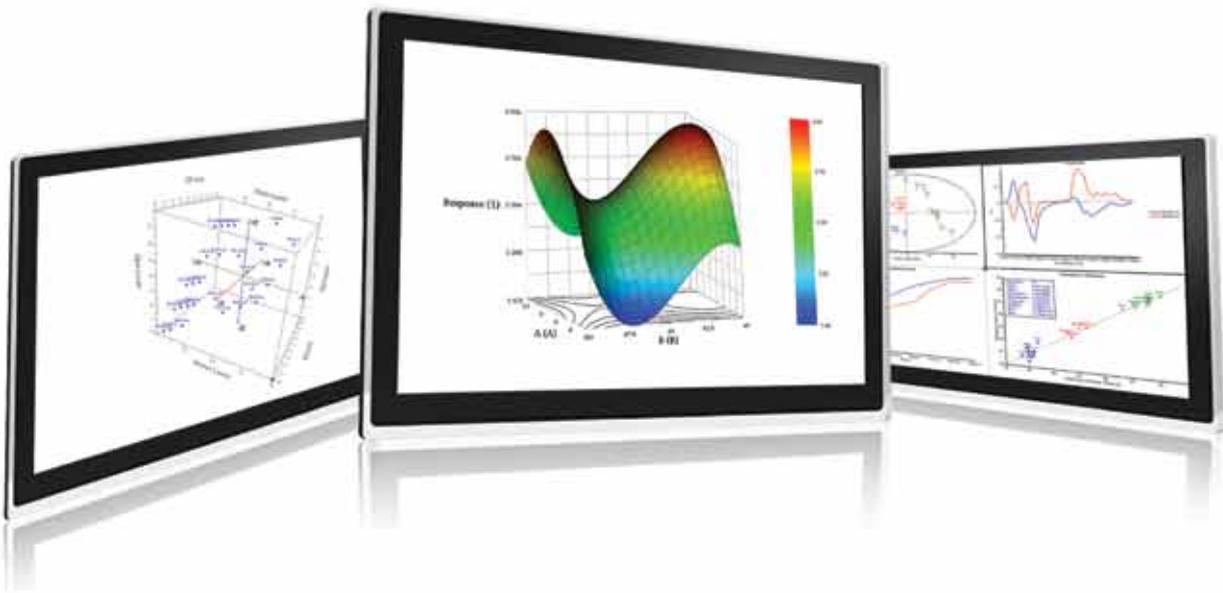




The Unscrambler[®]X

Version 10.3



All-in-one Multivariate Data Analysis and Design of Experiments software

- Powerful multivariate analysis methods and design of experiments >
- Easy data importing options with intuitive workflows and interface >
- Outstanding graphics, plots and interactive data visualization tools >

“Cutting through complex data sets to underlying structures... is simplicity itself”

**scientific
computing world**

“This intelligent engine borders upon data mining, as it cuts through prediction and classification problems”

**Scientific
Computing**

Bring data to life

“The Unscrambler is much more intuitive and has all the features I need plus more advanced methods than generalist statistical software”

Søren Bech, Head of Research, Bang & Olufsen

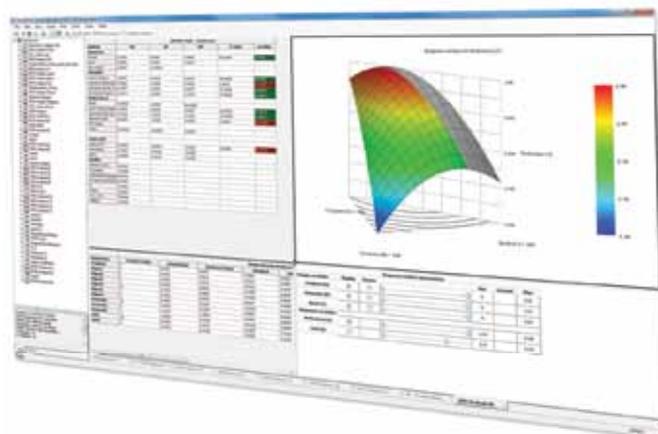
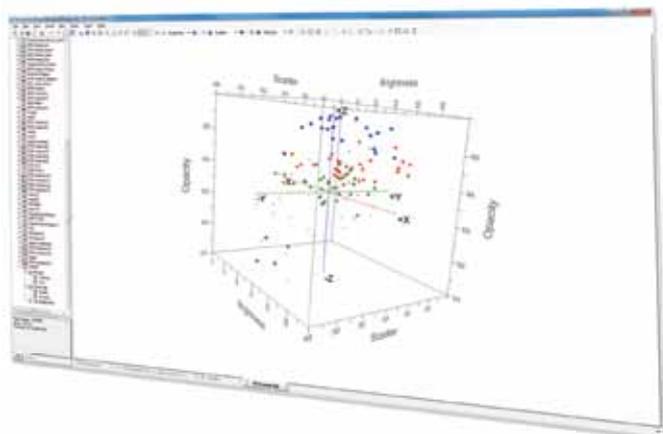


