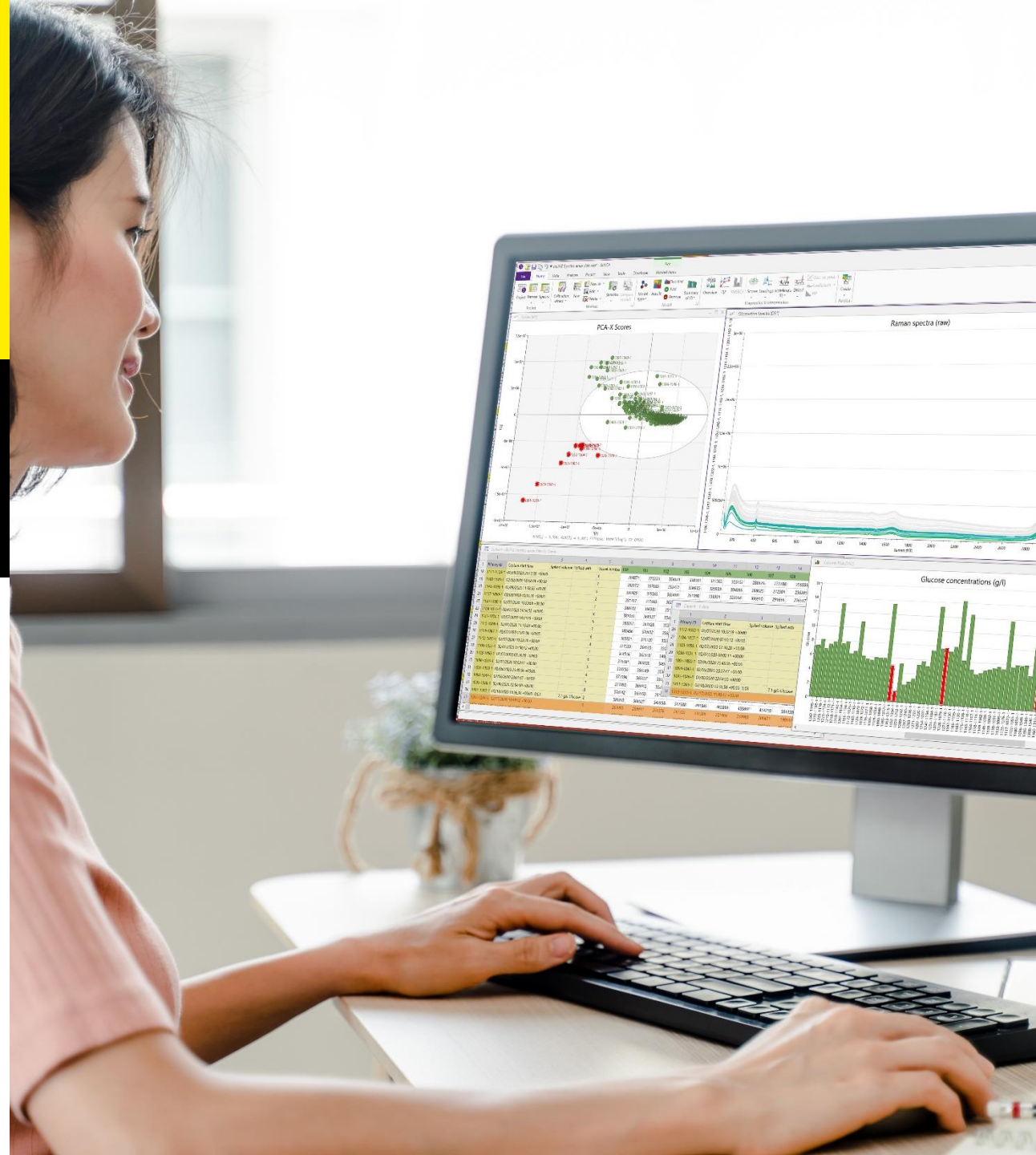# SARTORIUS

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SIMCA® 17 – What's New?

Release February 9, 2021

SIMCA® 17 Overview

- Umetrics® suite SIMCA® is focused on delivering a full data analysis experience, from data organization to data based decision making supported by multivariate models.

- SIMCA® 17 is focused on improving spectroscopy data analysis by providing tools to make multivariate calibration easy and reliable

- With SIMCA® 17 you get a complete solution for preprocessing your spectral data to enhance prediction performance
  - Extended library of preprocessing algorithms in an easy-to-use wizard

- Calibration wizard providing instant model quality visualization after each preprocessing choice helping you chose the best prediction model

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SIMCA® 17 Highlights

- Spectroscopy Project
  - Set, or generate Spectral ID at import
  - New spectra visualization
  - Extended library of preprocessing algorithms
  - Preprocessing wizard
  - Calibration wizard for 1 Y models

- Batch Data and Database Import
  - Possibility to control Batch alignment
  - BCC from dataset
  - SimApi:s available at installation and database interface improvements

- Plot Interactivity
  - Color by Rank – new option for better vector coloring
  - Reverse and log axis control in properties pane
  - Color BCC by batch condition vectors

- Other Improvements
  - Multiple file import for CSV, TXT and DIF files
  - Import configuration template
  - Python news and additions
  - Dataset properties
  - Dataset merge to keep un-matched content
  - New bias vectors (MBE)
  - SIMCA® 16 compatibility
  - Performance

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Learning What's New in SIMCA® 17

- In the following slides you will get an overview of the changes and additions made in SIMCA® 17

- For more details on how to use the features, please watch the what's new videos that you can reach from the start page of SIMCA® 17

- Please also check out more videos on SIMCA® and other Umetrics® suite products by looking up Sartorius Data Analytics on YouTube

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SIMCA® 17 What's New – Spectroscopy Project

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Spectroscopy Project – Spectral ID

- A new integrated Spectroscopy project
  - Requires a Spectral ID vector
  - X-data (spectra) and Y-data are split in separate datasets

