



CAMO

The Unscrambler[®]

A Handy Tool for Doing Chemometrics

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Camo Process AS

Topics

- **The Unscrambler[®] by Camo**
 - Many possibilities for Analysing Data
- **Examples**
 - NIR-Spectra
 - Fluorescence Excitation Emission Spectra
- **Life Demonstration**
 - 3-way Data Handling

The Unscrambler[®] Main Features

Exploratory Analysis

- Descriptive statistics
- Principal Component Analysis (PCA)

Multivariate Regression Analysis

- Partial Least Squares regression (PLS)
- Principal Component Regression (PCR)
- Multiple Linear Regression (MLR)
- Prediction

Classification

- Soft Independent Modeling of Class Analogies (SIMCA)
- PLS-Discriminant Analysis

Experimental Design

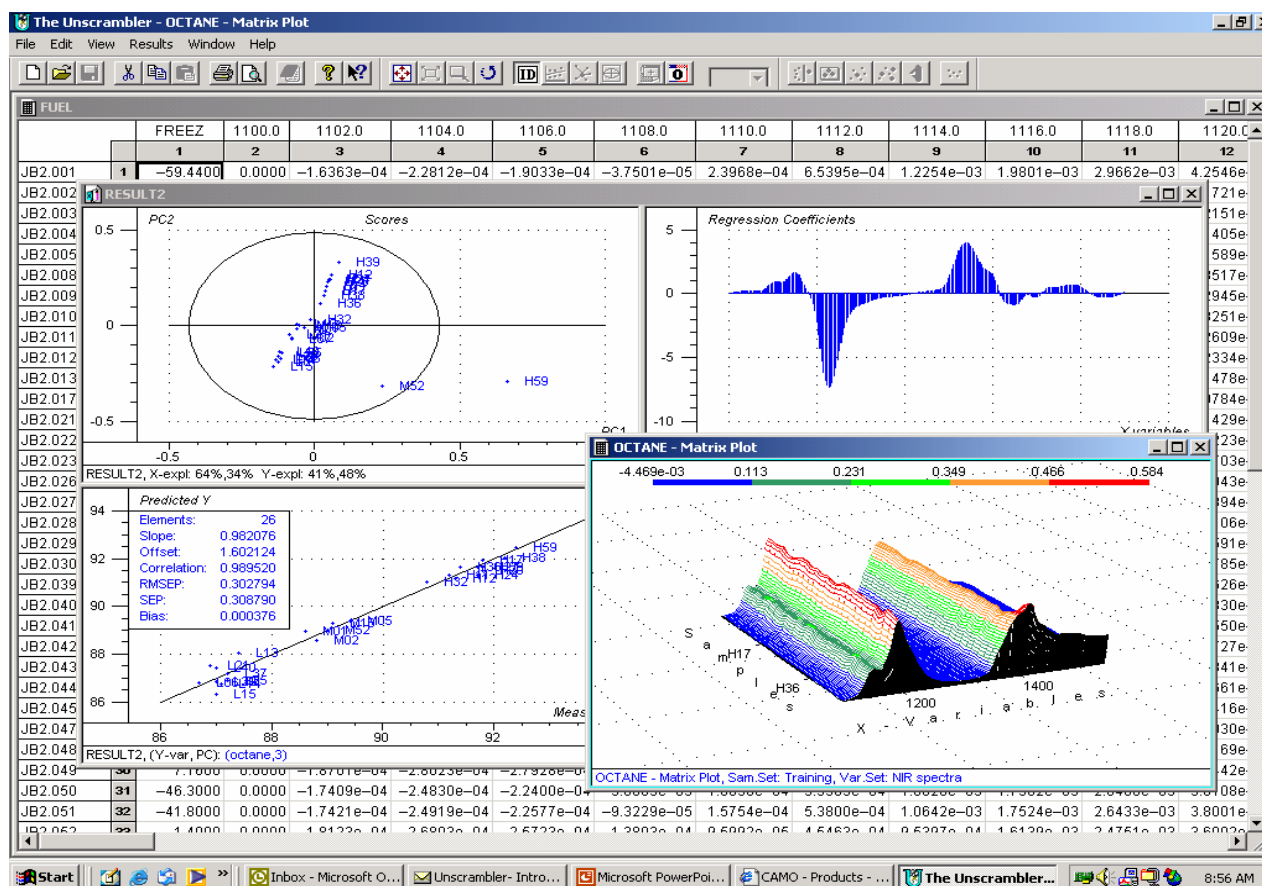
- Fractional and full factorial designs, Plackett-Burmann, Box Behnken, Central Composite, Classical mixture designs, D-optimal designs
- ANOVA, Response Surface ANOVA, PLS-R





The Unscrambler® Also Features...

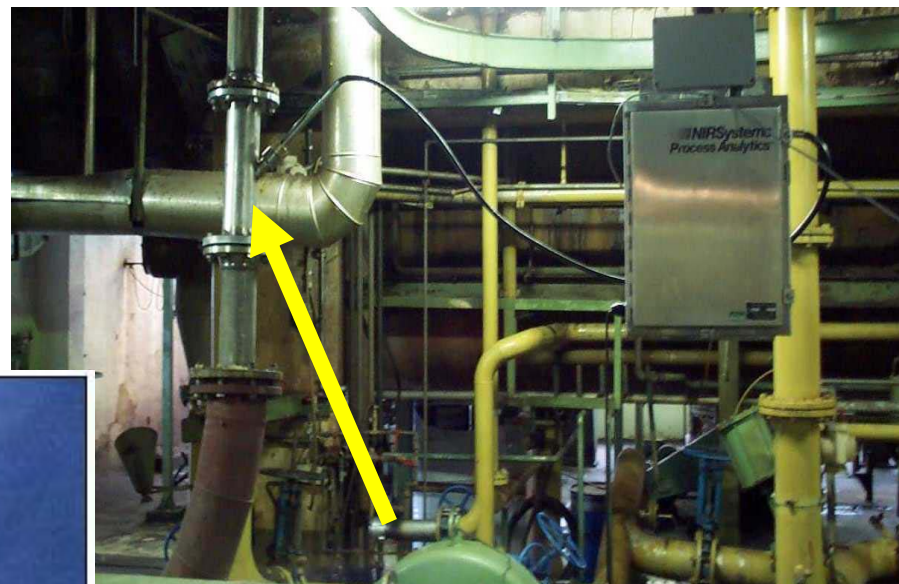
- Raw data checks
- Data preprocessing
- Over 100 pre-defined plots
- Automatic outlier detection
- Automatic variable selection
- ... and more