Software for every industry

For almost 30 years, The Unscrambler® has enabled organizations across many industries and research fields to improve product development, process understanding and quality control through deeper data insights.

- Pharmaceuticals
- Chemicals/Petrochem
- Agriculture
- Food & Beverage
- Pulp & Paper
- Mining & Metals
- Oil & Gas
- Manufacturing
- Research & Academia
- Energy/Renewables
- Automotive
- Medical Devices
- Electronics
- Engineering
- Retail
- Semi-conductors
- Marketing
- Aerospace





- Multivariate data analysis is a highly visual approach that helps you identify and understand patterns in large or complex data sets. Easily accessible raw data plots are a very useful tool in the analysis.
- In the 3D Scatter Plot above, data from paper manufacturing is shown, where each of the samples can be seen in relationship to its level of scatter, opacity and brightness. This plot can be rotated to see sample groups from different perspectives and zoomed in on individual data points.
- The Unscrambler® X is the only major multivariate data analysis software that includes a seamlessly integrated Design of Experiments (DoE) module, giving you a powerful all-in-one tool for your data analysis needs.
- Multivariate analysis and Design of Experiments often go hand in hand. The Unscrambler® X combines both of these powerful tools so you can use multivariate models to analyze experiments that are not well suited for classical analysis (i.e. ANOVA).

Deeper data insights, faster & easier than ever

When CAMO software was founded in 1984, we were pioneers and leaders in multivariate data analysis. Almost 30 years later, The Unscrambler® X continues to set the standard in chemometrics and multivariate data analysis software with over 25,000 data analysts, researchers, engineers and scientists across a wide range of industries and research fields using the program.

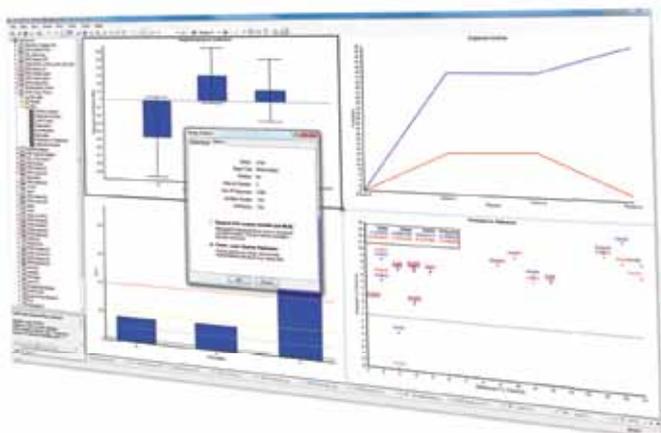
We believe that while your data might be complex, your software shouldn't be. That's why we focus on making The Unscrambler® X easy to use. An intuitive user interface, tutorials within the software and project-based workflows make it easy to find the data, plots and results you need quickly.

And as data sets have become even more complex The Unscrambler® X has also evolved, with improved handling of big data and advanced multivariate analysis tools to cut through even the most challenging data for faster, easier results.