- Set your Spectral ID at import
  - Spectral ID will be used as X-axis in plots
  - Triggers access to the Calibration wizard

- Select your spectral ID, or type in a custom name
  - Generate your own numerical vector if none exist

- Center (ctr) scaling is set as default for spectral data

Spectroscopy Project – New Spectra Visualization

- New selection tool in spectra plot
  - Spectra selection instead of variable selection
  - ctrl click to select more than one spectrum
  - Tooltip follow selected spectra for easy comparison

- SIMCA® recognizes spectra as observations and links the plot selections accordingly

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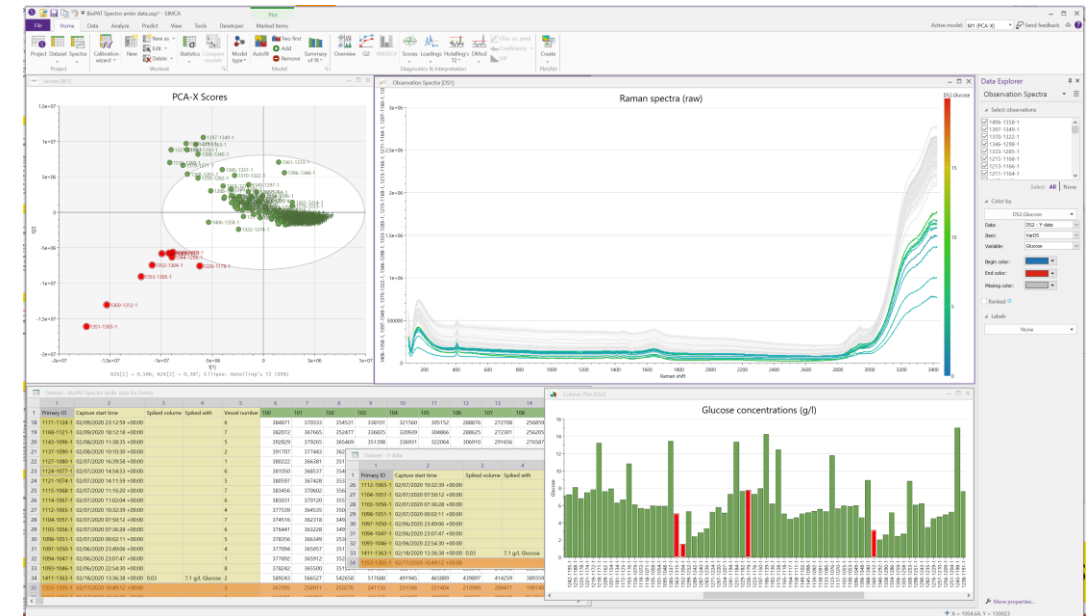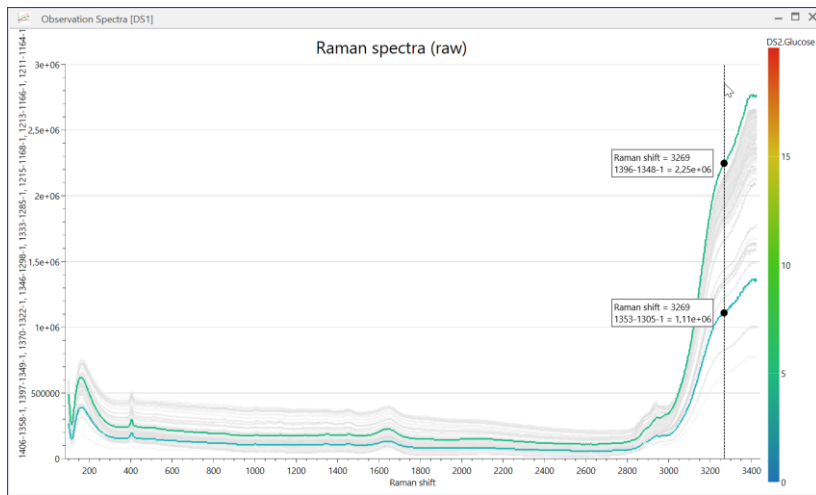
Preprocessing Library Additions

SIMCA® 16 preprocessing

- Smoothing
  - *Savitzky-Golay*
  - *EWMA (left filter)*
  - *Wavelet denoising*

- Normalization
  - *SNV*

- Baseline correction
  - *Row center*

- Other (Spectra enhancement)
  - *MSC*
  - *Wavelet compression*
  - *Derivatives (Savitzky-Golay) 1st-3rd*
  - *OSC*

SIMCA® 17 additions

- Smoothing
  - Moving window
    - average and median
  - EWMA (symmetric filter)
  - AsLS

- Normalization
  - peak height
  - peak area

- Baseline correction
  - Offset, linear baseline, AsLS

- Other (Spectra enhancement)
 - Derivatives (Savitzky-Golay) 4th

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Preprocessing Wizard

- Extensive selection of spectral preprocessing
  - Individual or chained filters

- Interactive, graphical, wizard for filter settings
  - Direct visualization of filter transformation effect

- Python based preprocessing filters are easily added to any of the categories in the wizard

- All filters are automatically applied to predictions
 - Also in SIMCA® -Q and SIMCA®-online

