

# Setting Standards in Multivariate Data Analysis & Experimental Design



## The Unscrambler® 9.6

Simple to use



### Highlights

- Exploratory Statistics
- Regression Analysis
- Prediction
- Design of Experiments
- Data Pretreatments
- Classification

The Unscrambler® is the complete multivariate analysis and experimental design software, equipped with powerful methods including Principal Component Analysis (PCA), Multivariate Curve Resolution (MCR), Partial Least Squares Regression (PLS-R), 3-Way PLS Regression, K-Means Clustering and SIMCA Classification.

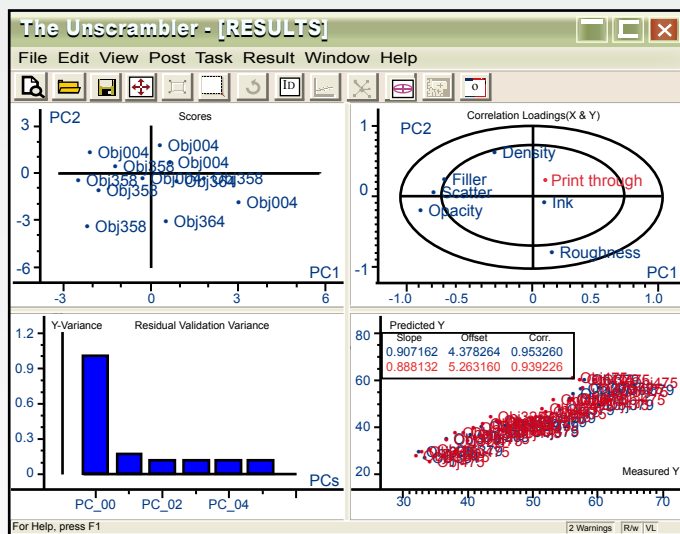
Extensively used across a wide range of research and industrial applications including advanced Chemometrics, Spectroscopy and cutting-edge Sensometrics, this market-leading software yields demand-driven formulations, process optimization, cost-savings and increased ROI in product development, process control, quality control and R&D.

It is used in the Chemical, Pharmaceutical, Food Processing, Pulp and Paper, Consumer Products and Agricultural industries.

### Benefits

An inventive multivariate software that incorporates the latest and most efficient advances in data analysis and interpretation, The Unscrambler®:

- Combines ease-of-use with comprehensive data analysis methods
- Supports various instrument file formats and offers numerous data preprocessing capabilities
- Ensures greater ROI by reducing the number of experiments required
- Generates models that can be used for on-line prediction and classification in CAMO Software's On-Line Unscrambler Predictor (OLUP) & On-Line Unscrambler Classifier (OLUC)
- Generates models that can be used for faster product and process optimization in CAMO Software's Product Optimizer.



### Application Areas

- Spectroscopy
- Chemometrics
- Sensometrics
- Quality Control
- Process Analytical Technology (PAT)
- Product Development

## Analysis Methods

- Descriptive statistics (Mean, Standard Deviation, Box-Plot, skewness, kurtosis, correlation matrix)
- Principal Component Analysis (PCA)
- Multivariate Curve Resolution (MCR)
- Regression (MLR, PCR, PLS-R, 3-way PLS-R)
- Prediction from PCR, PLS-R and 3-way PLSR models
- Clustering (K-Means) New
- Classification (SIMCA, PLS-DA)
- ANOVA and Response Surface ANOVA
- Validation options: Leverage Correction, Cross-Validation (freely choose number of samples per segment), Test Set
- Variable Scaling options: Scaling is free on each variable. Suggested options: Auto-scaling, Constant, Passify
- Interaction and square terms can be included in PCA, MLR, PCR and PLS-R models

## Smart Tools for Analysis

- Automatic detection of significant X-variables in PCR & PLS-R
- Model stability in PCA, PCR and PLS-R
- Automatic outlier detection in PCA, MLR, PCR, PLS-R and Prediction
- Message list of recommendations in MCR modeling
- Interactive analysis:
  - Mark samples and/or variables on plots
  - Recalculate With or Without Marked samples or variables
  - Recalculate With Passified Marked or Unmarked variables
  - Extract Data from Marked or Unmarked
- Automatic Pretreatments in Prediction and Classification
- Interactive help
- Tutorial exercises guiding you through the use of all The Unscrambler® modeling techniques in application examples

## Design of Experiments (DoE)

- Design Wizard: takes you through the stages of building a design
- Fractional and Full Factorial designs
- Plackett-Burman designs
- Central Composite designs
- Box Behnken designs
- Mixture designs (Simplex-Lattice, Axial, Simplex-Centroid)
- D-Optimal designs of mixtures and non-mixtures
- Effects plots of main effects and interaction effects; response surface plots

## Result Viewer

- Over 100 pre-defined plots (Scores, Loadings, Loading weights, Correlation Loadings, Stability Plot, Bi-plot, Leverages, Variances, RMSE, Regression coefficients, Predicted vs. Measured, Residuals, Response Surface....)
- Many plot options: Sample grouping with colors or symbol; Insert text; Remove grid; Display plot as Line/Bars/Accumulated bars...
- Live rotation of 3D plots
- PC navigation tool: navigate along model components in a click

## Data Pretreatments

- Smoothing: Moving Average, Savitzky-Golay, Median filter New, Gaussian filter New
- Normalize: Area, Unit vector, Mean, Maximum, Range, Peak
- Spectroscopic conversions: absorbance/reflectance, reflectance/Kubelka-Munk, wavenumber/nanometers New
- Multiplicative Scatter Correction (MSC) & Extended MSC (EMSC)
- Noise
- Derivatives: Norris Gap, Gap-Segment, Savitzky-Golay
- Baseline offset, Linear baseline correction
- Standard Normal Variate (SNV)
- Mean centering, New standard deviation scaling New
- User-defined Transformations, programmed e.g. in Matlab or C++ & utilized in The Unscrambler® as a DLL

## Spreadsheet Editor

- No size limit
- 2D and 3D tables supported
- Continuous, discrete and mixture variables supported
- Sample and variable names of up to 49 characters
- Raw data plots (Line, 2D scatter, 3D scatter, Normal probability, Histogram, Matrix, Matrix 3D)
- Set Editor: allows to work freely either on the whole table or on a selection of samples and/or variables
- Sort samples / Sort variables
- Transpose
- Mathematical array manipulations
- Fill missing values
- Undo/Redo functionality

## Interactions with Other Software

- Drag'n drop functionality from Excel to The Unscrambler®
- Copy/Paste data or plots to Microsoft Office applications
- Data import of 2D and 3D data tables with over 20 file formats supported: ASCII, spreadsheet software (Excel, Lotus), statistical software (NSAS, Matlab) and instrument software: JCAMP-DX, Tracker (Foss), APC, Grams (Thermo Electron), MVACDF, Indico (Analytical Spectral Devices), CLASS-PA & SpectrOn (Guided-Wave), F3D (Hitachi), BFF3 (Brimrose) New
- User-Defined Import: allows to import any file format using a pre-programmed DLL.
- Data export in various formats (ASCII, Matlab, JCAMP-DX...)
- Model export in various formats (ASCII, NSAS, Vision, Tracker)

## System Requirements

**Processor:** Pentium 100 MHz or higher  
**OS:** Windows 98/ME/2000/XP/2003 or NT 3.51 or higher  
**RAM:** 64 MB minimum; higher is recommended  
**Hard disk space:** 150 MB