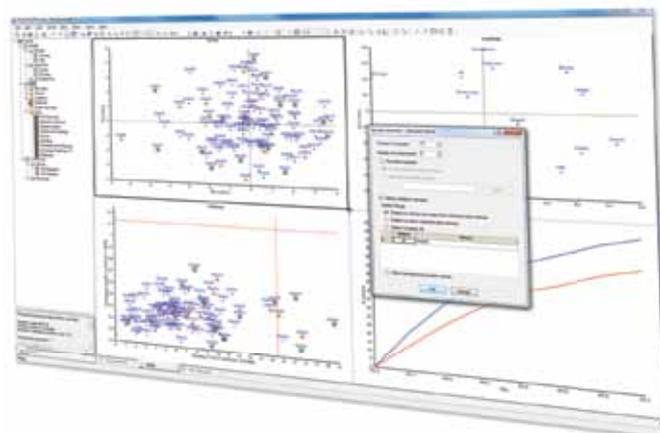
All-in-one multivariate analysis & design of experiments

The latest version of The Unscrambler® X builds on its tradition of powerful multivariate analytical methods and ease of use, adding even more integration options, enhanced ability to handle process data, improved Design of Experiments module and useful features for creating spectroscopic calibrations.

- Multivariate regression and prediction methods
- Multivariate classification methods
- Exploratory data analysis tools such as PCA
- Extensive data pre-processing tools for spectra
- Classical statistics and statistical tests
- Integrated Design of Experiments module
- Easy data importing in wide range of formats
- Intuitive and user-friendly



- The plot above shows Partial Least Squares (PLS) regression analysis of designed data. PLS analysis is a useful alternative to classical DoE (ANOVA) when constraints or missing data give a non-orthogonal design that cannot or should not be analyzed using ANOVA.
- From the dialog box, users can choose classical ANOVA or PLS analysis depending on the orthogonality of the design and correlation between responses. Statistics are shown in the dialog box to help guide the choice of analysis.



- The figure above shows a scores plot with PCA overview using Kennard-Stone sample selection, where the points marked in green are calibration samples and points marked in orange are validation samples. Kennard-Stone sample selection is used for selecting an evenly separated set of observations for robust calibration. This is useful if the data are huge or poorly distributed.

Highlights in version 10.3

Better handling of process data

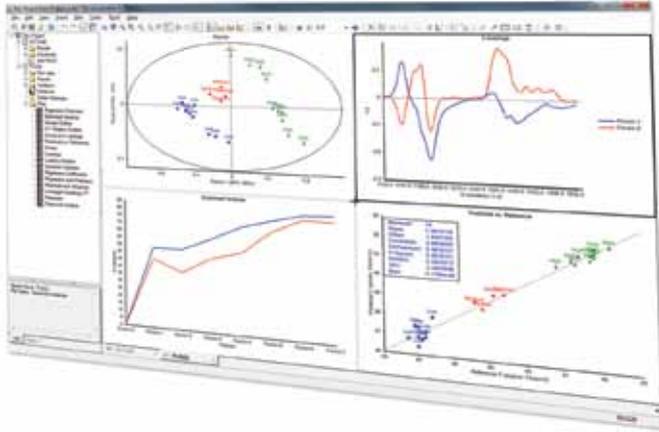
- Option to define units and tags for input variables to be saved with models
- Ability to set alarm and warning limits for calibration models for use in run-time applications
- Improved integration options through OSISOFT PI* and OPC DA* (*Not included as standard part of The Unscrambler® X)
- Hierarchical Modeling*, Instrument Diagnostics* and more (*Not included as standard part of The Unscrambler® X)

Improved Design of Experiments module

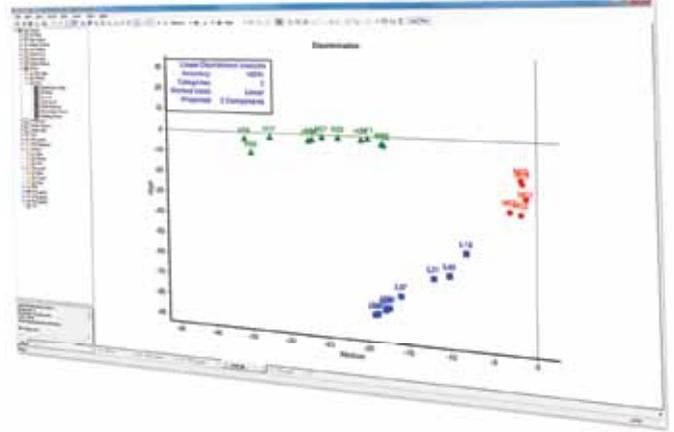
- Enhanced D-Optimal Designs augmented with space filling points for more robust designs
- Better handling of non-simplex mixture and process/mixture designs
- DoE PLS for flexible analysis of non-standard or modified designs
- New response surface plots include control panel sliders for greatly improved interactivity and graphical optimization

Improved calibration and validation sample selection

- Double Kennard-Stone sample selection for selecting representative samples for calibration and validation
- Improved features for creating sample ranges for NIR or other spectroscopic calibrations
- Enhanced sample labelling for easier interpretation
- New outlier detection tools and plots



- The image above shows a Partial Least Squares (PLS) Regression analysis of petrochemical data in a number of different plots including Scores, Loadings, Explained Variance and Predicted vs Reference values. The samples are clearly divided into their octane levels from low (blue) to medium (red) and high (green).
- PLS is a powerful regression method which finds the best possible linear combination of indirect variables for predicting the desired outcome e.g. product quality or yield. The Unscrambler® X allows you to see several different plots on the same screen, giving you a complete picture of your data from different perspectives for easier interpretation and analysis.



- The image above shows a plot of petrochemical data analyzed with Linear Discriminant Analysis (LDA) to classify octane levels. As shown, the samples group very clearly according to their octane levels.
- LDA is a powerful classification method which finds the best separation between classes using linear or quadratic discrimination functions. When combined with PCA, LDA can be used on data with any number of correlated variables such as spectra.

Regression and Prediction methods

Develop models from existing data and predict the value of new samples with the powerful regression analysis tools in The Unscrambler® X. These models can also be used for monitoring processes on-line, at-line or in-line.

The Unscrambler® X includes:

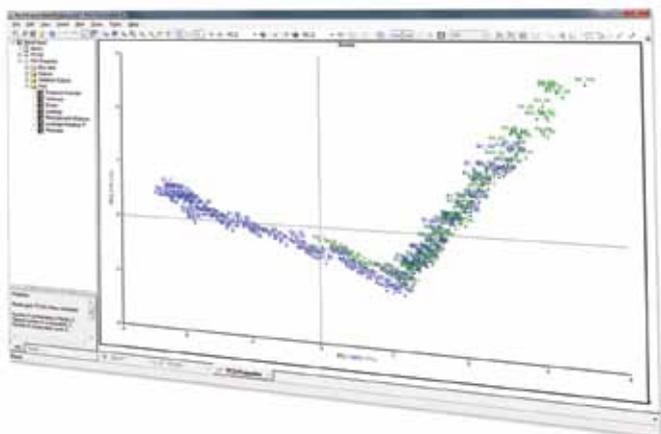
- Multiple Linear Regression (MLR)
- Principal Component Regression (PCR)
- Partial Least Squares Regression (PLSR)
- L-shaped Partial Least Squares Regression (L-PLSR)
- Support Vector Machine Regression (SVM-R)

Multivariate Classification methods

Predict which category a sample belongs to with advanced classification methods in The Unscrambler® X. Classification is the separation, or sorting, of a group of objects into one or more classes based on distinctive features in the objects.

The Unscrambler® X includes:

- Linear Discriminant Analysis (LDA)
- Support Vector Machine Classification (SVM-C)
- Partial Least Squares Discriminant Analysis (PLS-DA)
- Soft Independent Modeling of Class Analogy (SIMCA)



- The Unscrambler® X includes a number of advanced data mining methods including Principal Component Analysis (PCA), which is a powerful tool to see, for example, how a process evolves by measuring the trajectory of samples. PCA will also help identify the variables with the most influence on a model.
- In the image above, PCA was used to model batch process data for a pharmaceutical product, with the calibration sample in blue showing how the batch evolves. A subsequent batch was projected onto the model (green), with the data showing the batch started later but closely following the calibration model's trajectory, indicating it is in the desired operating range.



- Pre-processing data is important when analyzing spectral data or building robust process models. The Unscrambler® X includes all of the most common pre-processing options as well as more advanced tools unique to the software, such as Extended Multiplicative Scatter Correction (EMSC), which allows you to discard interference in spectra but retain interesting information relating to the chemical constituents.
- The Unscrambler® X also has the option to preview spectra with treatments applied, so you can see the effect of the pre-processing before doing it to real data, as shown in the dialogue box above.

Exploratory data analysis tools

Cut through complex data to find patterns easily using the powerful exploratory data analysis tools in The Unscrambler® X. Exploratory data analysis, or data mining, finds hidden structures in large data sets. Descriptive statistics, principal component analysis and clustering are often used in initial explorations.

The Unscrambler® X includes:

- Principal Component Analysis (PCA)
- Cluster Analysis
- Multivariate Curve Resolution (MCR)
- Descriptive statistics and classical statistics including T-tests, F-tests

Advanced pre-treatment options

Ensuring data is clean and in shape to be analyzed is essential, especially with instrument data, such as spectra. The Unscrambler® X offers the most comprehensive and advanced range of data pre-treatment tools, making it the ideal software for spectroscopic applications.

The Unscrambler® X includes:

- Smoothing
- Normalization
- Derivatives
- Baseline correction
- Standard Normal Variate (SNV)
- Multiplicative Scatter Correction (MSC) and Extended MSC
- Orthogonal Signal Correction (OSC)

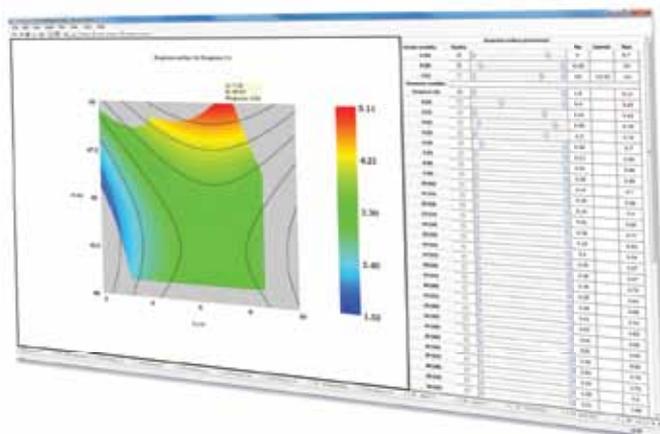
“ Using The Unscrambler, we were able to resolve a product quality problem which has saved us \$1M per year. It also gave us better process understanding which we have used to optimize other manufacturing processes ”

Siri Sølberg, Senior Process Engineer, Nidar AS





- The enhanced DoE in The Unscrambler® X includes ANOVA and response surface analysis also on constrained (D-Optimal) designs.
- The screen above shows a DoE overview where a corner of the response surface is removed as it is outside of the specified design region. The D-Optimal algorithm ensures the design can still be analyzed using classical ANOVA.



- The latest version of The Unscrambler® X has greatly improved graphics and interactivity. For example, the new response surface plot includes sliders for setting the levels of non-plotted design variables as well as constraints on both design and response variables. This lets you find the parameter settings that give the optimal response, irrespective of the constraints in the design.

Design of Experiments (DoE)

The DoE module in The Unscrambler® X has been improved with enhanced D-Optimal Designs, graphical optimization and DoE PLS for more flexible analysis of non-standard or modified designs.

The Unscrambler® X includes:

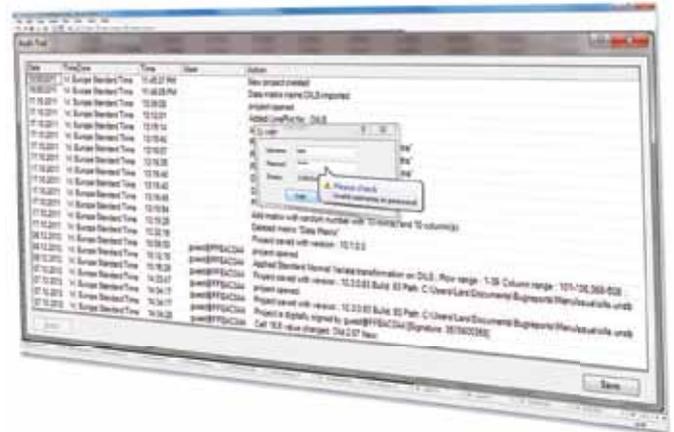
- Complete range of full and fractional factorial designs
- Enhanced optimization designs including Central Composite and Box-Behnken
- Mixture designs including Axial, Simplex Lattice and Simplex Centroid
- ANOVA tables, cube plots, response surfaces, Analysis of Effects, interactive tables

Exceptional data visualization

Understanding complex data is easy with the excellent visualization tools in The Unscrambler® X. Patterns can be clearly shown, and individual samples or groups of data can be visualized from a number of perspectives. Produce publication standard plots which can be annotated as needed.