Example: Fiber Board Production In-situ Measurements of Fibres in Blowpipe



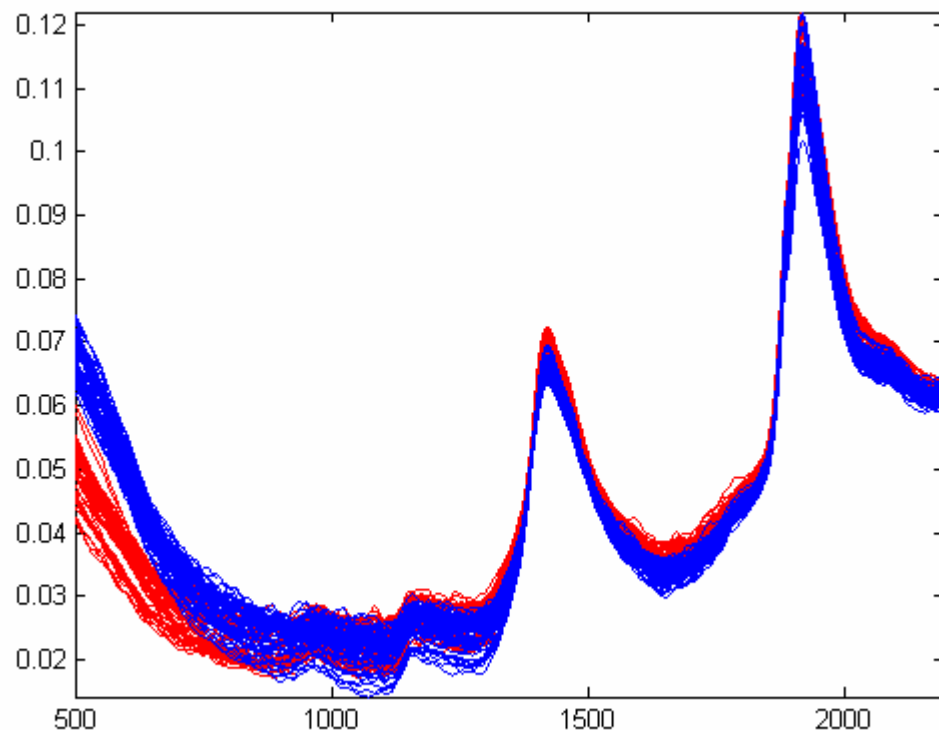
NIR FOSS Process Spectrometer with fibre bundle and diffuse reflectance probe 400 - 2200 nm



Blowpipe:
~ 180°C
~ 5 bar
~ velocity of fibres ~ 20 m/s

Fiber Board Production

NIR-Spectra of Fibres in Blowpipe



Spectra contain the following information:

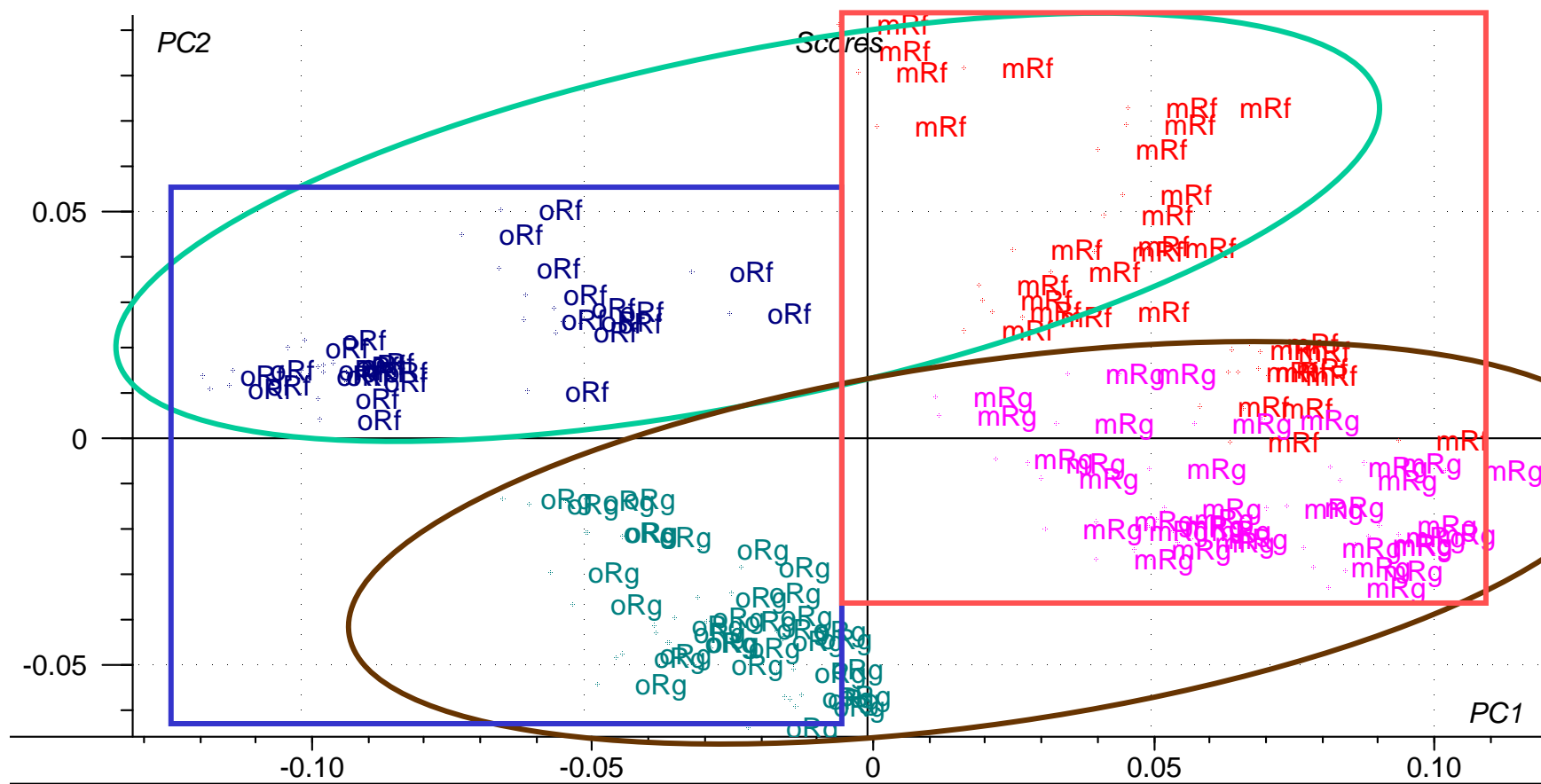
- kind of wood
- fineness
- degradation of lignin

