

Product Specification for SIMCA-P+ 12



For many years SIMCA-P+ has been the standard tool for scientists, researchers, product developers, biochemists, and others who have large datasets to cope with. With a few clicks, the data transforms into information, which makes it possible to make quick and confident decisions.

New features in
SIMCA-P+ 12.0
marked in red

General

- Analysis Advisor to interpret plots and guide you through the next step
- Flexible report generator in html, customizable as user templates
- Plug-in for display of chemical structures from SMILES codes
- Audit trail 21 CFR Part 11 compliant

Import / Export

Supported file formats

- EXCEL 5 to **EXCEL 2007**, **MATLAB 5**, LOTUS (wk1 format), DIF and TEXT, UNSCRAMBLER ASCII, NSAS (NIR Systems) v 2.0, MVA CDF v 2.0, Brimrose and Galactic (*.spc) v 2.0, **JCAMP-DX v 6.0**, Andi Net-CDF (Chromatography)
- SIMCA and MODDE, all Windows versions
- Export models and datasets from SIMCA-P+
- Direct import from databases using ODBC and MS Query
- Image analysis import
- Possibility for importing any formatted file using "plug-in" DLL
- **Improved support for CSV-files**

Import Wizard functionality

- View SIMCA-P+ datasets
- Transpose matrices
- Change variable and observation names
- Edit the data with cut, copy, paste and insert
- Qualitative variable imported as is, expansion into dummy variable automatic in computation
- Display a map of missing values
- Up to 100 secondary IDs for both variables and observations

- Specify X/Y defines the default workset
- Zoom
- Flexible merging and appending of files
- Downsizing number of observations during or **before import**
- Workset wizard opens and guides you through fitting the model
- Possibility to add secondary IDs to the dataset
- **Import by pasting entire dataset**
- **Improved date/time handling**
- **Class ID specification**
- **Local centering of dataset**

Data Viewing, Preprocessing

Data viewing

- Display missing values map, trimming overview map
- Plots can be made directly from dataset or any open spreadsheet (list) by marking columns or rows.
- Non contiguous columns can be marked
- Plotting spectra directly from dataset, workset, plot or list
- Fast statistics in Quick Info
- Listing of the number of samples, variables, missing values, minimum, maximum, mean, median, standard deviation, skewness and kurtosis for each selected row or column
- Frequency histogram, Spectrum/Time series, Auto- or cross-correlation, Power spectrum
- Trimming/Winsorizing of selected variables or the whole dataset
- Quick Info connected to all lists and plots
- Trimming can be done on a section (time period) for a variable

Data Preprocessing

- Orthogonal Signal Correction (OSC)
- Multiplicative Signal Correction (MSC)
- Standard Normal Variate (SNV)
- Wavelet denoising of spectral data
- Wavelet transform and compression, row wise or column wise
- Decimation
- **First, second and third derivatives**
- **EWMA**
- **Savitsky-Golay**
- Chaining of filters
- Filter summary
- Denoising of secondary datasets
- **Spectral filter Plug-In**

Generate new variables

- Variables as functions of existing ones or as functions of result variables
- Operators +, -, ^, *, /
- Functions available: Log10, Ln, Exp, Lag, First difference, Second difference, Seasonal difference, Average, SD, Sum, Binning
- Results from existing models: DModX, T, TSquare, U, TPS, etc
- Possibility to establish user specific functions

Workset

- Workset spreadsheet with quick info and Trimming/Winsorizing variables
- Default workset can be changed and saved as new default
- **User defined default scaling**
- Find feature
- Workset statistics
- **Selecting model type in workset dialog**

Variables

- Transforms: Linear, Log, Neglog, Logit, Exponential, Power
- Quick info in the transformation page
- Exclude variables and specify X and Y block
- Different X and Y block for different classes and **blocks**
- Lag time series data
- Square, Cross, and Cubic terms
- Variable and Block scaling
- Flexible scaling from file, secondary IDs or manually entered
- Average and standard deviation displayed in scale page
- **Qualitative Y variables supported**

Observations

- Exclude/Include observations
- Group observations by classes
- Ability to generate classes from variables or scores values
- **User defined class names**

Analysis

Models

- Unlimited number of models in a project.
- All methods work with missing data.
- PCA, PCA of classes
- PLS, PLS of classes
- PLS discriminant analysis
- PCA and PLS time series
- **OPLS/O2PLS, OPLS/O2PLS of classes**
- **OPLS/O2PLS discriminant analysis**
- **Cluster analysis with PLS-Trees**
- Hierarchical models
- **Automatic generation of Hierarchical Models after assigning variables to blocks**
- Automatic fit of class models