The Unscrambler® X includes:

- The ability to see several plots on one screen simultaneously for easier interpretation
- The option to rotate certain plots to see data from different angles
- Annotate and add comments or lines to plots as required



- The Unscrambler® X has a wide range of data import options for standard formats such as Excel and ASCII as well as various scientific instrument formats.
- The software has a range of useful data import preview options, as shown above. For example auto-selection and interpolation enables similar spectra collected on different wavelengths (instruments) to be matched, and displays the spectral files in your folder with details on wavelength regions, size of spectra, step size etc.

- When The Unscrambler® X is installed in compliance mode, the user is required to input their Windows credentials to log on.
- The audit trail will show who has logged on and which changes they have made.

Easy data importing

In many statistical programs, getting data into software in a format that is usable can be the first hurdle, but it is easy in The Unscrambler® X. The software accepts data from a wide range of scientific instruments, ASCII and Excel, making importing easy.

The Unscrambler® X includes:

- Drag and drop data directly from Excel
- Preview data and see preview plots to ensure it looks as expected
- Works with most leading spectrometer data formats
- Accepts OS/soft PI* and OPC DA* (*Not included as standard part of The Unscrambler® X)

Data security

If you are working in a regulated industry, you'll understand the importance of data security. The Unscrambler® X has greatly improved security options to help you meet your compliance needs. It is also helpful if you want to have models developed centrally then distributed to analytical centers.

The Unscrambler® X includes:

- Compliance mode
- Digital signatures
- Audit trail
- Meets requirements of 21 CFR Part 11 (Electronic Records)

Technical Specification Overview

Exploratory Data Analysis

Descriptive Statistics

- > Mean/Std Dev/Quartiles/ Cross Correlations/Scatter Effects

Statistical Tests

- > Normality Test/t-Tests/F-Tests/Mardia's Multivariate Test

Cluster Analysis

- > K-Means
- > Hierarchical Cluster Analysis (HCA) with many distance measures and cluster methods

Principal Component Analysis (PCA)

- > Choice of using NIPALS or SVD algorithms
- > Rotation methods including Varimax, Equimax, Quartimax and Parsimax

Multivariate Curve Resolution (MCR)

- > Resolve time evolving data such as chemical reaction or chromatographic data into pure constituent profiles and pure spectra

Regression and Classification

Regression Methods

- > Multiple Linear Regression (MLR)/Principal Component Regression (PCR) and Partial Least Squares Regression (PLSR) + SVR
- > Choice of algorithms, NIPALS and SVD for PCR and NIPALS, Kernel Methods and Orthogonal Scores for PLSR
- > L-PLS, incorporating three data tables for greater insights into data structure

Advanced Classification Methods

- > Projection using PCA and PLS models
- > Soft Independent Modelling of Class Analogy (SIMCA)
- > Linear Discriminant Analysis (LDA)
- > Support Vector Machines (SVM)
- > Classification with numerous kernel types

Data Pretreatments

Spectral Functions

- > Smoothing
- > Derivatives: Moving Average/ Norris Gap/ Savitsky-Golay
- > Baseline Correction
- > Normalization

Scatter Correction and Advanced Functions

- > Multiplicative and Extended Multiplicative Scatter Correction (MSC/EMSC)
- > Standard Normal Variate (SNV)
- > Orthogonal Signal Correction (OSC)
- > Deresolve
- > Detrending

General Transforms

- > Choice of Centre and Scale options
- > Spectroscopic: Reflectance / Transmission/ Kubelka-Munck / Basic ATR correction **NEW**
- > Interaction & Squares and Individual Variable Weighting
- > Compute General
- > Fill Missing Values
- > Correlation Optimization Warping (COW)

