

SIMCA

Multivariate Data Analysis Solution

Readme SIMCA 17.0.1

May 18 2021

Thank you for your interest in SIMCA® 17.

SIMCA® 17.0.1 is a minor release that introduces a new licensing system. This release also addresses some bugs that were found in SIMCA 17.

SIMCA is a versatile multivariate data analysis software, praised for its accessibility and ease of use and this release has a focus on making analysis of spectroscopy data easier, faster and more intuitive. This involves context-based ribbons, extended library of spectral preprocessing and a calibration wizard that make creating multivariate calibration models easier. All users of SIMCA will also benefit from the improvements in performance and plot responsiveness that has been made in this version.

Changes in SIMCA 17.0.1

- Changed third party licensing system
- Addressed stability issues found in SIMCA 17
- Fixed issues with downsizing at import

New features and changes in SIMCA 17:

- Integrated spectroscopy project
 - o Context based ribbons with spectra focus
 - o User defined Spectral ID used in plots
 - New spectra visualization
 - o Full range of spectral preprocessing options
 - Preprocessing wizard for single or chained filters
 - Calibration wizard for 1 Y prediction models
- Batch Data and Database Import
 - o Possibility to control Batch alignment
 - o BCC from dataset
 - o SimAPI:s available at installation
 - o Database interface improvements including node hierarchies
- Plot Interactivity
 - o Color by Rank new option for better vector coloring
 - o Reverse and log axis control in properties pane
 - o Color BCC by Batch condition vectors
- Other Improvements
 - o Multiple file import for CSV, TXT and DIF files
 - o Import configuration template
 - o CPython updated to version 3.7.9
 - NumPy, SciPy, and Pandas installed by default
 - o Possible to change name of dataset
 - o Dataset merge keep un-matched content in new dataset
 - New bias vectors (MBE)
 - Possibility to Save as version 16
 - Multiple performance related improvements

Information about this and other functionality in SIMCA is available at our website.



Installation

Administrator permissions are necessary to install SIMCA 17.0.1.

The Omics skin is included in the installation file. For information on how to enable the skin and more details on general installation and activation see "SIMCA 17 Installation instructions.pdf"

Licensing and Activation

To run the full version of SIMCA you need to have a valid license that has been activated. Due to the change of licensing system, a previous SIMCA 17 license will not work.

For single installations an activation key was delivered in your delivery e-mail.

If you have been instructed to connect to a license server, you may need information from your local IT department about which Host/IP to use.

Trial Limitations

SIMCA can be run as a trial for 30 days.

Virtual Machine

To run SIMCA on virtual machine, your license must specifically allow this. Contact your sales representative for more information.

Minimum System Requirements

- CPU: Intel Core i5-4460, 4:th generation, (3.20GHz) or AMD FX-6300
- RAM: 4 GB
- Disk space: 700 MB available disk space
- OS: Microsoft Windows 8.1 or 10
- Video card: Nvidia GeForce GTX 460, ATI Radeon HD 4850, or Intel HD Graphics 4400

Support

The latest information and support questions can be found in <u>Sartorius Data Analytics</u> Knowledge base.

For Technical support, contact $\underline{umetrics_support@sartorius.com}$.