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.
Customizing the Navigation Table

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.
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
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
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

- 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 **automation** of 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.

- Users selecting 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.
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