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 Exitation Emission Spectra
- Life Demonstration
  - 3-way Data Handling

The Unscrambler® Main Features

Exploratory Analysis

- Descriptive statistics
- Principal Component Analysis (PCA)

Multivariate Regression Analysis

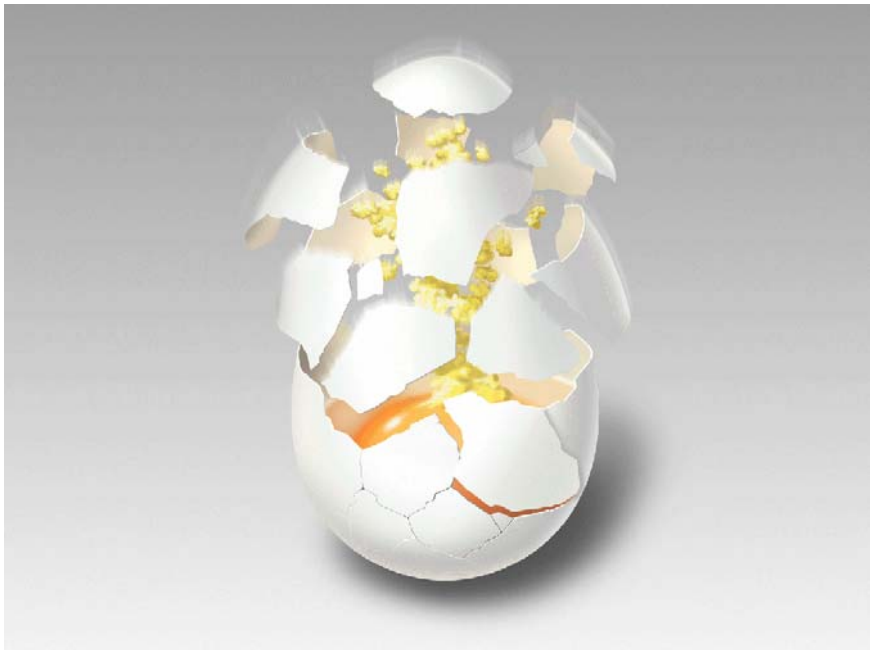
- Partial Least Squares regression (PLS)
- Principal Component Regression (PCR)
- Multiple Linear Regression (MLR)
- Prediction