Calibration Wizard

- Wizard for creating and comparing multivariate calibration models with 1 Y
  - Automatically available for spectroscopy projects
    - Spectral ID required
  - Creates a calibration session of models
    - Similar to Class models and Phase models
    - Workset observations consistent over session
  - Existing calibration sessions can be opened and new data can be added
    - But only new prediction (validation) data
  - Session report template available
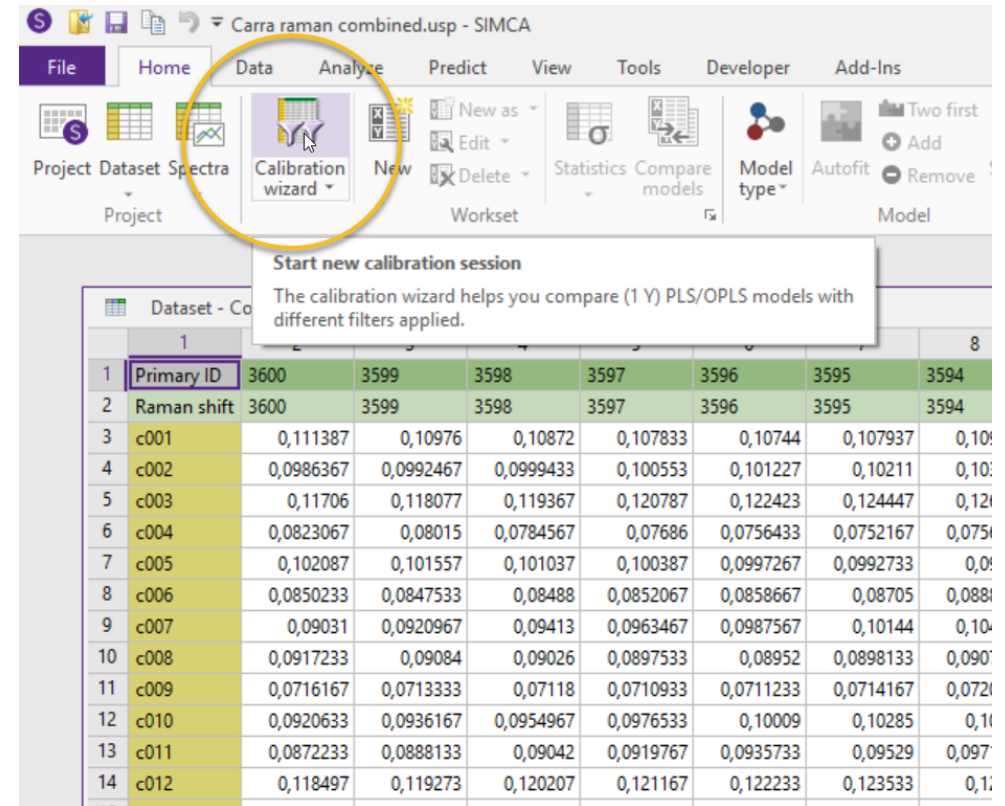
Calibration Wizard – Filter & Compare

- Same filter selection as in Preprocessing wizard
  - Select zero or many filters to apply

- Fit PLS or OPLS models
  - Access to cross validation group definition

- Model performance pane display model parameters and statistics
  - Calibration view (workset statistics)
  - Validation view (prediction set statistics)
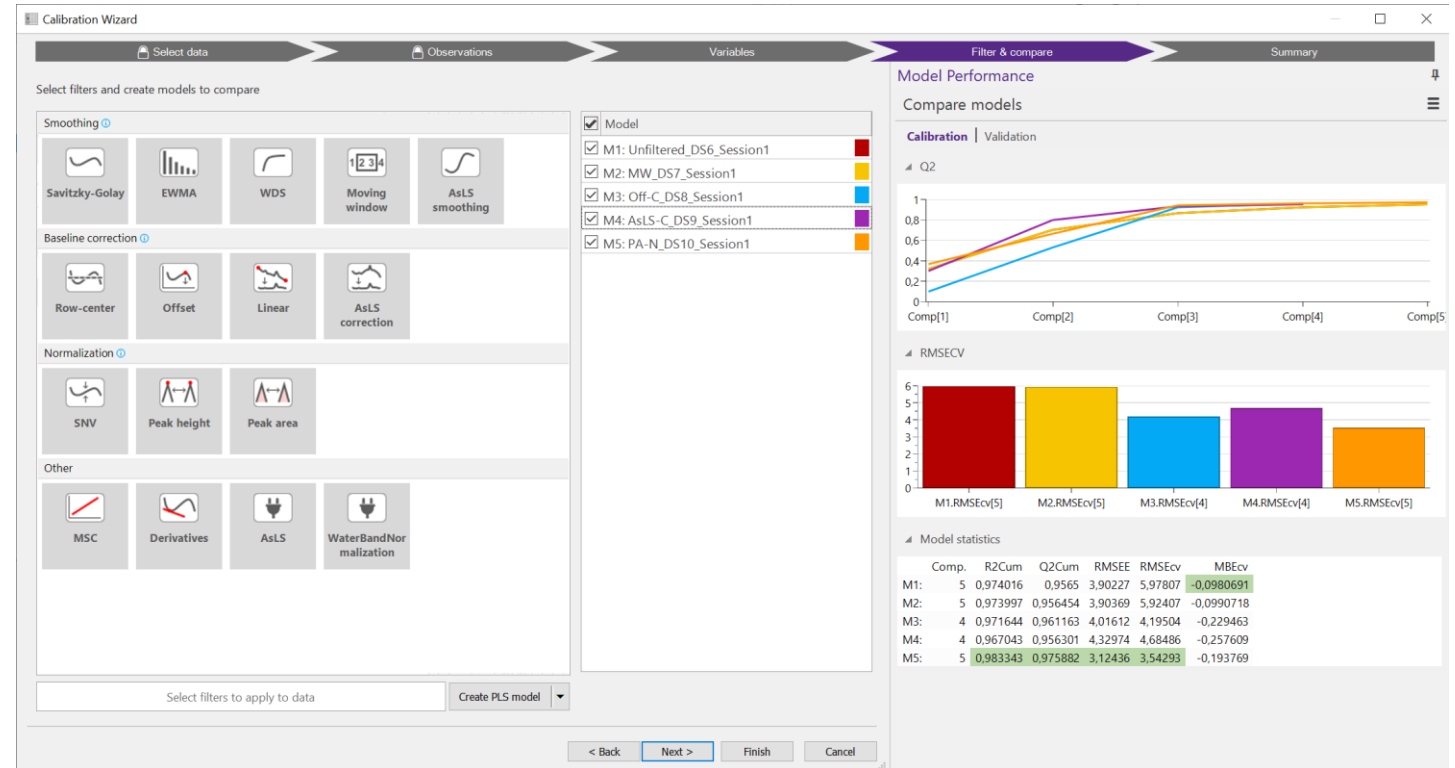
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SIMCA® 17 What's New – Batch Data and Database Import

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# Batch Alignment – New Batch Alignment Option

- New option to control the batch alignment vector

- The default SIMCA® alignment algorithm has been complemented with the possibility for user defined alignment vector

- For short batches (< 20 observations) there sometimes is a desire to control the alignment vector in detail

- In SIMCA® 17, it is possible to align Y according to an existing batch
  - Y alignment option in Workset dialog
  - Same batch for all phases
  - Short batches (<20 observations) have this as default

Batch Modelling Related Additions

- Variable BCC from dataset
  - No need to first create a model
  - Also in Quick info
  - Select and Exclude batches possible
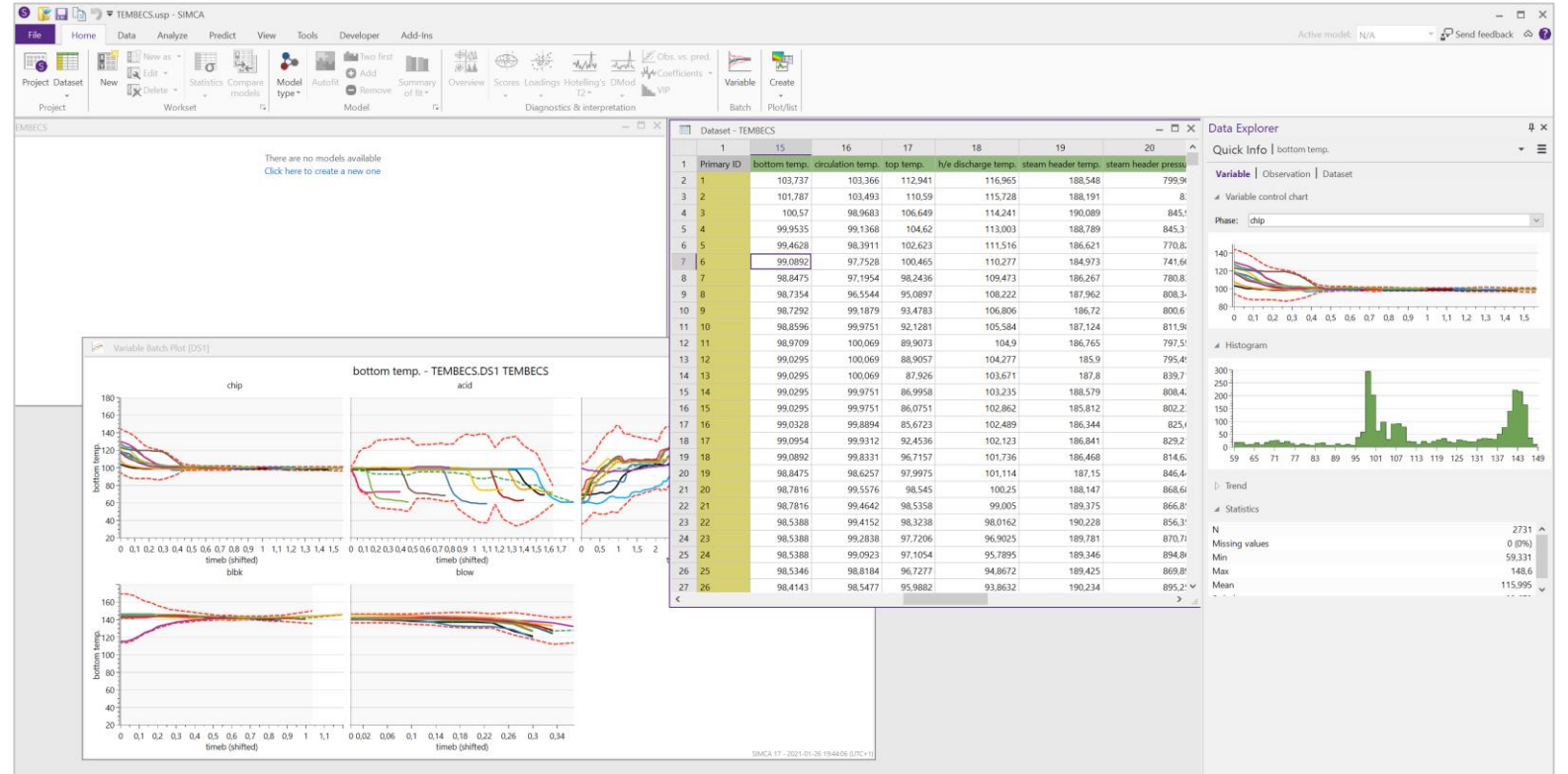
SimApi:S and Database Interface Improvements

- To assist users with process data to extract data directly from the process database some common SimApi:s have been made available during installation
  - No need to download and install the SimApi after SIMCA® installation
  - More SimApi:s are available on Sartorius Data Analytics webpage (link in SIMCA® Help)
- Database interface improvements
  - Hierarchies and node trees visible in database import
  - Database import of batch data where the process node is missing a Batch ID tag is now possible
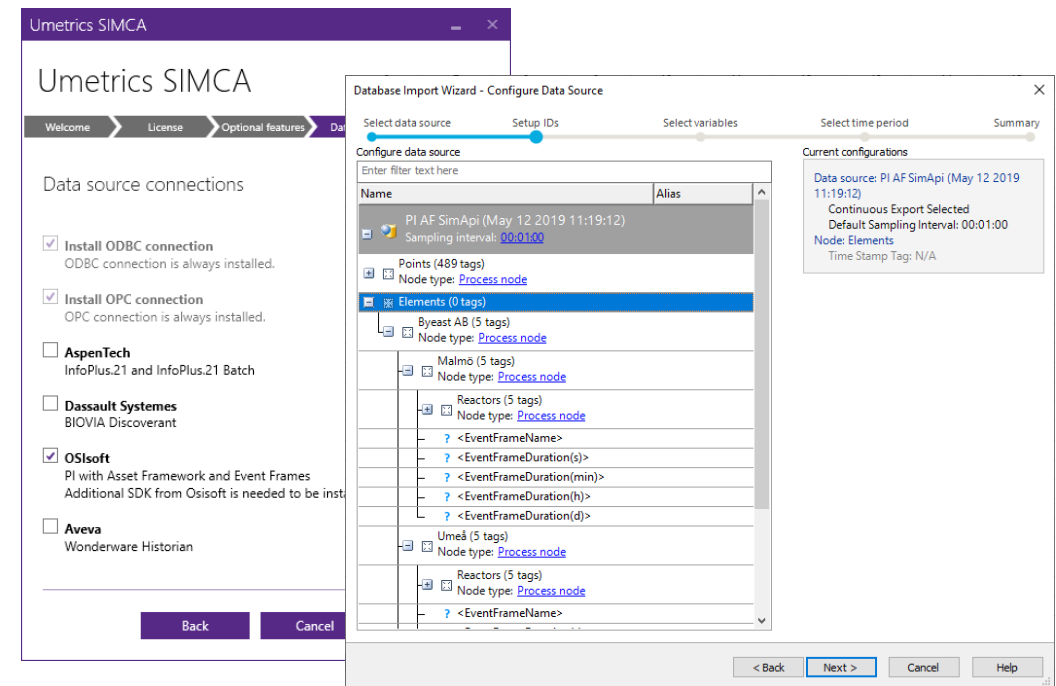
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SIMCA® 17 What's New – Plot Interactivity
and Other Improvements

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Plot Interactivity – Color by Rank

- Color by rank added as an alternative for Continuous coloring

- Ranked color is useful when the coloring vector values have a skewed distribution
  - Ranked color distributes the colors linearly over the full vector range
  - Available in the properties pane
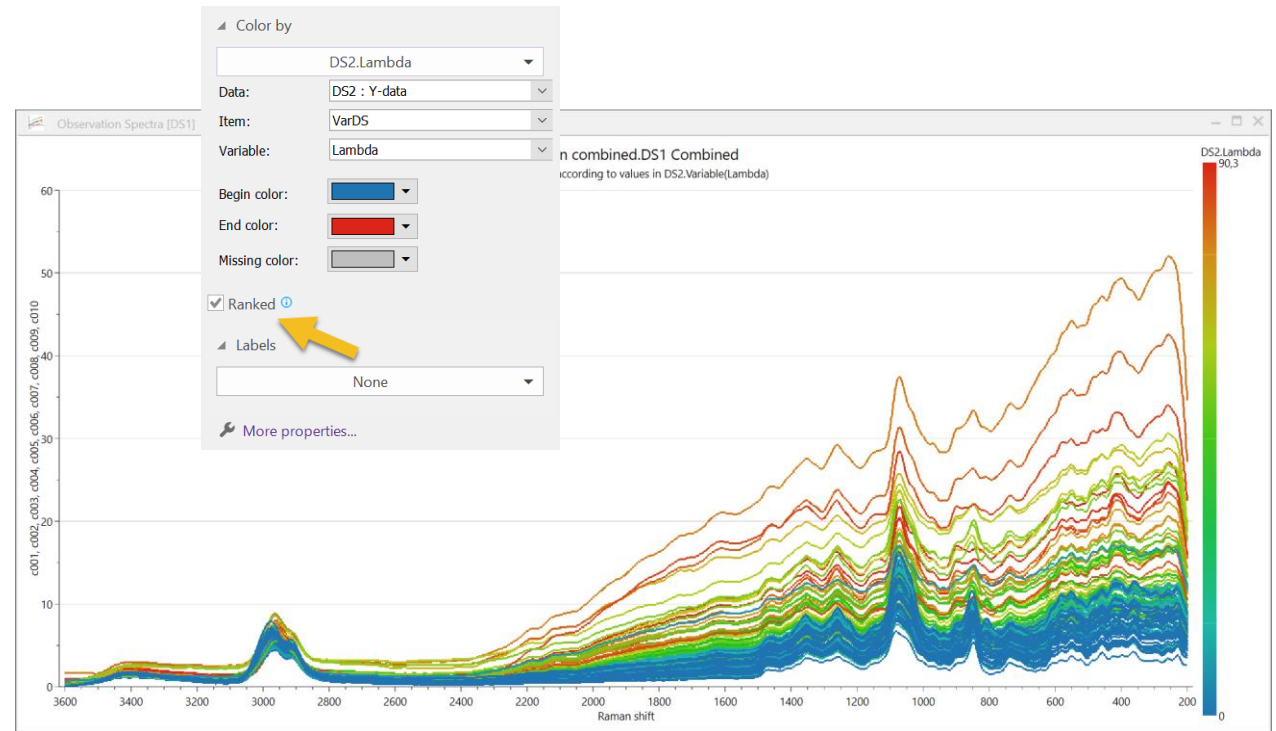
Plot Interactivity – Axis Options

- Reverse and Log axis available in the properties pane
  - Not only for spectra plot
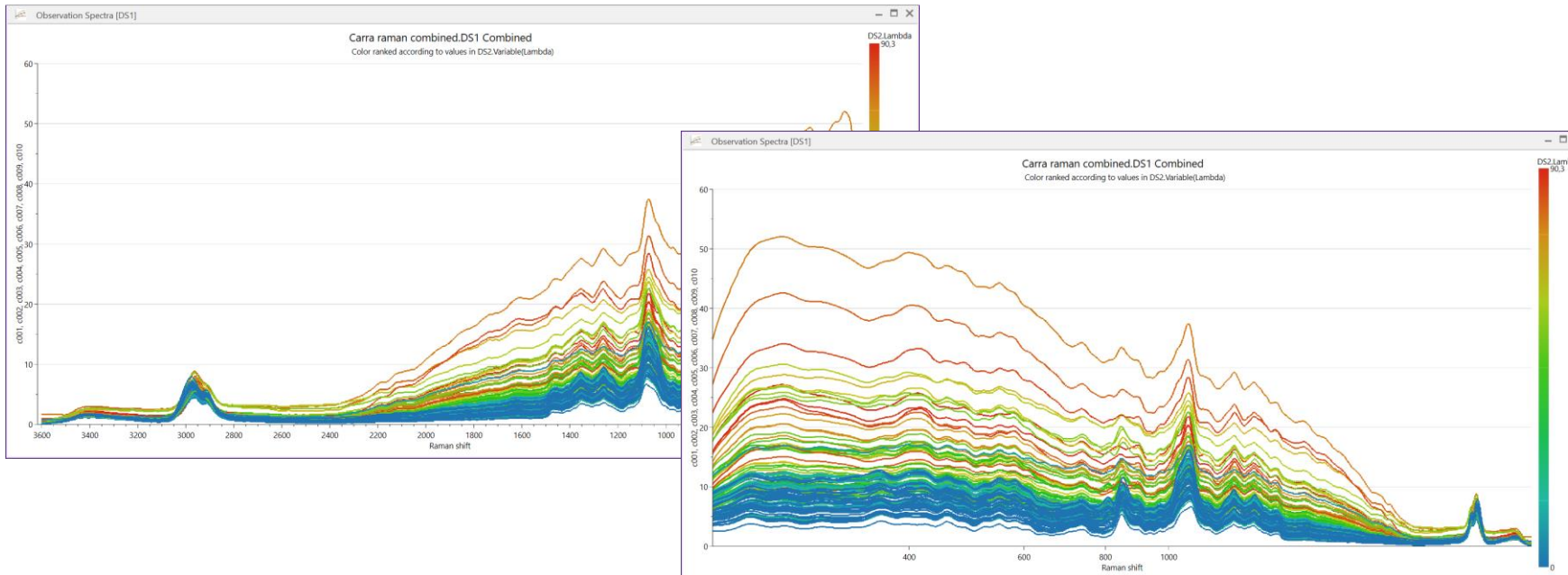
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Plot Interactivity – BCC Coloring

- BCC can be colored by batch conditions
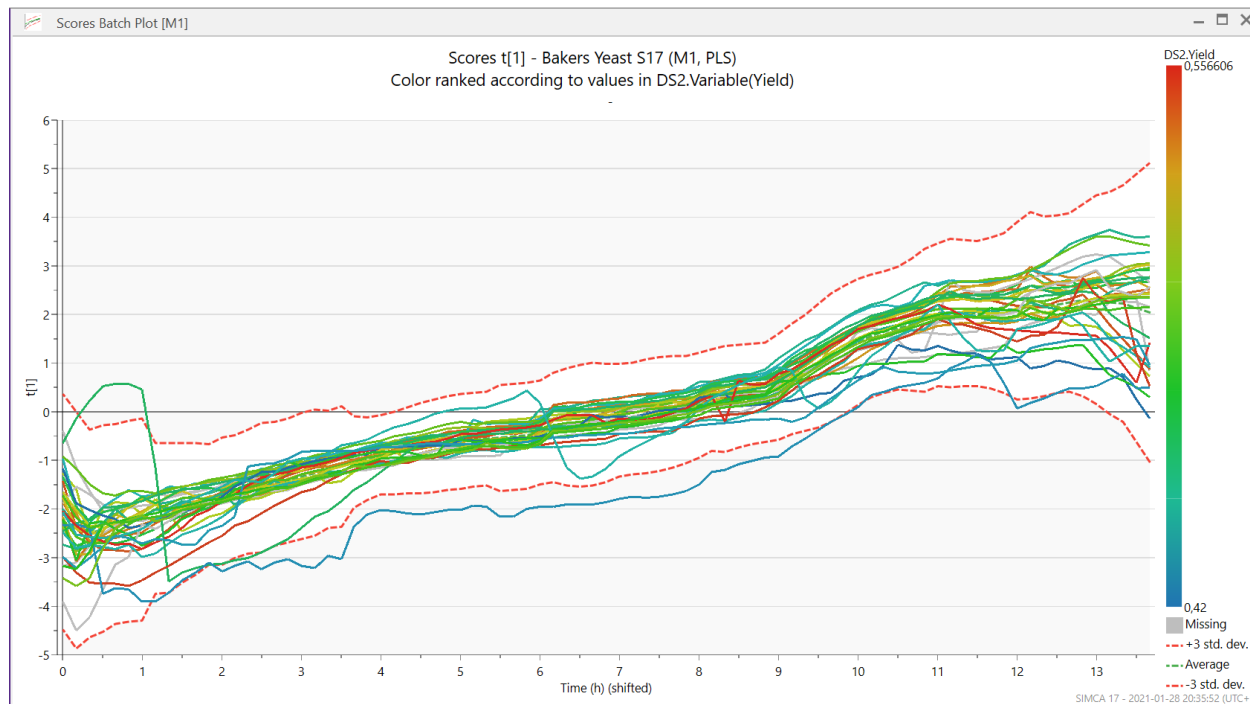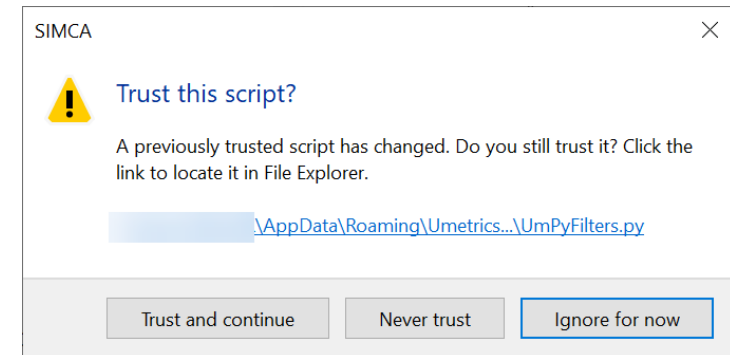
File Import – Templates and Multiple File Import

- Import multiple CSV, TXT and DIF files
  - SIMCA® supports multiple file import of text style file formats
- Template functionality during import
  - Template configures columns and rows
  - Copy current tab configuration to selected tabs
  - Save and load templates
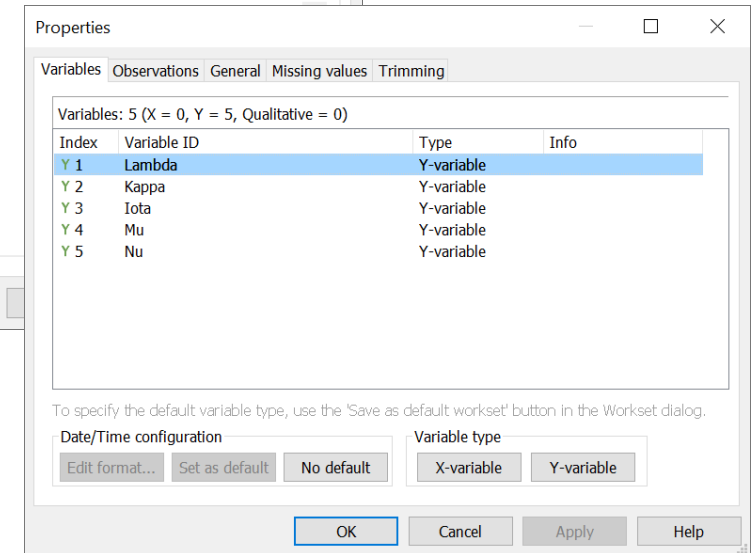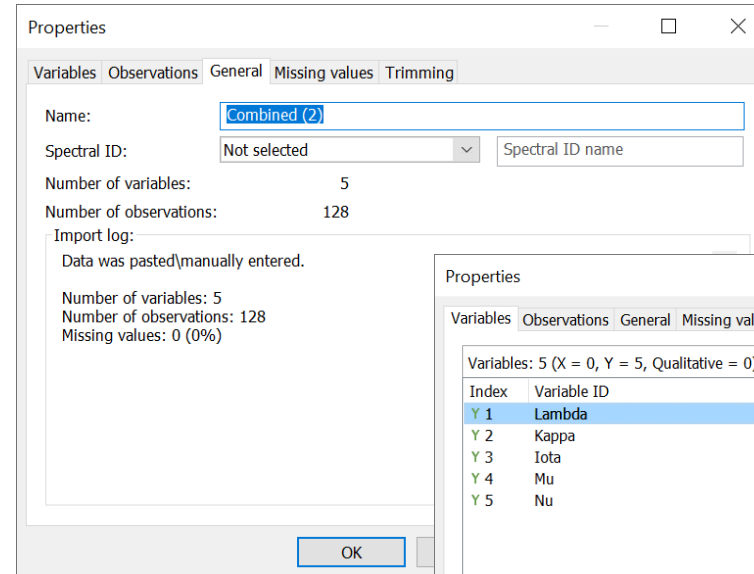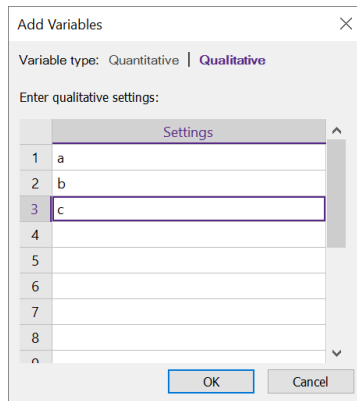
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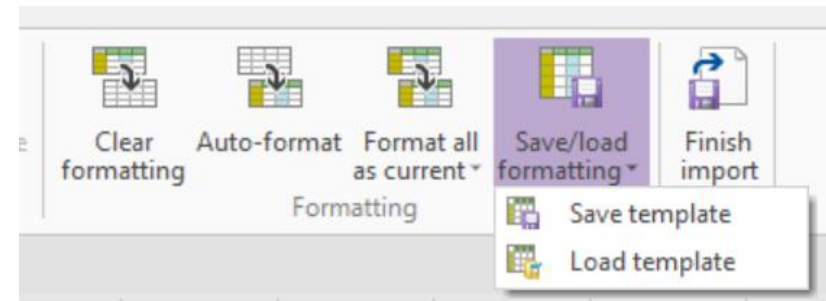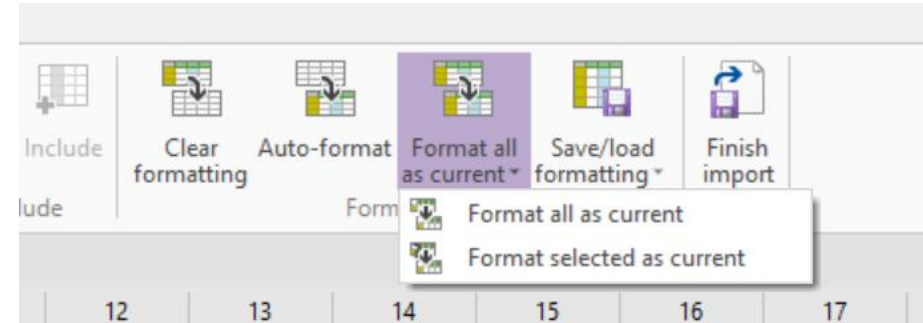
Python News and Additions

- Python updated to version 3.7.9

- NumPy, SciPy, and Pandas are pre-installed in the default virtual environment
  - Versions aligned with SIMCA®-Q and SIMCA®-online