Information is hidden within complete wavelength range
Information overlaps – separation by PCA



Principal Component Analysis

Separate the Overlapping Information



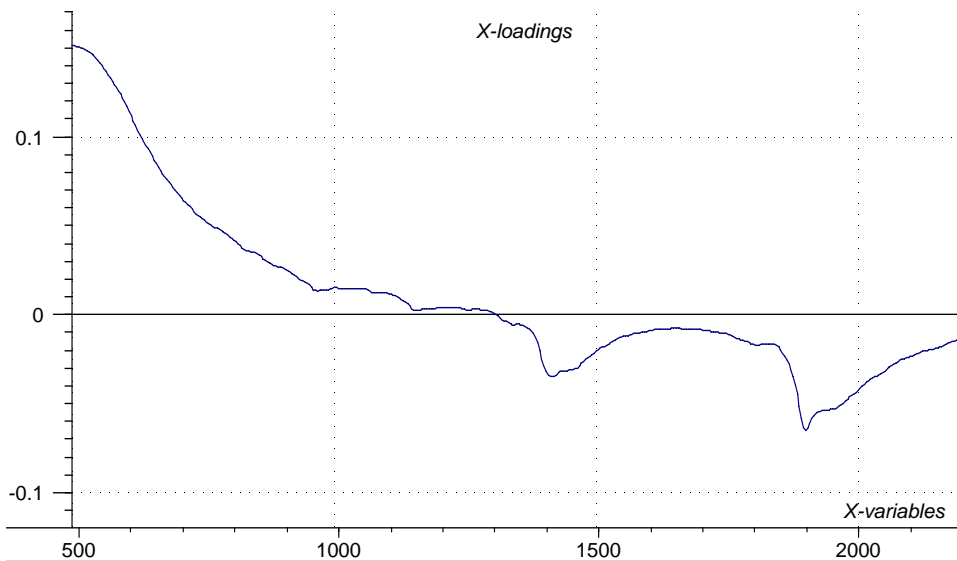
PC2 = Fineness
 ↑
 PC1 = kind of wood: **Spruce**

Spruce with bark



Principal Component Analysis

Scores and Loadings for PC1 and PC2

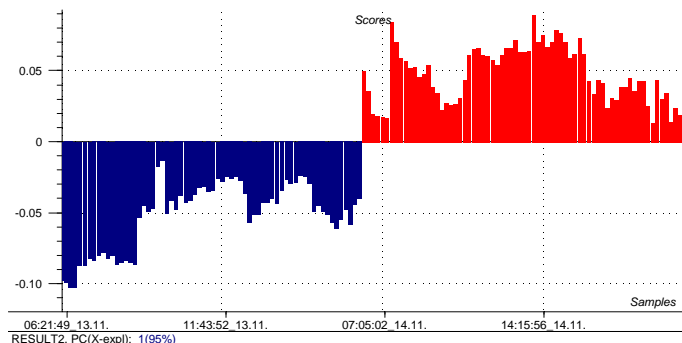


RESULT9, PC(X-exp): 1(72%)

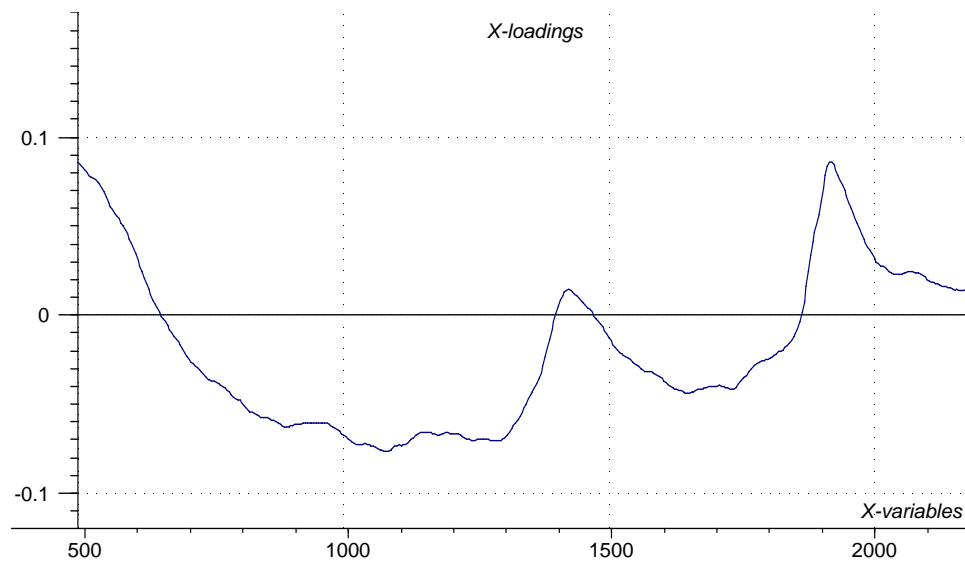
PC1: Kind of wood

Spruce
with bark

Spruce



RESULT2, PC(X-exp): 1(95%)

