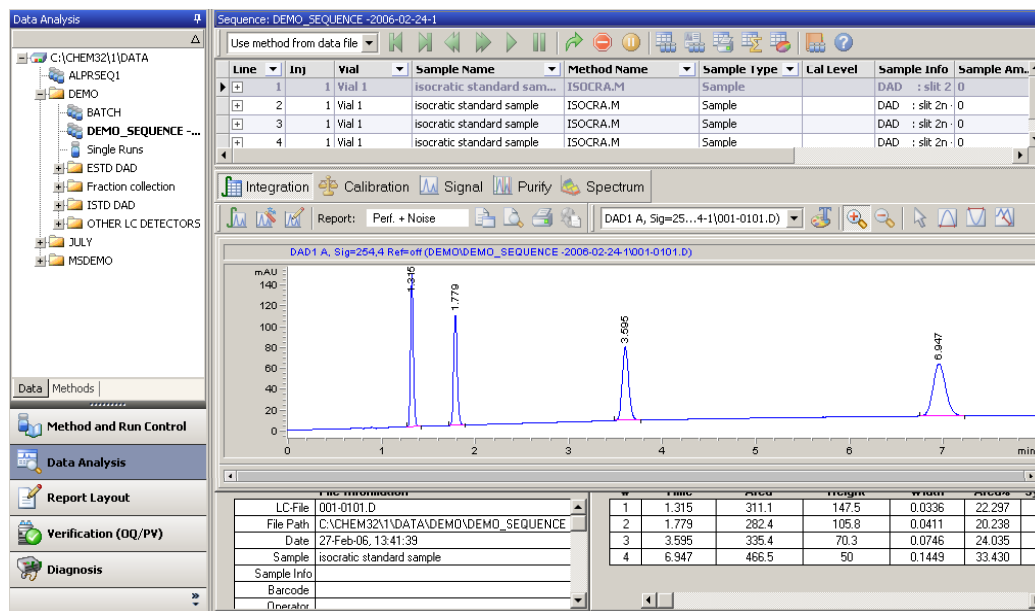


ChemStation B.03.01-What's New!

Agilent Technologies

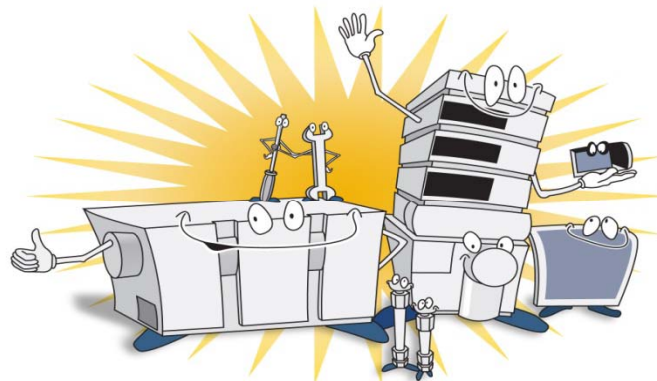
Katja Kornetzky

Product Manager
Lab Informatics



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:**

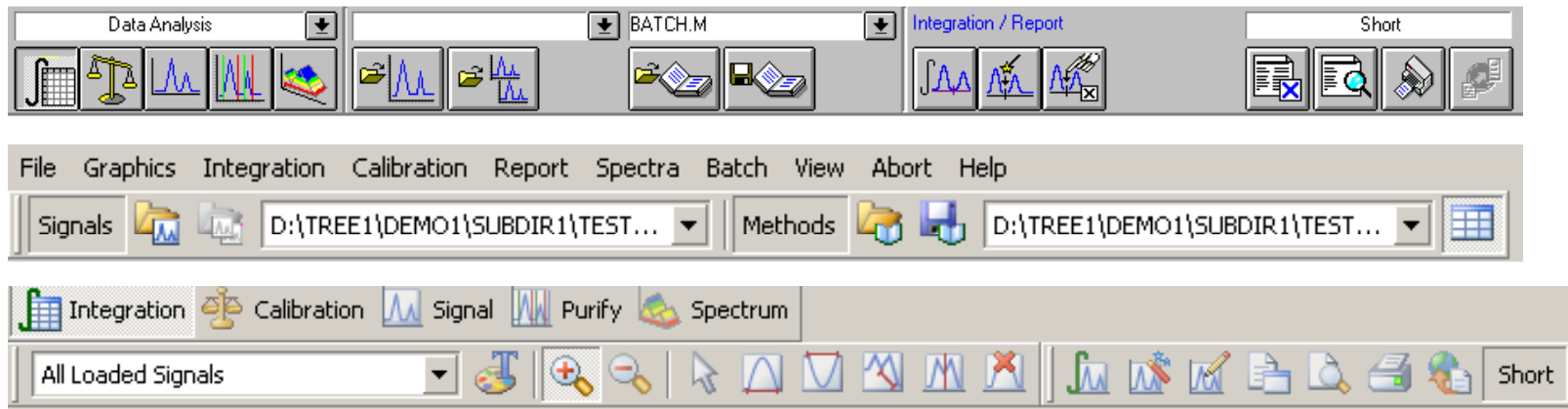
- ⇒ Modern Icons

- ⇒ 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.

Line	Inj	Vial	Sample Name	Method Name	Sample Type	Cal Level	Sample Info	Sample Am...	ISTD Amount	Multiplier	Dilution	Data File
1	1	Vial 1	cal 1	METHOD_NAME.M	Calibration	1		0	0	1	1	TRAINING00...
2	1	Vial 2	cal 2	METHOD_NAME.M	Calibration	1		0	0	1	1	TRAINING00...
3	1	Vial 3	cal 3	METHOD_NAME.M	Calibration	1		0	0	1	1	TRAINING00...
4	1	Vial 4	sample 1	METHOD_NAME.M	Sample			0	0	1	1	TRAINING00...
5	1	Vial 5	sample 2	METHOD_NAME.M	Sample			0	0	1	1	TRAINING00...
6	1	Vial 6	sample 3	METHOD_NAME.M	Sample			0	0	1	1	TRAINING00...

List of all runs belonging to a
sequence (read-only). Provides
easy access to load the file.