- Python security improvements
  - User to trust new or updated Python scripts and Plugins

- New Python functionalities
  - Create, copy, and save generic plots
  - Plot properties in BCC
  - Labels and colors in plots
  - All new SIMCA® 17 added functionality

```
>>> import umpypkg
>>> sys.version
'3.7.9 (tags/v3.7.9:13c94747c7, Aug 17 2020, 18:58:18) [MSC v.1900 64 bit (AMD64)]'
>>> umpypkg.list()
Package         Version
--------------- -------
numpy           1.19.5
pandas          1.2.0
pip             20.2.3
python-dateutil 2.8.1
pytz            2020.5
scipy           1.6.0
setuptools      50.3.0
six             1.15.0
wheel           0.35.1
```

SIMCA ⚠ **Trust this script?**

A previously trusted script has changed. Do you still trust it? Click the link to locate it in File Explorer.

\AppData\Roaming\Umetrics...\UmPyFilters.py

[Trust and continue] [Never trust] [Ignore for now]

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Dataset Properties

- In dataset properties you can
  - Change the name of the dataset
  - Changing X and Y assignment
  - Set, or rename, Spectral ID

- Add qualitative variables to an existing dataset

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Dataset Merge

- In SIMCA® 17 un-matched content is retained in a new dataset

New Vectors – Mean Bias Error

- Mean Bias Error (MBE)
  - Average prediction error in original unit and with sign
  - Indicates if model has a bias in the predictions
    - i.e. over or under predicts
  - The new Identity line (1:1) helps to visualize bias

- Available bias vectors
  - MBEE
    - Estimated from workset observations
  - MBEcv
    - Calculated from the CV-round predictions of Workset observations
  - MBEP
    - Calculated from (true) prediction set observations

- Compare models list found in Home and Predict tabs
  - Prediction performance for models with same Y
  - Best value in each column in green
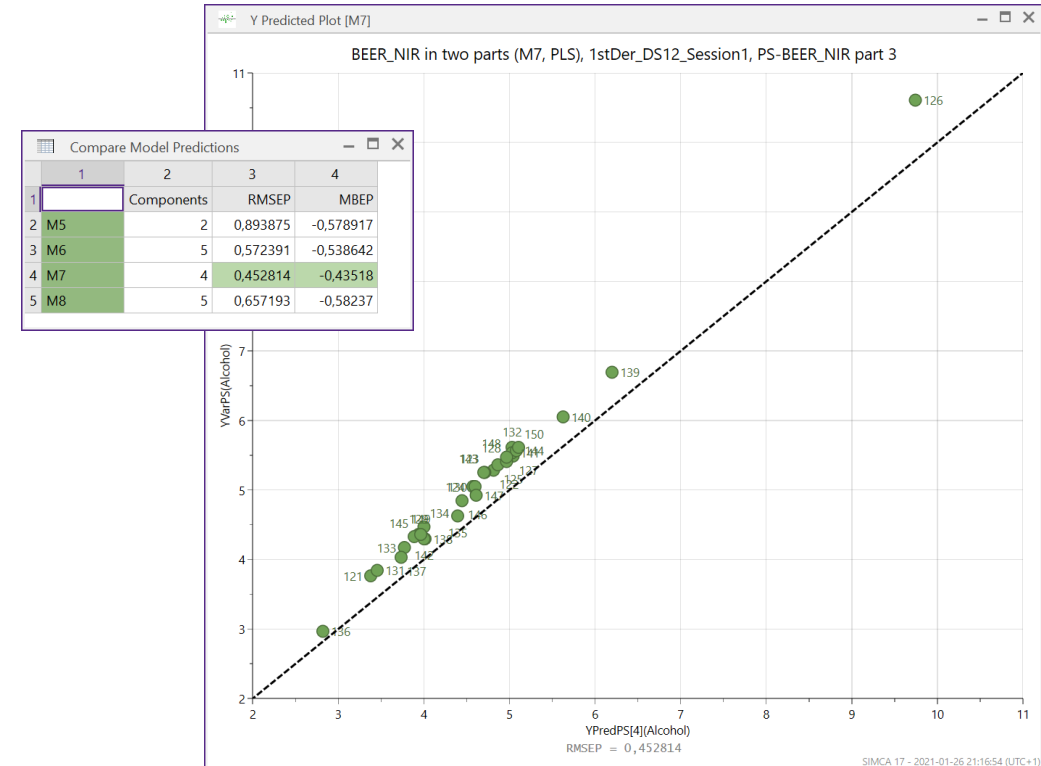
SIMCA® Compatibility

- SIMCA® 17 is compatible with
  - SIMCA® -Q 17 and SIMCA® -online 17
- Save as SIMCA® 16 introduced
  - But not available for preprocessing functionality added in SIMCA® 17
- SIMCA® Qpe format
  - A special format for embedded predictions. Need special implementation to be used
    - Only for OEM customers

- Filters in SIMCA 17 *not compatible* with SIMCA 16
  - Smoothing
    - Savitzky-Golay Quartic, Quintic
    - EWMA
    - Moving window
    - AsLS smoothing
  - Baseline correction
    - Offset
    - Linear
    - AsLS correction
  - Normalization
    - Peak height
    - Peak area
  - Other
    - Derivatives 1st Quartic, Quintic
    - Derivatives 2nd Quartic, Quintic
    - Derivatives 3rd Quartic, Quintic
    - Derivatives 4th Quintic

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Performance – Some Examples

- Many aspects of SIMCA® performance and responsiveness have been addressed in SIMCA® 17

- Plot creation and interactivity
  - e.g. line plots and coloring of line plots

- Opening of projects is approximately 67% faster

- Drop-down lists get populated with values in a fraction (<1%) of the time

- And many more things to improve the SIMCA® experience

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Thank You for Your Interest in SIMCA® 17

Don't forget to check out the instructional videos

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