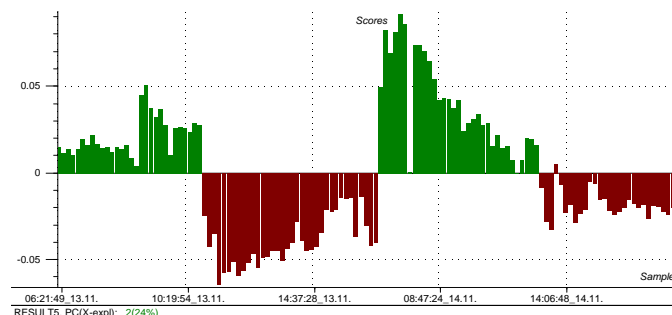


RESULT9, PC(X-exp): 2(24%)

PC2: Fineness

fine

coarse

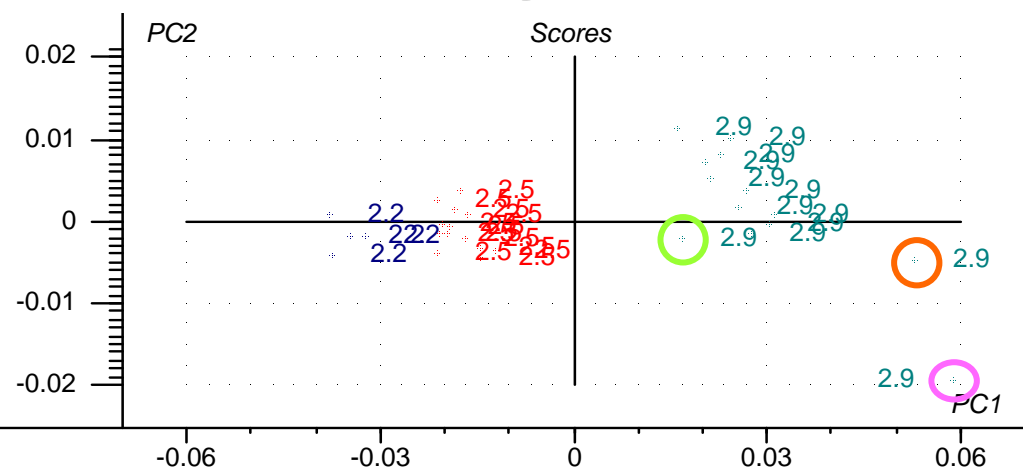


RESULT5, PC(X-exp): 2(24%)

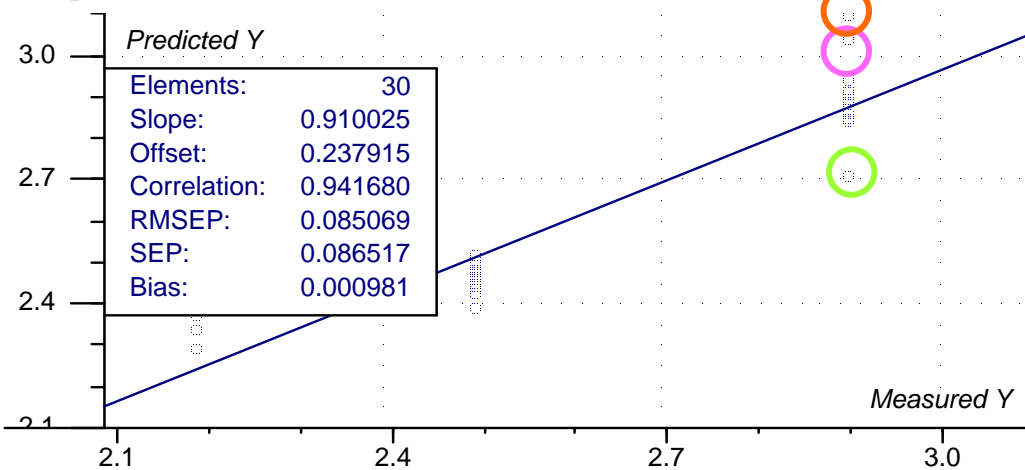


PLS Regression

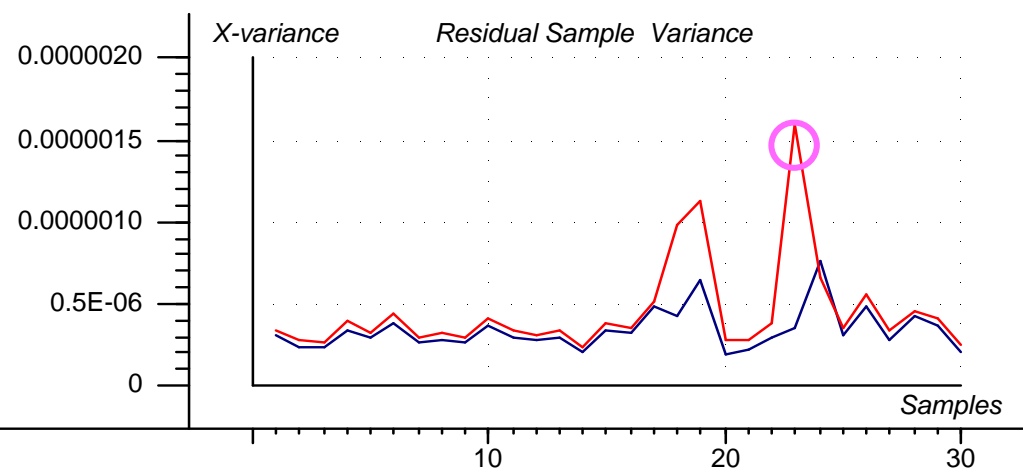
Degradation of Lignin for Spruce



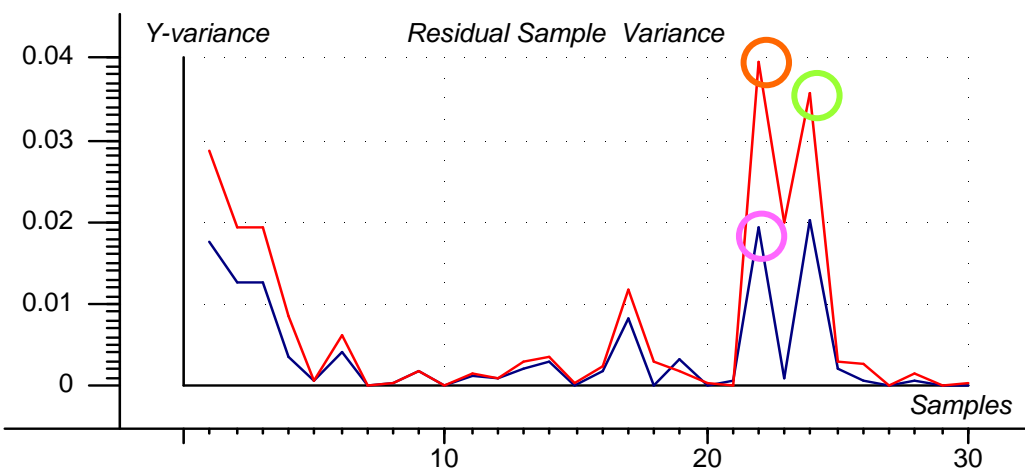
RESULT16, X-expl: 80%,5% Y-expl: 88%,6%



RESULT16, (Y-var, PC): (SFC,2)

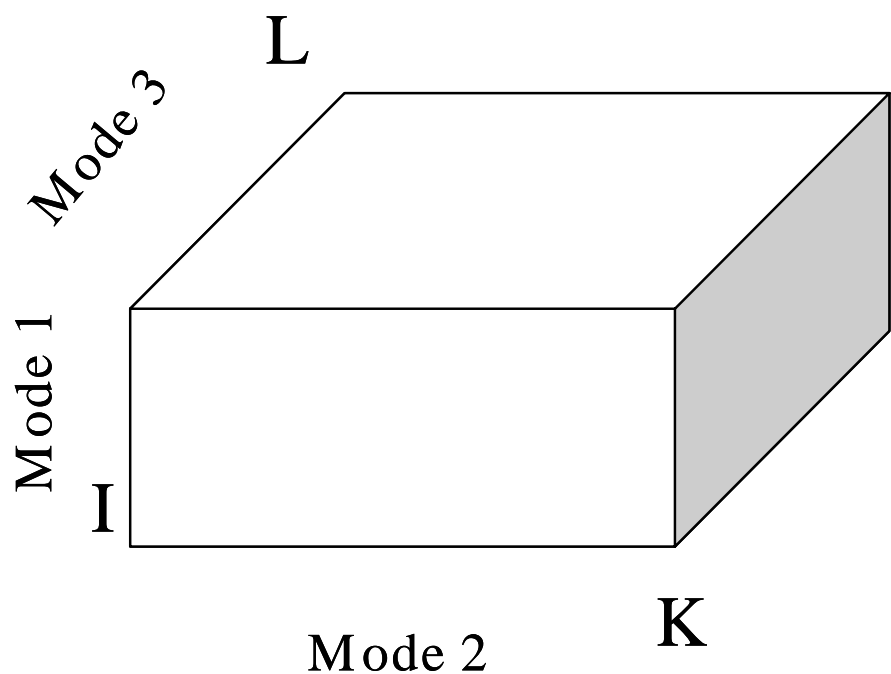


RESULT16, PC: 2 2



RESULT16, PC: 2 2

Analysing Three-Way Data



Two different types of modes are distinguished:

- Sample mode - O
- Variable mode - V

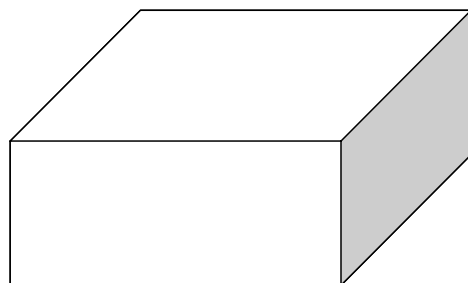
Sample mode - usually first mode

Variable mode - usually second and/or third mode

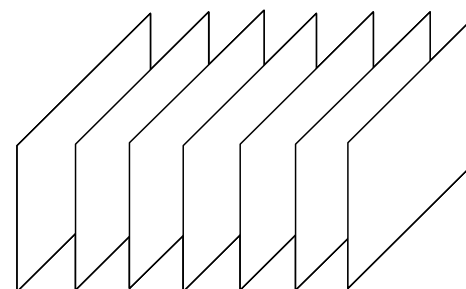


OV^2 or O^2V

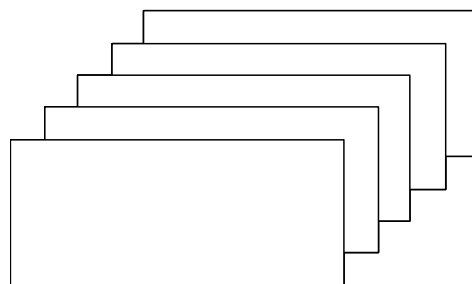
Substructures in Three-way Arrays



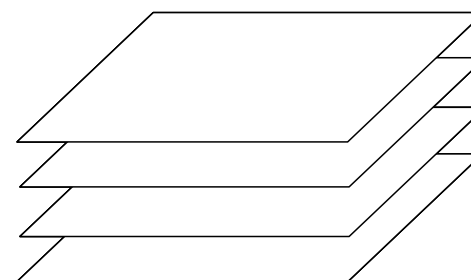
K vertical slices



L frontal slices



I horizontal slices



Three-way arrays can be divided into different slices
Decide which slices are put together to form a two-dimensional array