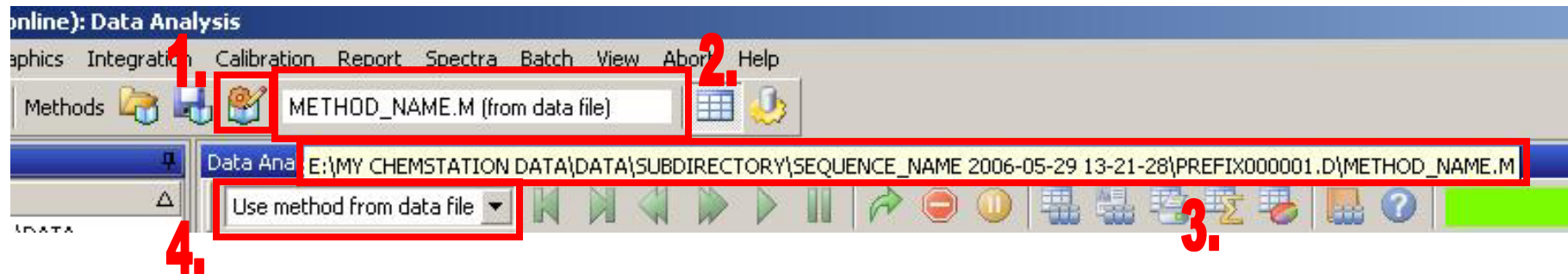
Customizing the Navigation Table

The screenshot displays the ChemStation interface with a navigation table. The table has columns: Line, Inj, Vial, Sample Name, Method Name, Cal Level, Sample Info, Sample Am..., ISTD Am..., and Data File. The first three rows are grouped under 'Sample Type: Calibration'. Row 3 is selected, and its details are expanded in the lower-left pane. Two context menus are shown: one for the 'Sample Name' column header and one for the selected row 3. Red boxes and numbers 1-4 highlight these key features.

Line	Inj	Vial	Sample Name	Method Name	Cal Level	Sample Info	Sample Am...	ISTD Am...	Data File
- Sample Type: Calibration									
+ 1	1	Vial 1	cal 1	METHOD_NAME.M	1		0	0	TRAINING00...
+ 2	1	Vial 2	cal 2	METHOD_NAME.M	1		0	0	TRAINING00...
- 3	1	Vial 3	cal 3	METHOD_NAME.M	1		0	0	TRAINING00...
Sample Type: Sample									
+ 4	1	Vial 4	sample 1	METHOD_NAME.M			0	0	1 1 TRAINING00...
+ 5	1	Vial 5	sample 2	METHOD_NAME.M			0	0	1 1 TRAINING00...
+ 6	1	Vial 6	sample 3	METHOD_NAME.M			0	0	1 1 TRAINING00...

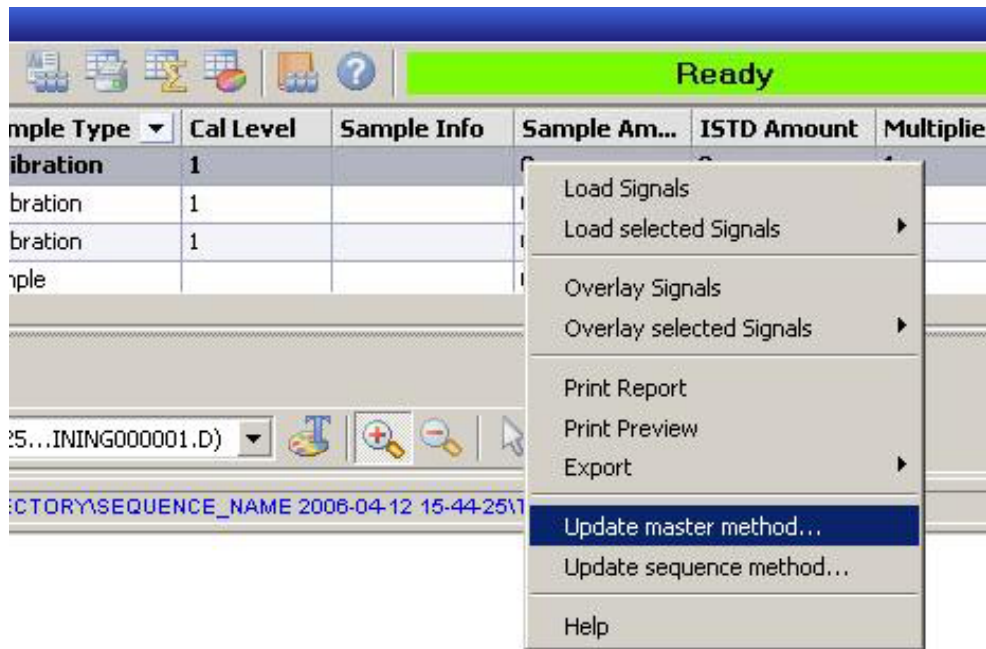
1. Right-click the column headers to configure the table.
2. Group the Table Rows by columns, e.g. by Sample Type.
3. Right-click a run to perform actions on the run.
4. Expand a run to view its details.

GUI Enhancements for Method Handling

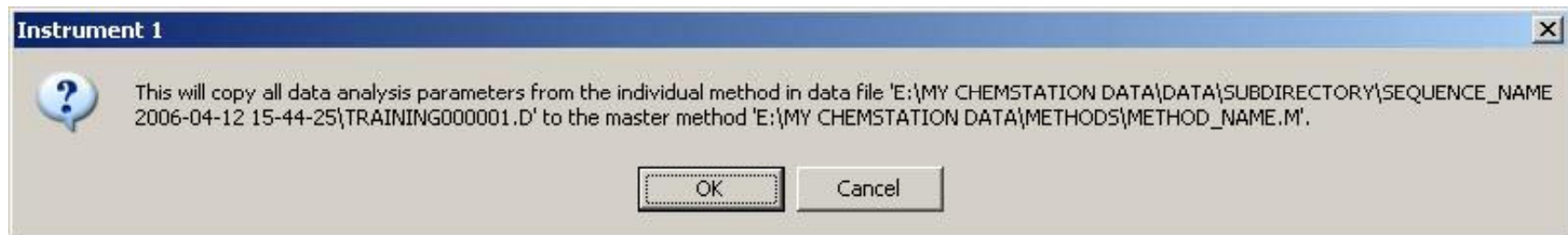


1. The method modification status is now displayed also in Data Analysis.
2. The method combo box was replaced by a static field always displaying the current method.
3. A tool tip displays the complete method path.
4. This dropdown box allows to change the method usage options of the Preferences dialog 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

