ChemStation B.03.01-What’s New!

Agilent Technologies

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What we will show you today

- Refreshed User Interface and New Data Organization in ChemStation
- Fast Navigation in Data Analysis
- Easy Data Reprocessing
- Supported Instruments and Add-on Software
- ChemStation Integration with Agilent Enterprise Content Management System
Refreshed User Interface and New Data Organization in ChemStation

Introduced with ChemStation B.02.01 SR1!
Modernized User Interface and Data Organization

• Modernized User Interface:
  ⇒ Modern Icons
  ⇒ Modern Navigation Features

• New Data Organization
  ⇒ linkage between a sequence, the data files, the results, and the method being used to create the results
ChemStation User Interface – New Icons

- Refreshed ChemStation icons
- New color scheme
- Icons have the same meaning as in older revisions.
- Icons remain at the “same” place.
The Navigation Table in Data Analysis: Review and Reprocess Data
Navigation Table

Review tools: convenient review of analysis results on run-per-run base

Reprocessing tools: analyze the complete sequence, including calibration table updates, change of multipliers, etc.

List of all runs belonging to a sequence (read-only). Provides easy access to load the file.
1. Right-click the column headers to configure the table.
2. Group the Table Rows by columns, e.g. by Sample Type.
3. Right-click a run to perform actions on the run.
4. Expand a run to view its details.
GUI Enhancements for Method Handling

1. The method modification status is now displayed also in Data Analysis.
2. The method combo box was replaced by a static field always displaying the current method.
3. A tool tip displays the complete method path.
4. This dropdown box allows to change the method usage options of the Preferences dialog directly from the UI. The available options depend on whether sequence or a single run is loaded. The option is applied the next time you load a run – it does not load a new method immediately.
Copying Data Analysis Parameters

- Depending on the currently loaded method, it is possible to update the master or sequence method.
- This function copies all data analysis parameters.
Demo 1: ChemStation Explorer and Navigation Table
Data Storage

• Central storage for **method and sequence templates**
• After acquisition, a sequence and the used method is stored in one folder
• It is possible to **define locations** for saving sequences and methods
  
  • define data paths, create a subdirectory
• You can browse for a method, and if you are on a network you can load the method from another ChemStation
• Very flexible naming of sequences enables easy identification of project related data
New Data Organization Concept - Why

• direct link between a sequence, the data files, the results, and the method being used to create the results
  ⇒ could previously only be achieved using reports

• The new concept provides possibility to easily archive consistent sets of data
  ⇒ prerequisite for better ECM integration
Sequence Acquisition

Sequences and all related data such as raw data, methods and results are stored in a **sequence container** and thus **easy to retrieve**. Sequences can be saved to defined locations such as external drives, and **multiple naming patterns** are possible.
Central Storage of Master Methods and Sequence Templates

- Loading methods *.m (master methods)
- Loading sequences *.s (sequence templates)
- Directories are displayed according to the settings in Preferences
Preferences Dialog: Paths and Sequence Tabs

The image shows a preferences dialog window with several tabs: Paths, Sequence, and Signal/Review Options. The Paths tab is highlighted, and there are options for Data Storage, Name Pattern, Sequence Paths, Data Paths, and Method Paths. The relevant paths are as follows:

**Sequence Paths:**
- C:\ChemStation\SEQUENCES\E:\My ChemStation Data\Sequences\

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

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

The dialog has buttons for Add, Remove, OK, and Cancel.
Define Subdirectory

Sequence Parameters: Instrument 1

- **Operation Name:** Darth Vader
- **Data File**
  - **Paths:**
    - My ChemStation Data1/大事
    - C:/Chem321/DATA/大事
    - My ChemStation Data1/大事
  - **Subdirectory:** SUBDIRECTORY
  - **Prefix/Counter**
    - Prefix: training
    - Counter: 00001
- **Part of methods to run**
  - **Wait:** 0 minutes after loading a new method
  - **Post-Run Commands/Scripts**
    - **Post-Run Commands/Scripts:**
      - According to Runtime Checklist
      - According to Runtime Checklist
      - Acquisition Only
      - Not Ready Timeout: 0 minutes
- **End Code Header**
  - **Use In Sequence:**
  - **End Code in Case of Error:**
    - Error code not matched
    - Do not inject anyway
    - Do not inject
- **Fraction Information**
  - **Fraction Start Location:**
  - **ChemSure:**
    - Transfer Settings...
- **Sequence Comment**
  - **Sequence Comment:**
  - Waiting sequence

OK  Cancel  Help
Share methods, eg. from another network drive

- Possibility to browse to any other method
- Method Path Pointer is set to the default master method folder defined in the Configuration Editor
**Data Organization – Summary**

1. Data Container according to the settings described above
2. Includes all methods used during the sequence
3. Includes batch files, log files (same like B.01.03)
4. Includes original sequence.s
5. All data files are stored with the actually used method
Using the Navigation Table: Review and Reprocess Data
Data Review in the Navigation Table

- is essentially a **single run review** with very convenient access to the runs of a sequence

- The **Preferences** dialog defines which actions are performed when a run is loaded from the Navigation Table

- The review tool buttons allow to **automate** the review
Sequence Reprocessing (1)

- now performed in Data Analysis

- works on the copies of the method and the sequence that are placed in the sequence container

- updates the calibration table and allows to change sequence table parameters like multiplier, sample amount, etc.
Sequence Reprocessing (2)

- updates the information in the Navigation Table
- updates the DA.M of a data file in case a different method is used during reprocessing
- copies new methods into the sequence container in case they haven’t been employed during acquisition
New Data Organization Concept – Changes

• The **master methods** and **sequence templates** are to be used in Method and Run Control view for acquisition, while the copies are to be used in Data Analysis for data review and reprocessing.

