.D</td>
</tr>
</tbody>
</table>

- **Sequence Logbook**
- **Sequence Batch File**

**ChemStation Rev. A - B.01.03**

**ChemStation Rev. B.02.01**

- **Individual Methods of the data file**
- **Seq. Logbook**
- **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.
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
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 Seq. Data Container - Counter

Sequence1.S  Sequence
Method1.M    Sequence
Method2.M    Methods
  Data1.D
  Data X.D
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

<table>
<thead>
<tr>
<th>Revision</th>
<th>Description</th>
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<tr>
<td>B.02.01</td>
<td>Introduction of sequence container concept</td>
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<tr>
<td>B.02.01 SR1</td>
<td>Enhancements of UI in Data Analysis view</td>
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<tr>
<td>B.02.01 SR2</td>
<td>Partial Sequence in Data Analysis view (Partial Reprocessing)</td>
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<td>B.03.01</td>
<td>Option to switch Unique Folder Creation off</td>
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<td>B.04.01</td>
<td>Partial acquisition into an existing sequence container</td>
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<td>Storage of manual integration results in the data file</td>
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<td></td>
<td>Introduction of a method menu in Data Analysis view</td>
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<td>Possibility to store a sequence file inside a sequence container as a sequence template</td>
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Partial Acquisition Sequence in ChemStation B.04.01
Acquiring Data into an Existing Sequence Container (1)

Select Sequence / Partial Sequence

ChemStation verifies that the sequence container and the sequence template are still consistent:

Only containers fulfilling this requirement are listed for selection!
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

- 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

Customer Trainings (NorthAmerica)
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:
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: