

SIMCA

Multivariate Data Analysis Solution

Spectroscopy skin for SIMCA 15 Quick guide

9 June 2020

Introduction

This guide describes the interface and functionality unique to the Spectroscopy skin, complementing the SIMCA 15 User Guide and Help.

The Spectroscopy skin was developed to offer a simplified and customized interface designed for a specific application area. Compared to the standard 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 standard SIMCA.

Access and activate

The Spectroscopy skin is installed as part of the standard SIMCA 15 installation. If you wish to use them and they are not shown as options under **File | New**, enable them in **File | Options, SIMCA options, Skins** section. Set **Yes** on the skins you wish to enable.

The skin is automatically activated when a spectroscopy project is created using **File | New | Spectroscopy project**. The skin can also be activated for an existing project from the View tab. Select Spectroscopy from the Skins group. It is recommended to switch on the Spectroscopy skin before import of data but it is possible to change skins at any time and switch back and forth between the Default and Spectroscopy skin.

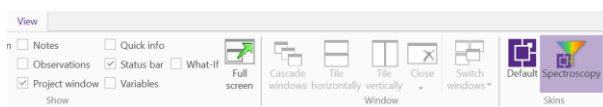


Figure 1: Activate the skin in the Skins group on the View tab.

Settings for the spectroscopy skin

Upon activation of the skin the appearance of SIMCA changes as the default ribbon structure is changed to

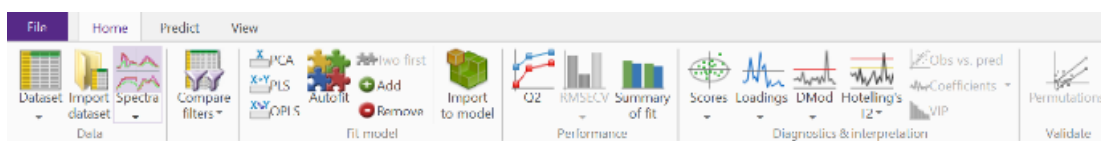


Figure 2: Spectroscopy skin Home tab

the Spectroscopy skin layout. In the tabs Home, Predict and View, skin specific plots and functionality are located. Some functions are the same as in the default SIMCA layout while others have different defaults or even are unique for the skin.

In addition to the user interface there are other adaptations not immediately visible to the eye:

- By default X-variables are centered and not scaled as opposed to the default SIMCA setting center and Unit variance scaling. Centering only is a suitable base for most spectral data. Scaling and centering can be changed in the Workset for each model separately or saved as a project default.
- In the Spectroscopy skin loadings and coefficients are by default plotted on a numerical spectral axis.

Plot, analyze and compare spectral filters

The **Spectra** function in the Data group on the Home tab gives a dialog where up to four different datasets can be selected for plotting. Selected datasets will be displayed in individual spectra plots. By default the spectra are colored according to the first Y-variable.

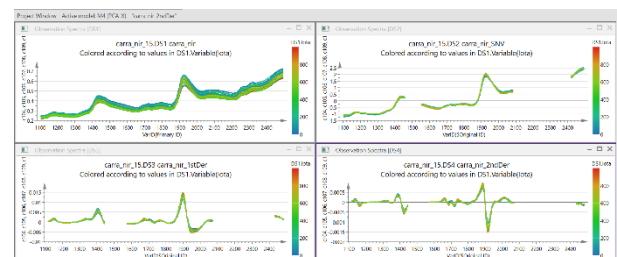


Figure 3: Representation of raw and filtered spectra.

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, OPLS or 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. One model on raw data plus three models based on different filters.

The wizard includes the following steps:

Select spectral range

Parts of the spectra not to be used in the model are graphically excluded by marking in the plot. The list can also be used to exclude regions. The same spectral region(s) will be used for all filters.

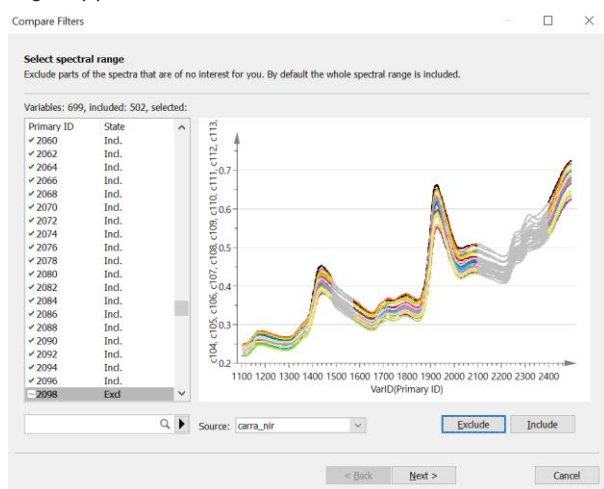


Figure 4: Select spectral range page

Select spectra

Spectra which should not be included in filtering and modelling are graphically selected by clicking a spectra or mark them in a list. Click Exclude to omit them from filtering and further analysis.

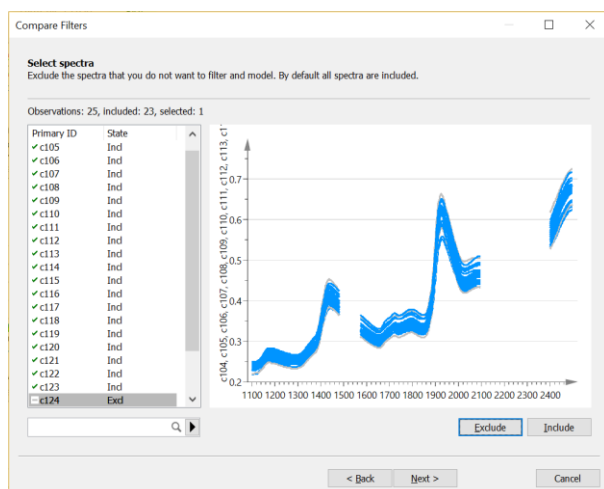


Figure 5: Select spectra page

Specify filters

On the Specify filters page you can assign up to three filters, or sets of chained filters, to apply to the dataset. The preset filters are 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 an OPLS or PLS model, or leave empty to fit PCA models.

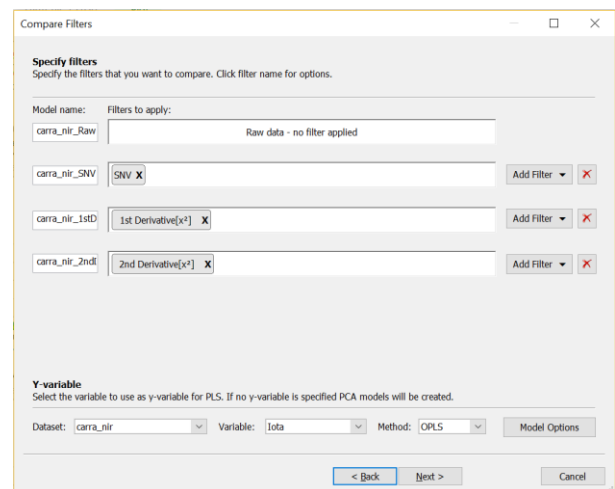


Figure 6: Specify filter page

Filtered spectra

The last page displays spectra plots for the new filtered datasets as well as for the raw data. Upon clicking Finish the filtered datasets are created, one workset is created per filter and the model for each is calculated.

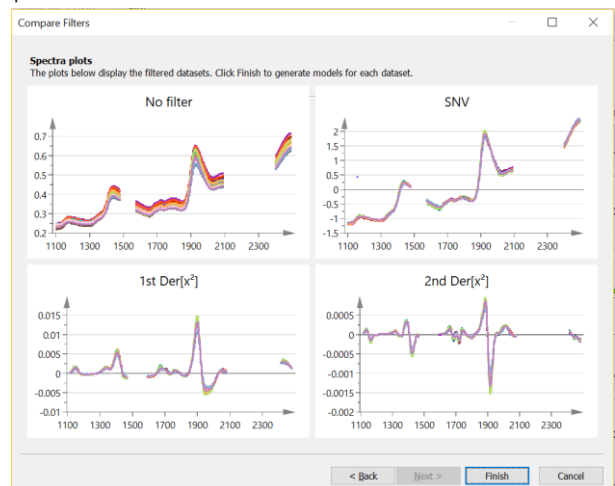


Figure 7: Spectra plots page

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 $Q^2(\text{cum})$ versus component. A high Q^2 value for the final model is desired. The Q^2 values are identical to the Q^2 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

The **Import and predict** feature located on the Predict tab combines importing data and specifying them as prediction set. This feature correspond to clicking Import dataset on the Home tab followed by specifying prediction set As dataset on the Predict tab and speeds up the prediction process compared to regular SIMCA.

RMSEP plot

Another skin specific feature on the Predict tab is the **RMSEP** plot. This plot is similar to the RMSECV plot and compares the model performance of a set of selected models by plotting the average prediction error estimated from the prediction set (RMSEP). One RMSEP value is displayed for each model, based on the number of components fitted for the individual models.