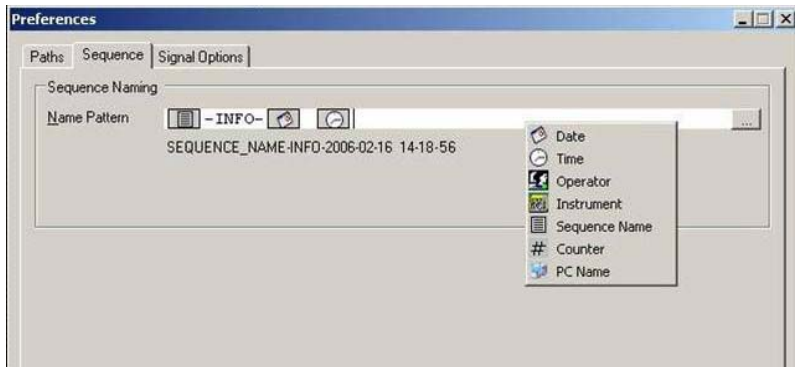
Data Storage

- 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

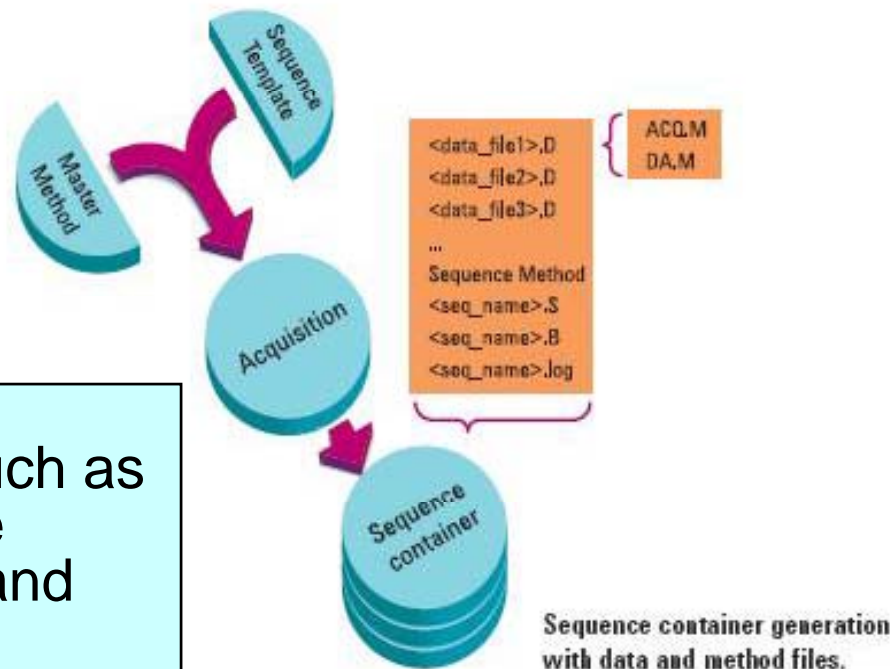
- direct link between a sequence, the data files, the results, and the method being used to create the results
 - ⇒ could previously only be achieved using reports
- The new concept provides possibility to easily archive consistent sets of data
 - ⇒ prerequisite for better ECM integration

Sequence Acquisition



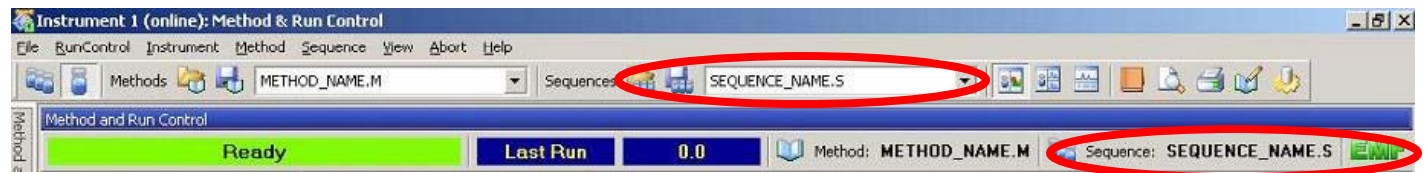
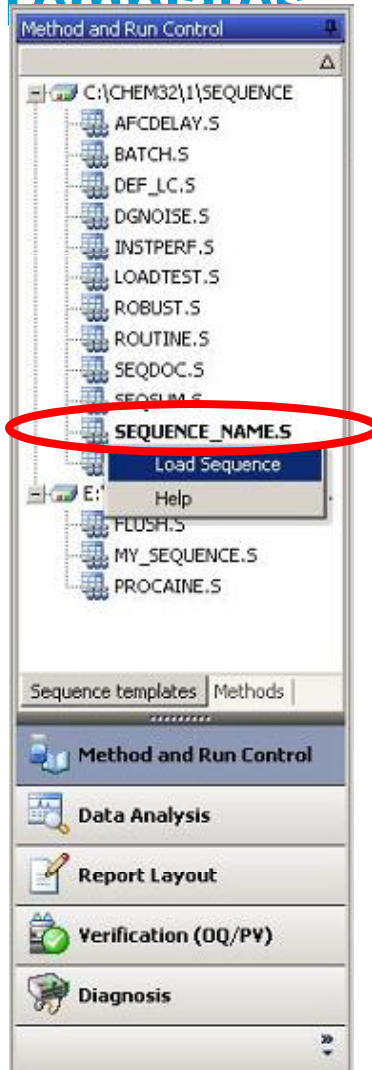
Sequences and all related data such as raw data, methods and results are stored in a **sequence container** and thus **easy to retrieve**.

Sequences can be saved to defined locations such as external drives, and **multiple naming patterns** are possible.



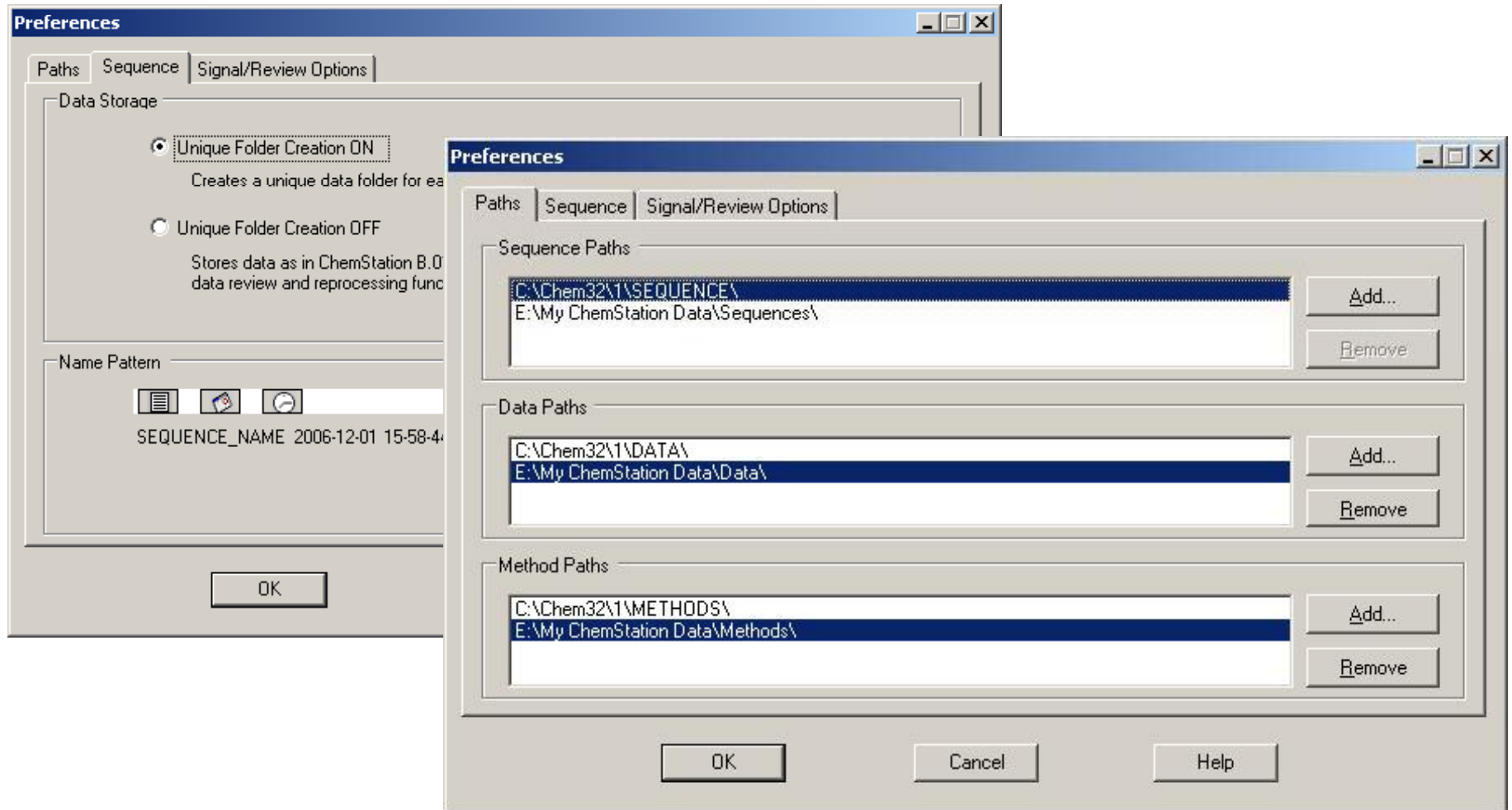
Central Storage of Master Methods and Sequence

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



Define Subdirectory

Sequence Parameters: Instrument 1

Operator Name:

Data File

Path: Subdirectory:

Auto

Prefix/Counter

Prefix: Counter:

Part of methods to run

Wait minutes after loading a new method

Shutdown

Post-Sequence Command/Macro

Not Ready Timeout: minutes

Bar Code Reader

Use In Sequence

On a bar code mismatch

Inject anyway

Don't inject

Fraction Information

Fraction Start Location:

ChemStore

Sequence Comment:

Share methods, eg. from another network drive

Sequence Table: Instrument 1

Currently Running
Line: Method:

Sample Info for Vial 1:

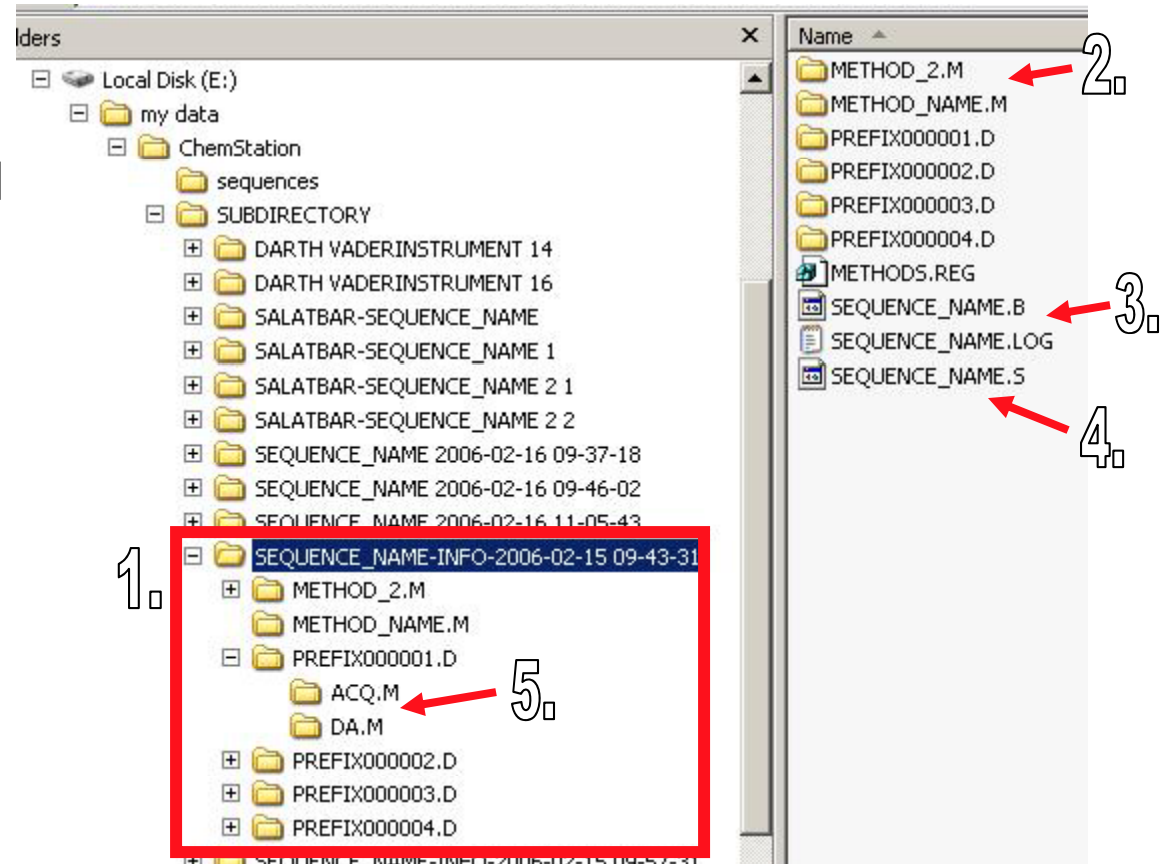
Line	Vial	Sample Name	Method Name	Inj/Vial	Sample Type
1	Vial 1	this is a test	BATCH	1	Sample
2	Vial 1	this is a test	BATCH	1	Sample
3	Vial 1	this is a test	BATCH	1	Sample
4	Vial 1	this is a test	<input type="text"/>	1	Sample

LOADTEST
MULTISIG
PURITY
SYSPERF
STRESSUI
Browse...

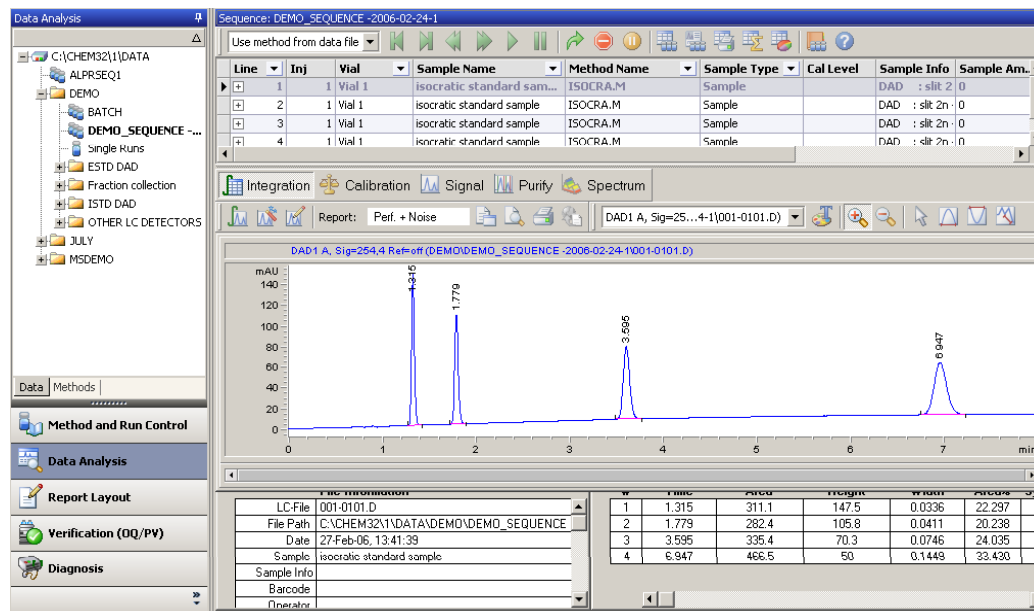
- Possibility to browse to any other method
- Method Path Pointer is set to the default master method folder defined in the Configuration Editor

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

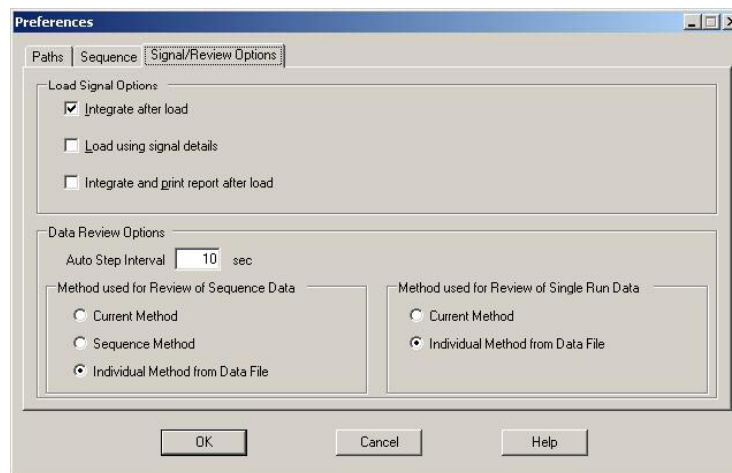


Using the Navigation Table: Review and Reprocess Data



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

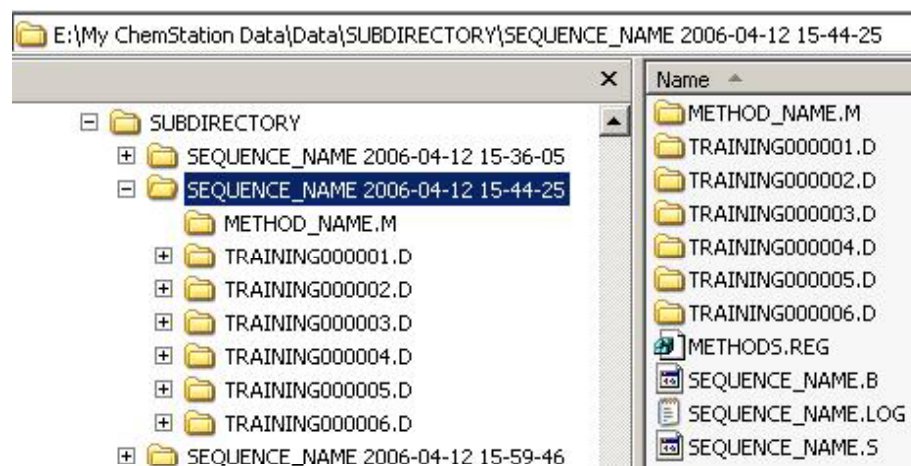


Sequence Reprocessing (1)

- 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

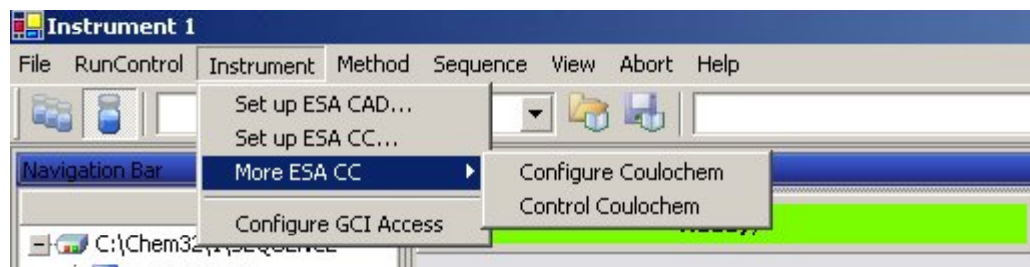
- Easy to use interface for 3rd party devices (LC technique only)
- Supports detector feature sets, including 2D signals and spectra
- Available in online plot and instrument actuals
- Additional features need implementation by the 3rd party device driver itself

Following 3rd party drivers are supported:

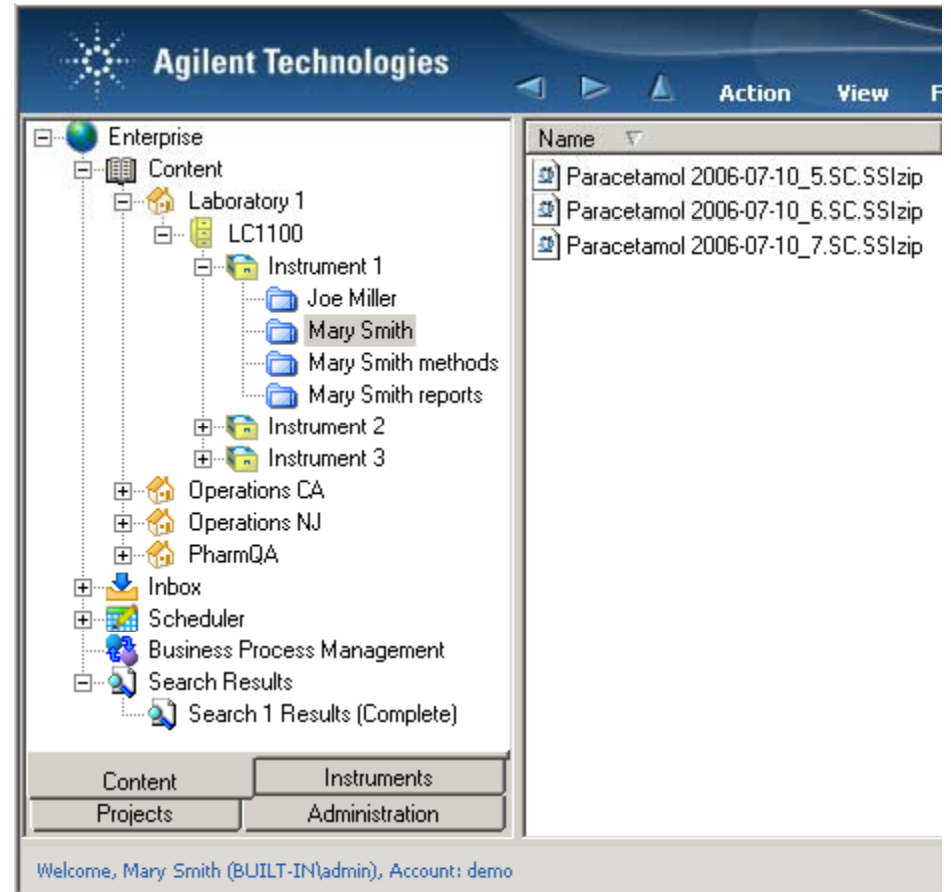
Company: **ESA Biosciences**

CAD Corona (Charged Aerosol Detector)

CC Coulochem III (Electrochemical Detector)



ChemStation ECM Integration



What Is ECM?