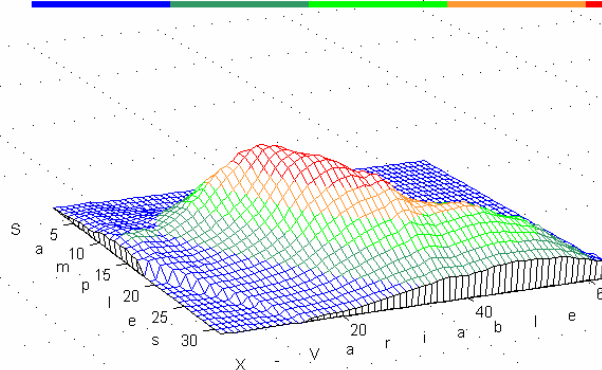
Three-way Data Example: Fluorescence Excitation Emission Spectra

- **Samples:** 32 fibres from steam treated and ground woodchips
- **X-Data:** Fluorescence Excitation-Emission spectra
(250 - 575 nm) x (300 - 600 nm)
- **Y-Data:** Kind of wood (beech and spruce)
Severity of treatment (a combination of time and temperature)
Age of wood (fresh and old)
Plate gap of grinding (fine and coarse).



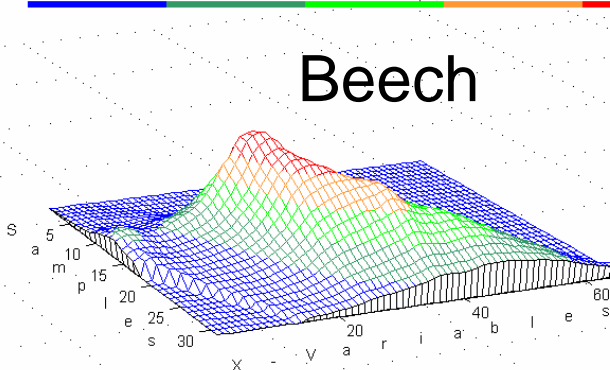
Three-way Data Example: Fluorescence Excitation Emission Spectra

0.000 109.841 219.682 329.523 439.364



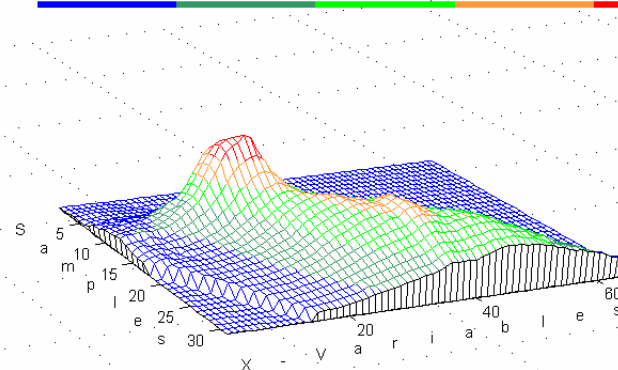
bf_sfc32x(66x31) - Matrix Plot, Sam.Set: Secondary Variables, Var.Set: Primary Variables

0.000 100.753 201.506 302.259 403.012



bf_sfc32x(66x31) - Matrix Plot, Sam.Set: Secondary Variables, Var.Set: Primary Variables

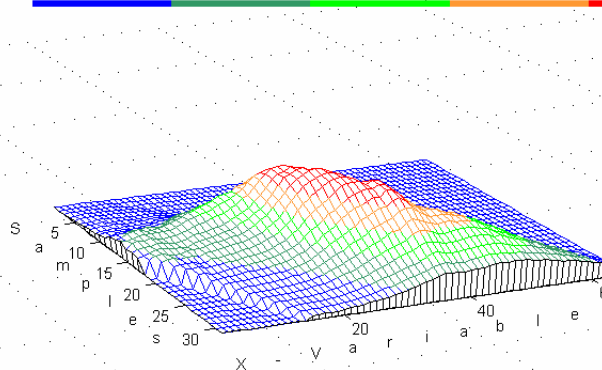
0.000 57.511 115.022 172.532 230.043



bf_sfc32x(66x31) - Matrix Plot, Sam.Set: Secondary Variables, Var.Set: Primary Variables

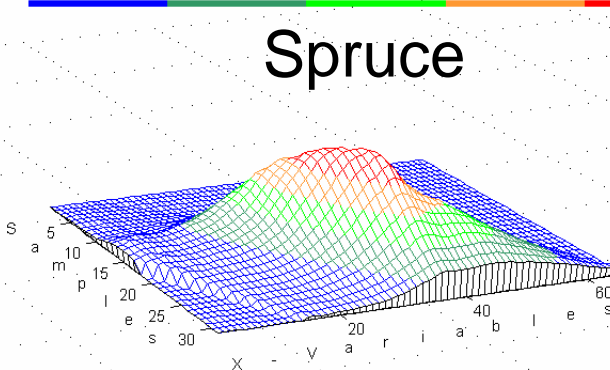
Beech

0.000 62.158 124.315 186.473 248.630



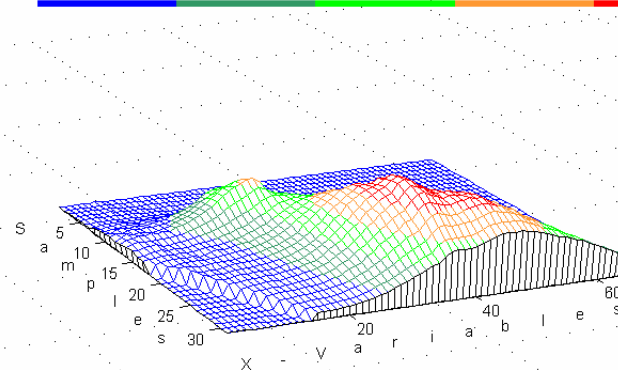
bf_sfc32x(66x31) - Matrix Plot, Sam.Set: Secondary Variables, Var.Set: Primary Variables