• **Reprocessing** is only possible in **Data Analysis** view.

• Once a sequence has been run, the **sequence log** can only be viewed in Data Analysis.

• During acquisition, Data Analysis is only accessible in the Offline Instrument.
New Data Organization Concept - Changes

• Snapshots can only be created in Offline Instrument.

• The new **ChemStation Explorer** supports the new data organization concept with fast access to the correct folders.

• The new **Preferences** dialog is introduced for options where the sequence container is located and which of the methods is loaded for data review.

• Customers who use **Average** and not **Replace** option for update at the beginning of the sequence have to copy their method to the master method directory after a sequence run, including calibration samples.
Demo: Setting of Preferences in Acquisition, Review Settings in Data Analysis
ChemStation B.03.01: Supported Instruments
ChemStation: Supported Instruments

• The ChemStation B.03.01 has been developed to support the 7890 GC
• ChemStation has been especially designed to fully support the 1200 series
• It is fully backwards compatible
• And additionally, ESA detectors are supported, too
Common Instrument Control (CID) / ESA drivers

- Easy to use interface for 3rd party devices (LC technique only)
- Supports detector feature sets, including 2D signals and spectra
- Available in online plot and instrument actuals
- Additional features need implementation by the 3rd party device driver itself

Following 3rd party drivers are supported:
Company: **ESA Biosciences**
- CAD Corona (Charged Aerosol Detector)
- CC Coulochem III (Electrochemical Detector)
ChemStation ECM Integration
What Is ECM?

**Enterprise Content Manager**

is a web-based electronic library that collects, organizes, indexes, stores, archives and shares any electronic file – from raw analytical data and lab reports to compliance records, molecular drawings, Adobe Acrobat documents, Microsoft Office documents, web pages, pictures, video and audio.

ECM allows users to easily search and review all of their data. ECM automatically extracts searchable metadata from files and provides powerful search capabilities.
ChemStation ECM Integration Functionality

- The ChemStation ECM integration adds a pull-down menu and some ECM icons to the ChemStation interface.
- You can store data, master methods and sequence templates from ChemStation directly to ECM, similar to a local directory.
- Open data, master methods and sequence templates stored in ECM directly into ChemStation.
- The ECM node in the Explorer shows the last sequence uploaded from ECM to ChemStation.
Settings of Data Transfer to ECM

- Data in ECM are organized in a four-level hierarchy.
- Users can define within ChemStation where data are stored in ECM.
- Data can be automatically uploaded after acquisition or re-processing.
Each time ChemStation is started, the user has to authenticate himself against the ECM server. Alternatively, he can start ChemStation without access to ECM.
Recommended Literature
Information on the new ChemStation Revision and on Upgrading

- “Upgrade Preparation Guide for ChemStation”
  Publication Number: G2170-90226
- Upgrading from 16 to 32 bit: technical info sheet:
  Publication Number 5989-5444EN
- ChemStation B.03.01 Feature Overview:
  Publication Number 5989-6505EN
- ChemStation B.02.01/B.02.01 SR1 - New Concepts of Data Organization:
  Publication Number: 5989-5589EN
- Application Notes
- The ChemStation Treasure Chest - Part 1: Create a calibration table in virtually no time
  Publication Number: 5989-6602EN
Learn More about ECM & ECM Integration

- ECM Product Page:  

- New ChemStation ECM Interface manual:  
  P/N G2170-90030

- Technical Note: Integration of ChemStation with Agilent OpenLAB ECM:  
  5989-5552EN

- Agilent ChemStation and Agilent OL Enterprise Content Manager integrate seamlessly to facilitate compliant data management  
  5989-6238EN
Summary

• **ChemStation B.03.01** is continuing the new method- and data storage settings introduced with ChemStation B.02.01.

• It gives you the **flexibility** to **configure** the software according to your lab workflows

• Integration with Agilent OpenLAB ECM enables data sharing and review across different locations within a company. This is useful for sharing documents, results and methods
Thank You!
Do you have revalidation concerns with upgrading to the new version of ChemStation?

Sign-up for our next eSeminar on Thursday, September 13, 2007 – 11:00am EDT

Register at www.agilent.com/chem/CSupgrade

Save time! Save money! Act now!
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www.agilent.com/chem/CSupgrade1
# Next eSeminar: Revalidation after Upgrade from A to B Versions

## ChemStation Upgrade

Series aimed at ChemStation users working currently with revision lower than B.02.01 and wishing to learn more about the feature set of the new ChemStation.

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