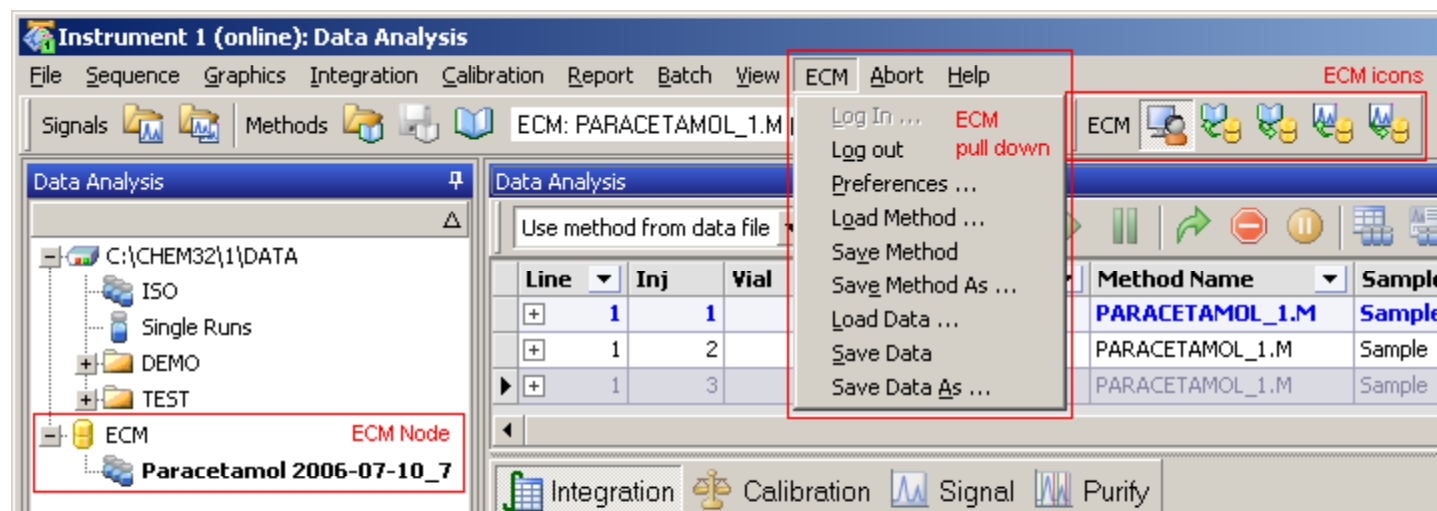
Enterprise Content Manager

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.

The screenshot displays the OpenLAB ECM Explorer interface within a Microsoft Internet Explorer browser window. The address bar shows the URL: `http://olweb1/ecm/Enterprise.asp?SessID=163432`. The main content area features a tree view on the left and a data table on the right.

Tree View Hierarchy:

- Enterprise
 - Content
 - Laboratory 1
 - LC1100
 - Instrument 1
 - Joe Miller
 - Mary Smith
 - Mary Smith methods
 - Mary Smith reports
 - Instrument 2
 - Instrument 3
 - Operations CA
 - Operations NJ
 - PharmQA
 - Inbox
 - Scheduler
 - Business Process Management
 - Search Results
 - Search 1 Results (Complete)

Data Table:

Name	Status	Version #	# of signatures	Date Uploaded
Paracetamol 2006-07-10_5.SC.SSI.zip		1	0	10.07.2006 17:07:20 (GMT +02:00)
Paracetamol 2006-07-10_6.SC.SSI.zip		1	0	10.07.2006 17:56:11 (GMT +02:00)
Paracetamol 2006-07-10_7.SC.SSI.zip		2	1	10.07.2006 18:16:17 (GMT +02:00)

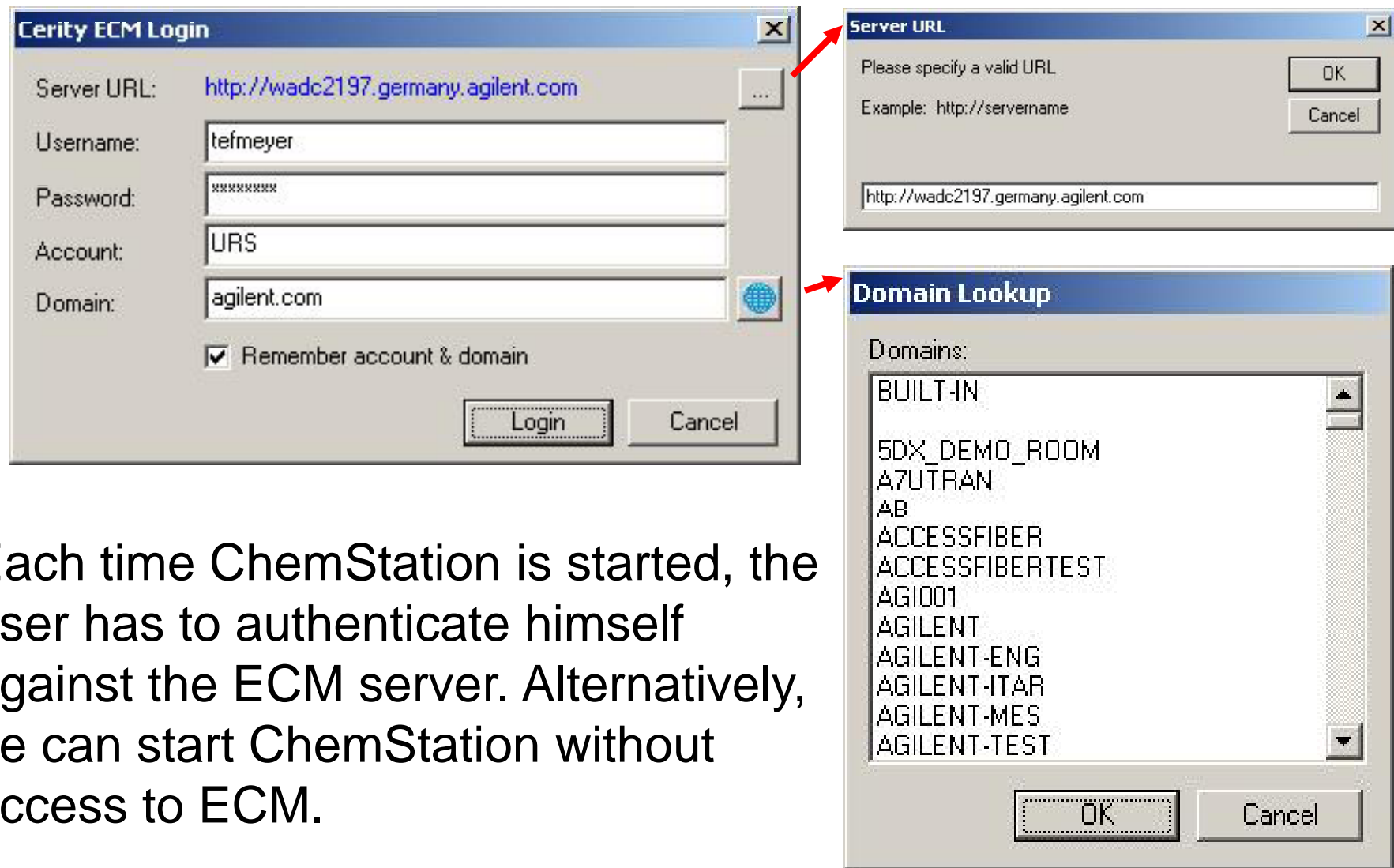
Preferences Dialog Box (ECM Tab):

The Preferences dialog box is open, showing the ECM tab. It includes the following settings:

- ECM Data Path:** A "Select ECM Path" button is present. Below it, fields for Location, Cabinet, Drawer, and Folder are shown. The Location is "Laboratory 1", Cabinet is "LC1100", Drawer is a dropdown menu with "Instrument Name" selected, and Folder is "[Operator]".
- Transfer Settings:**
 - save data automatically to ECM after completion of single run/sequence
 - save data automatically to ECM after reprocessing

Buttons for OK, Cancel, and Help are located at the bottom of the dialog box.