0.000 160.357 320.714 481.070 641.427



bf_sfc32x(66x31) - Matrix Plot, Sam.Set: Secondary Variables, Var.Set: Primary Variables

0.000 67.845 135.690 203.535 271.380



bf_sfc32x(66x31) - Matrix Plot, Sam.Set: Secondary Variables, Var.Set: Primary Variables

Spruce

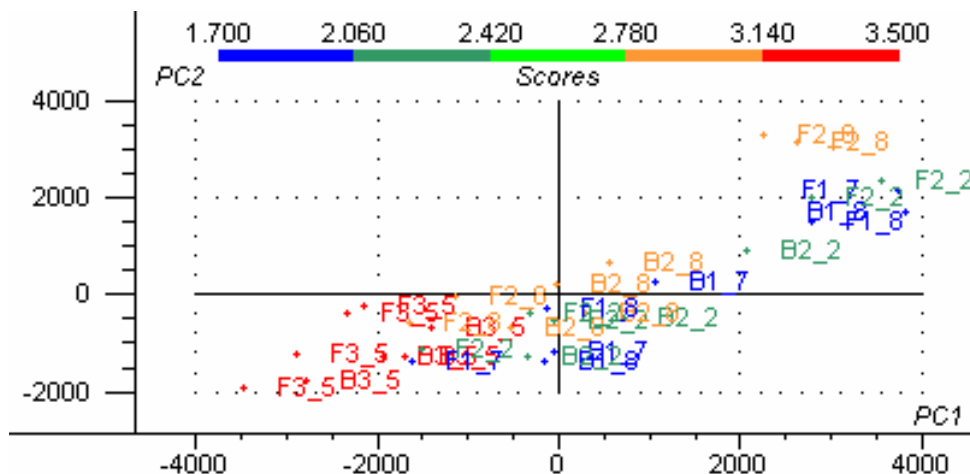
Treatment: low

middle

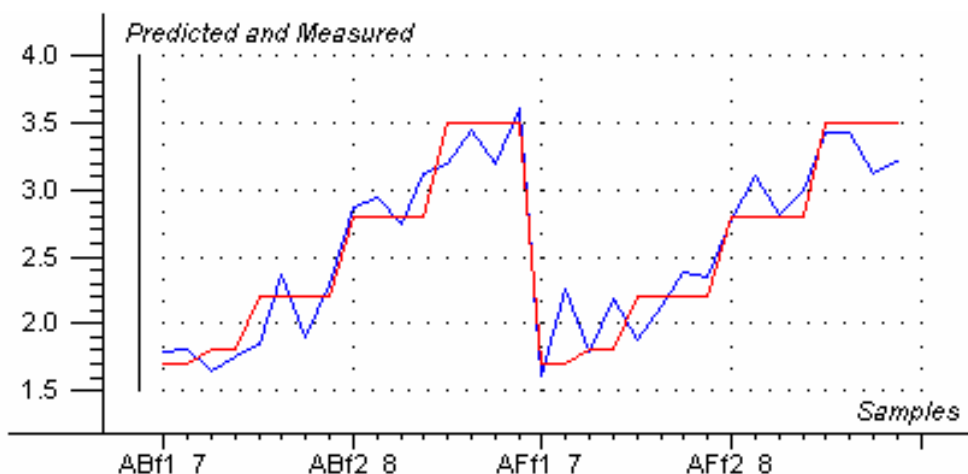
severe



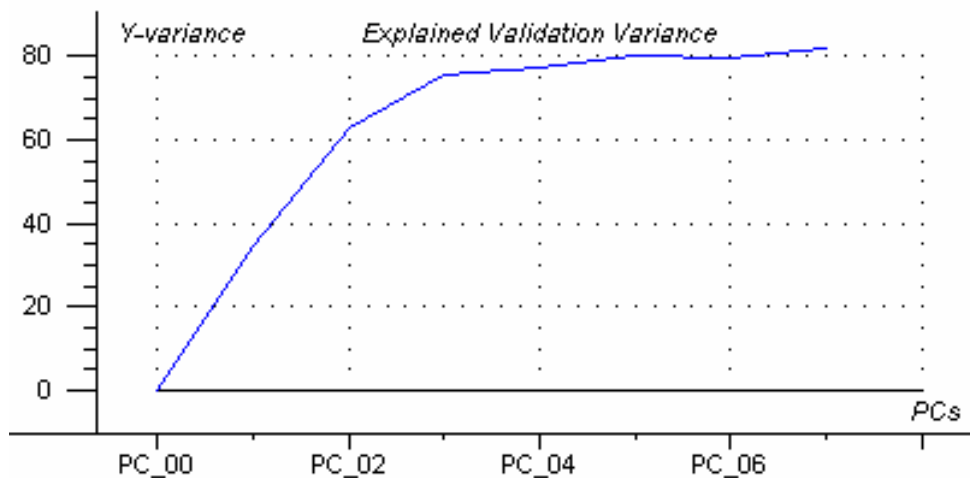
Fluorescence Excitation Emission Spectra Results of N-PLSR



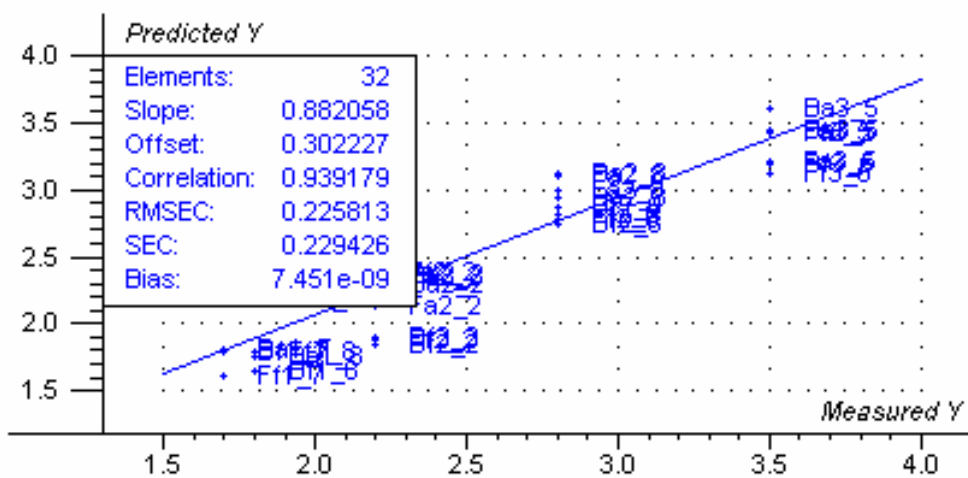
RESULT4, X-expl: 58%,19% Y-expl: 40%,26%



