Quick Guide to SIMCA Spectroscopy skin

1. Introduction
This guide describes the interface and functionality unique to the Spectroscopy skin, complementing the regular SIMCA 13 User Guide and Help.

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Motivation for Spectroscopy skin
The SIMCA Spectroscopy skin was developed to offer a simplified and customized interface designed for a specific application area, namely spectroscopic data. Compared to the regular SIMCA interface, some default settings, default plot options and shortcuts for typical routine operations were introduced to suit spectroscopy data and normal model procedures within this community.

The plot library, model types and calculations are identical to those performed in regular SIMCA.

How to open the Spectroscopy skin in SIMCA
On the View tab, in the Skins group, click Spectroscopy to switch to the customized interface for spectroscopy data.
2. Settings for Spectroscopy skin

Scaling
By default X-variables in PCA/PLS/OPLS models are centered only (scaled with ctr) which is suitable for spectral data.

Line plots
Loadings and coefficients plots are by default plotted on a numerical spectral axis.

3. Home tab
The interface of the Spectroscopy skin Home tab is displayed below. New plots and functionality specific for the Spectroscopy skin are marked with arrows and described in this section.

Spectra
Clicking Spectra in the Spectroscopy skin opens a dialog where you can select up to four datasets to display in individual spectra plots.

The four spectra plots display XObs of all observations in a line plot. By default the spectra are colored according to the first Y-variable.
Compare Filters wizard

With the Compare Filters wizard, up to three different spectral filters can be applied and compared with the original raw spectra. Three new filtered datasets are created and in the case where a y-variable has been specified, PLS models are fitted, otherwise PCA-models are fitted. In total four models are fitted when clicking Finish on the last page of the Compare Filters wizard. (raw data + 3 filtered data)

The wizard contains following steps:

a. **Select spectral range**
   If there are parts of the spectra that should not be included in the filtering, these can be excluded graphically or in the list by marking and clicking Exclude. The selected spectral ranges will be used for all filters. By default the whole spectral range is included.

b. **Select spectra**
   If there are spectra that should not be included in the filtering and modeling, these can be excluded graphically or in the list by marking and clicking Exclude. By default all spectra are included.

c. **Specify filters**
   On the Specify filters page you can assign up to three filters to apply to the dataset. There are three default filters: SNV, 1st Derivative and 2nd Derivative. Customize as desired by removing filters or adding one or more filters. Note that adding more than one filter results in a chained filter.
   Under Y-variable, select which Y-variable to use to fit a PLS model, or leave empty to fit PCA models.

d. **Spectra**
   The last page displays the spectra plots for the new filtered datasets and the original dataset. Clicking Finish results in new filtered datasets and autofitted models.
Import to Model

Import to Model combines importing data and including the new spectra in a copy of the active model. Application example: Spectra are recorded from 60 samples during one period. Data are imported to SIMCA and a PLS model with a quality parameter as Y is developed and optimized with respect to selection of filter and spectral range. Afterward 60 new spectra are measured. With the desired model marked clicking Import to Model and importing the new spectra automatically creates a new model as a copy of the active model complemented with the new spectra.

Q2 plot

The Q2 plot compares the model performance of the selected models in a line plot. Each model is displayed as a line in a plot of Q2(cum) versus component. A high Q2 value for the final model is desired. The Q2 values are identical to the Q2 values shown in the Summary of Fit plot.
RMSECV plot
The RMSECV plot compares the model performance of the selected models by plotting the average prediction error estimated from the cross validation (RMSECV). One RMSECV value is displayed for each model, based on the number of components fitted for the individual models. Thus, the model complexity (A) may differ for the different models displayed. The lower the RMSECV value obtained, the better the model performance.

<image>

4. Predict tab

Import and Predict
The Import and Predict combines importing data and specifying them as predictionset. In regular SIMCA this correspond to clicking Import Dataset on the File tab followed by specifying predictionset As Dataset on the Predict tab.

RMSEP plot
The RMSEP plot compares the model performance of the selected models by plotting the average prediction error estimated from the predictionset (RMSEP). One RMSEP value is displayed for each model, based on the number of components fitted for the individual models.