Startup of ChemStation – Login

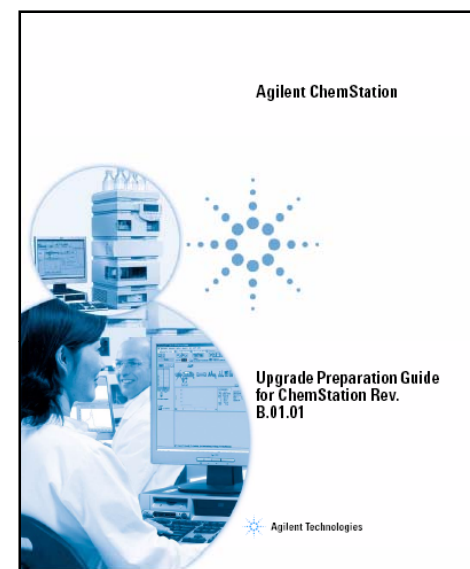


Each time ChemStation is started, the user has to authenticate himself against the ECM server. Alternatively, he can start ChemStation without access to ECM.

Recommended Literature

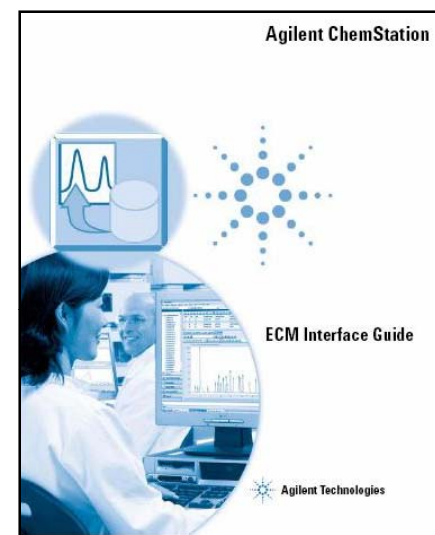
Information on the new ChemStation Revision and on Upgrading

- “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:
<http://www.scisw.com/products/ecm/index.htm>
- 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

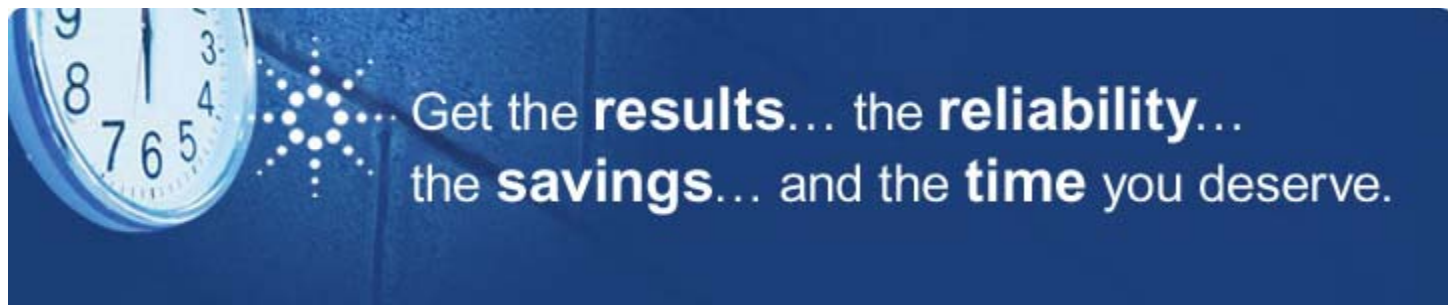


Summary

- **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!

Upgrade now and save 30% off a new instrument LAN card. Request a quote =

www.agilent.com/chem/CSupgrade1

Get ready to push a button... walk away... and know with confidence your sequence will be complete when you return. The new **32-bit ChemStation B.03.01** provides increased reliability plus a host of time-saving enhancements.

Best of all, you'll enjoy 30% savings.

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.

Date & Time	Event	Panelists Info	Status
August 21, 2007 11:00 am - 12:00 pm Eastern DT	ChemStation B.03.01 - What's New	Katja Kornetzky, Lab Informatics Product Manager, Agilent Technologies, Inc.	Enroll
September 13, 2007 11:00 am - 12:00 pm Eastern DT	ChemStation - Revalidation after Upgrade from A to B Versions	Katja Kornetzky, Lab Informatics Product Manager, Agilent Technologies, Inc.	Enroll

Task	Responsibility
Provide software revisions that have been developed and validated in a quality control environment following accepted software development quality procedures	Vendor responsibility – may be verified with audit questionnaire to vendor
Update of design qualification with new functionality in most recent revision of software	User responsibility – supported with change documentation from vendor
Provide new revisions of operating system and PC hardware	User responsibility – exact task and ownership should be defined for the project according to internal organization and procedures
....
Change control documentation	User responsibility – supported through documentation from vendor
Update and re-execution of system IQ/OQ	User responsibility – available as service from vendor
Hardware and software upgrade installations	User responsibility – available as service from vendor
End-user training	User responsibility – available as service from vendor
....
Risk assessment	User responsibility – vendor contributes key information for risk assessment, see appendix B of this document
Final project approval	User responsibility

<https://agilenteseminar.webex.com/mw0302l/mywebex/default.do?siteurl=agilenteseminar>