Review the model with plot and lists

- Summary of the model fit Q2, R2
- Scores and loadings
- Diagnostics (Residuals, DModX, Observed vs. Predicted)
- Calibration diagnostics: RMSEE and RMSEP for predictions
- Coefficients and Variable influence
- Contribution plots displayed by clicking on observations in plots
- Group contribution
- **Resolution of coefficients and contributions of Hierarchical Models**
- Options at property page
- Confidence intervals from jack-knifing
- Measure of leverage and Observation Risk
- Observation profiles generated from any observation plot
- Reconstructed observation profile
- Scaling plots by variance explained
- Rotated coefficients
- **Y-related profiles for OPLS/O2PLS**
- **Change model title from Project Window**

Model validation

- Cross validation
- Permutation test
- Possibility to specify how cross validation groups should be set up
- **CV-ANOVA table**

Prediction

- Import of prediction set from file
- Classification list using selected class models
- Option to trim prediction set as workset
- Prediction results presented as lists, plots, and diagnostics
- Prediction set automatically preprocessed as calibration set
- Exponentially weighted

adaptive predictions

- Color coding for list of PLS-DA predictions
- What If feature to simulate different scenarios
- **Improved misclassification table for PLS-DA and SIMCA classification**
- Import center values for prediction set
- **Find feature when creating prediction set**

Plots and Lists

- Coloring by values of variables or scores
- Connected plots and lists
- Easy to use interface for customizing plots
- Creating plots from lists and lists from plots
- Plots and lists of scores, loadings and coefficients from every cross validation round
- Auto- and cross correlation, power spectrum, wavelet coefficients and EWMA transformations
- Wavelet structure and power spectrum plots
- Interactive tool to remove or group observations from observation plots
- Interactive tool to remove model terms directly from loading, coefficient and VIP plots
- Plot types: 2D and 3D Scatter, Line, Column, Histogram, Time Series, Contour, Response Surfaces, Normal Probability, **Dendrogram**
- Control Charts both of scores and individual variables: Shewhart, EWMA, CuSum, EWMA/Shewhart
- Summary of preprocessed models
- Step response plot
- Use any observation or variable ID as labels on points or axes
- Property bar to quickly change content in plots, e.g. component, variable, model
- Find feature supporting chained search criteria
- Trend plot of a variable by double clicking it in a plot.
- Fast button for visualization

plots

- **Improved flexibility in saving of plot settings**
- **Coloring improvements**
- **Limits can be changed directly in plots**
- **Full screen mode**
- **Improved sorting of column plots**
- **Size by vector in scatter plots**

Multivariate Batch Analysis

- Batch conditions imported with primary dataset at observation level or as a secondary dataset at batch level
- Friendly import interface
- Tabs to switch between observation level and batch level
- Contribution plots in batch level can be resolved regular or **combined** to observation level
- Option to automatically generate observation level models after removal of outliers in batch level

Observation Level

- Batches can have different phases
- Phases can have different variables
- Ability to delete, merge and rename phases
- Conditional delete
- Local centering
- User specified time or maturity
- Different maturity variables for different phases
- Maturity monotonic in a phase
- Piece wise smoother for noisy maturity
- Automatic fitting of all phases
- Cross validation rule for batches
- Exclude tool removes entire batch
- Items selection in properties page by batch and phase
- Plots of aligned vs unaligned
- Plots of all vectors aligned
- Plots of smoothed vs observed maturity
- Batch control charts

- Alignments are done "on the fly" on any specified model
- Out of control summary plot
- Linear time warping
- Import scaling from file for all phases.
- Configuration of time or maturity

Batch Level

- Flexible creation of batch level projects
- Automatic partial models
- Automatic merging of batch conditions
- OSC will apply automatically to prediction set
- Batch VIP plot available for all types of models
- Automatic creation of hierarchical batch level models
- Source of variation plot
- **Secondary IDs brought to batch level project**

Additional Features

- Sort of datasets, lists and column plots
- Automation object, SIMCA-P+ can be started from external programs and data, and results exchanged with SIMCA-P+
- Unlimited number of observations or variables
- Option to have several projects opened simultaneously with tabs to switch in between
- Possibility to select personal pictures to display on progress bar
- Command to save reduced project files (.usp)
- Only affected models are deleted after changes in dataset
- Favorites including dataset and project
- **Export and Import of Favorites**

Minimum System Recommendations

Pentium II 300 MHz, 50 MB hard disk space, 128 MB RAM, graphic card 8 MB RAM, screen resolution 800x600, high-colour (16 bits), Windows 2000, Windows XP and Windows Vista.



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