Design Of Experiments

Improved Design Wizard

- > Interactive design setup with full descriptions and Beginner/ Expert modes
- > Complete range of full and fractional factorial designs
- > Enhanced optimization designs including Central Composite (CCD), Inscribed (ICC), Face Centred (FCC) and Box-Behnken (BB) designs.
- > Enhanced mixture designs including Axial, Simplex Lattice and Simplex Centroid designs.
- > A new D-optimal design module with option to augment design with space-filling points **NEW**
- > A completely new response surface plotting module with high resolution, fast graphics rendering and improved plotting controls for graphical optimization **NEW**

Choice of Analysis Algorithms

- > Intuitive analysis dialog helps select the best method **NEW**
- > Classical DoE handles most orthogonal and weakly constrained designs
- > Scheffé's polynomial model for mixture experiments
- > DoE PLS can be used for any design including mixture/process design **NEW**

Comprehensive Analysis Overview

- > ANOVA tables and other tabular results
- > Cube Plots
- > Response Surfaces
- > Analysis of Effects
- > Interactive Tables

Process Data

- > New Alarms tab in analysis dialogs of PCA, MLR, PCR and PLSR and right-click option for setting alarm limits in the project navigator (these limits are applied for online prediction using some of our prediction engines) **NEW**
- > New dialog for assigning Scalar/Vector tags as well as units. This information is used for collecting data from various sources during online monitoring of processes **NEW**
- > General enhancements and bug fixes **NEW**

General Improvements

Project Navigator

- > Save data and analyses into projects
- > Send complete projects to colleagues for further analysis/investigation
- > Save and export models within a project to other applications

Interactive Data Import

- > Improved ASCII and Excel data import: View entire worksheets and interactively select data ranges before import simply using a mouse
- > Preview data before importing from 3rd Party applications
- > Wide range of spectral data imports

- including OPUS (Bruker), OMNIC (Thermo), NSAS (Foss NIRSystems), Indico (ASD), Brimrose, Guided Wave, Zeiss, Varian, Perten, JCAMP-DX, GRAMS, Matlab, previous Unscrambler versions, Perkin Elmer and Net-CDF files
- > Import from Databases and OPC servers (plug-ins)

Improved Security

- > Windows domain authentication
- > Revised 21 CFR Part 11 compliance including time stamping and time zone logging

New and Improved Algorithms and Methods

- > Basic ATR correction of absorbance transformed spectra **NEW**
- > Introduced Double Kennard-Stone sample selection for PLSR, PCR and PCA **NEW**

Plotting and Data Visualization

Wide selection of plotting options

- > Line, Bar and Scatter plots
- > 3D and Matrix plots
- > Histograms and Normal Probability plots
- > Multiple Scatter plots for pair wise comparison of multiple rows or columns

Enhanced Plotting Features

- > Colour coding of unlimited categorical variables
- > Easy access to analysis results matrices from the project navigator for plotting
- > Interactive marking of samples or variables from plots for defining data ranges for analysis
- > Add data to existing plots from other sources
- > View Hotelling's T² ellipses at multiple confidence intervals in PCA/ PCR and PLSR scores plots
- > Plot settings in 'Tools – Options – Viewer' can be used to change the default appearance of plots **NEW**
- > New plots and plot layouts for Residuals and Influence plots in PCA, PCR, PLSR and Projection, including F-residuals with confidence limits **NEW**
- > Point labeling using value of any matching variable (Sample Grouping) **NEW**

Additional CAMO Software Products & Services

Unscrambler® X Process Pulse

Real-time process monitoring software that lets you predict, identify and correct deviations in a process before they become problems. Affordable, easy to set up and use.

Analytical Engines

Software integrated directly into analytical or scientific instruments for on-line predictions, classifications or hierarchical models directly from the instrument.

Training

Our experienced trainers can help you use multivariate analysis to get more value from your data. Classroom, online or tailored in-house training courses from beginner to expert levels available.

Enterprise solutions

Customized solutions which can be integrated into automation and control systems to enhance their analytical capabilities. Available for client-server and web-based architectures.

Consultancy and Data Analysis Services

Do you have a lot of data and information but don't have resources in house or time to analyze it? Our consultants offer world-leading data analysis combined with hands-on industry expertise.

Our partners

CAMO Software works with a wide range of instrument and system vendors. For more information please contact your regional CAMO Software office or visit www.camo.com/partners

Find out more >

For more information please contact your regional CAMO office or email sales@camo.com

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