RESULT4, (Y-var, PC): (Severity,5) Predicted Measured



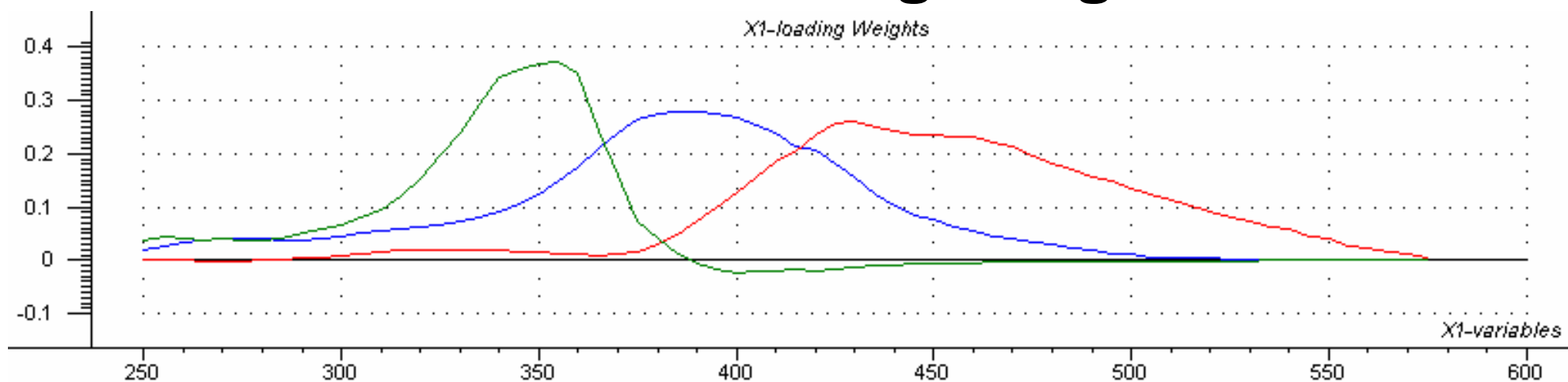
RESULT4, Variable: v.Total



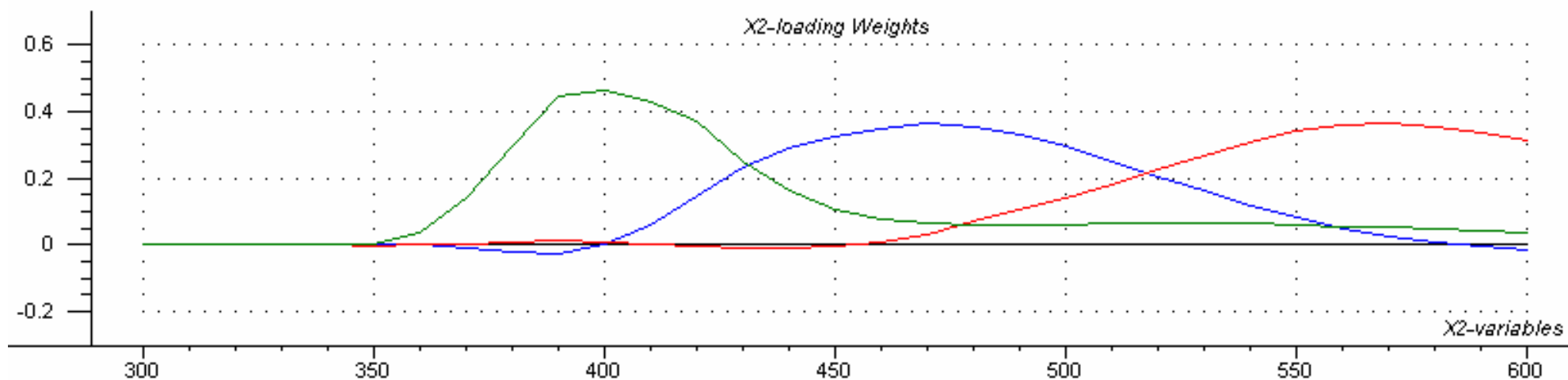
RESULT4, (Y-var, PC): (Severity,5)



Fluorescence Excitation Emission Spectra x1 and x2 Loading Weights



RESULT4, PC(X-expl,Y-expl): 1(58%,40%) 2(19%,26%) 3(12%,16%)



RESULT4, PC(X-expl,Y-expl): 1(58%,40%) 2(19%,26%) 3(12%,16%)

Possibilities for Three-way Data in The Unscrambler[®]

- **3D Data Import:** ASCII, Excel, JCAMP-DX, Matlab
- **Swapping:** toggle freely between the 6 OV^2 and 6 O^2V layouts of a 3D table
- **Matrix plots:** Contour and landscape plots of the samples
- **Variable sets:** Create Primary variable sets and Secondary Variables sets

The Unscrambler[®] Benefits

- Easy to make models
- Easy to interpret results
- High user-friendliness
- Less time spent doing data analysis,
more information extracted from your data
- Faster decision making

Try The Unscrambler[®] 9.2 for 30 days

Free trial version available on www.camo.com



- ✓ Fully functioning version
- ✓ Includes the Unscrambler user manual
- ✓ Includes 7 tutorial exercises and associated files
- ✓ Includes 3 demonstration tours

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