Classification

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

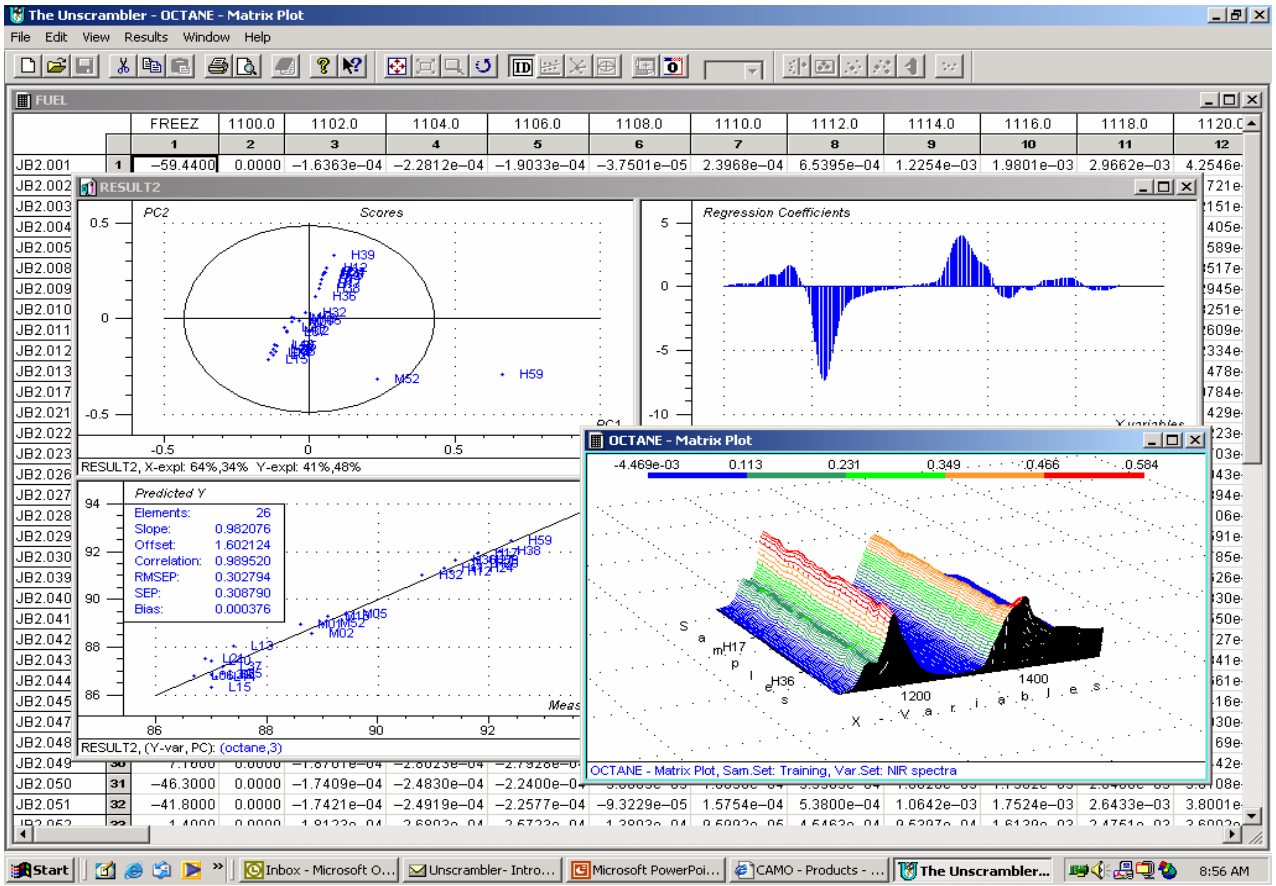
Experimental Design

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



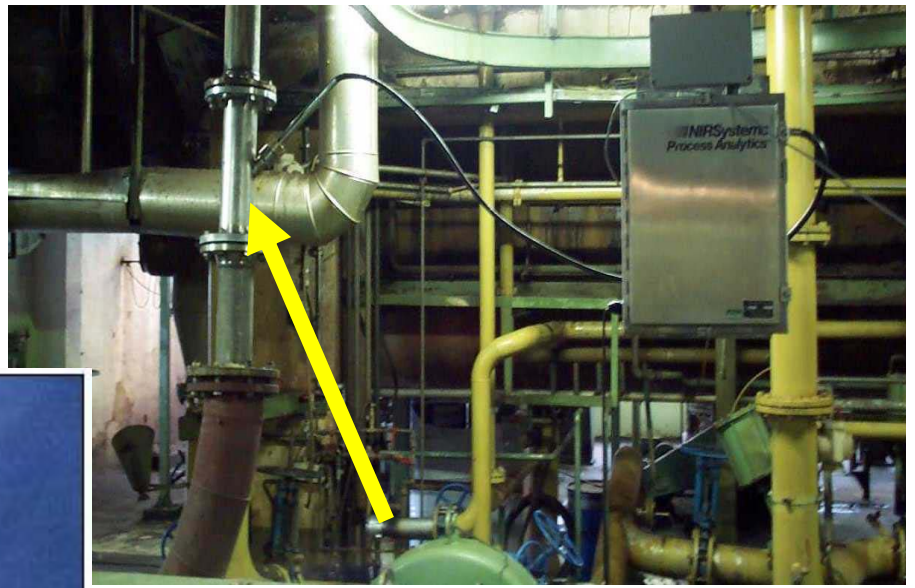
The Unscrambler® Also Features…

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



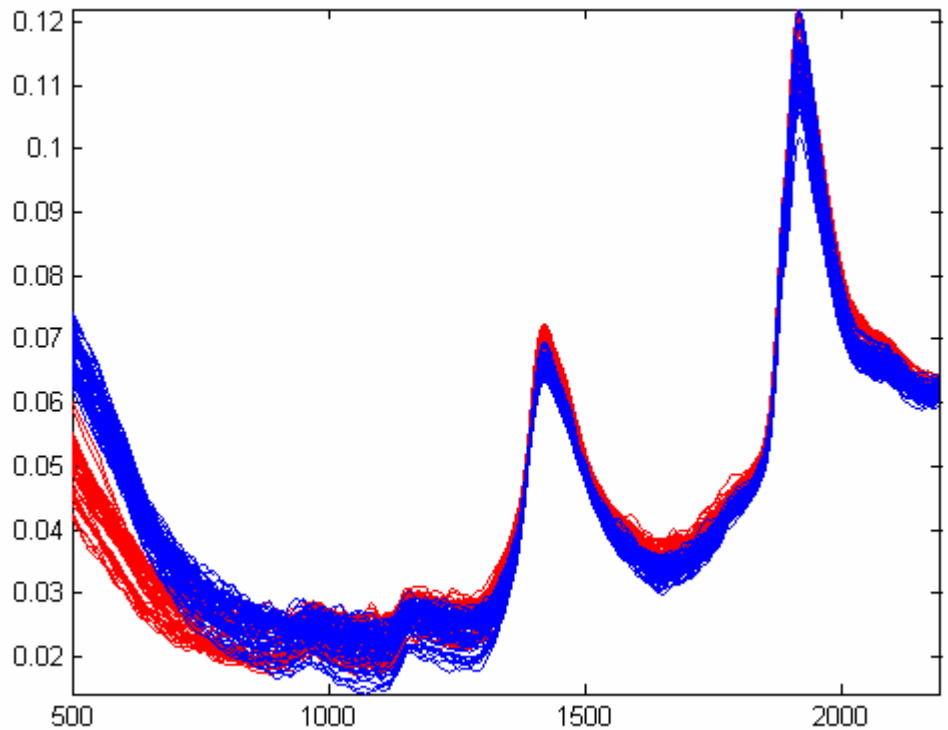
Example: Fiber Board Production
In-situ Measurements of Fibres in Blowpipe

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

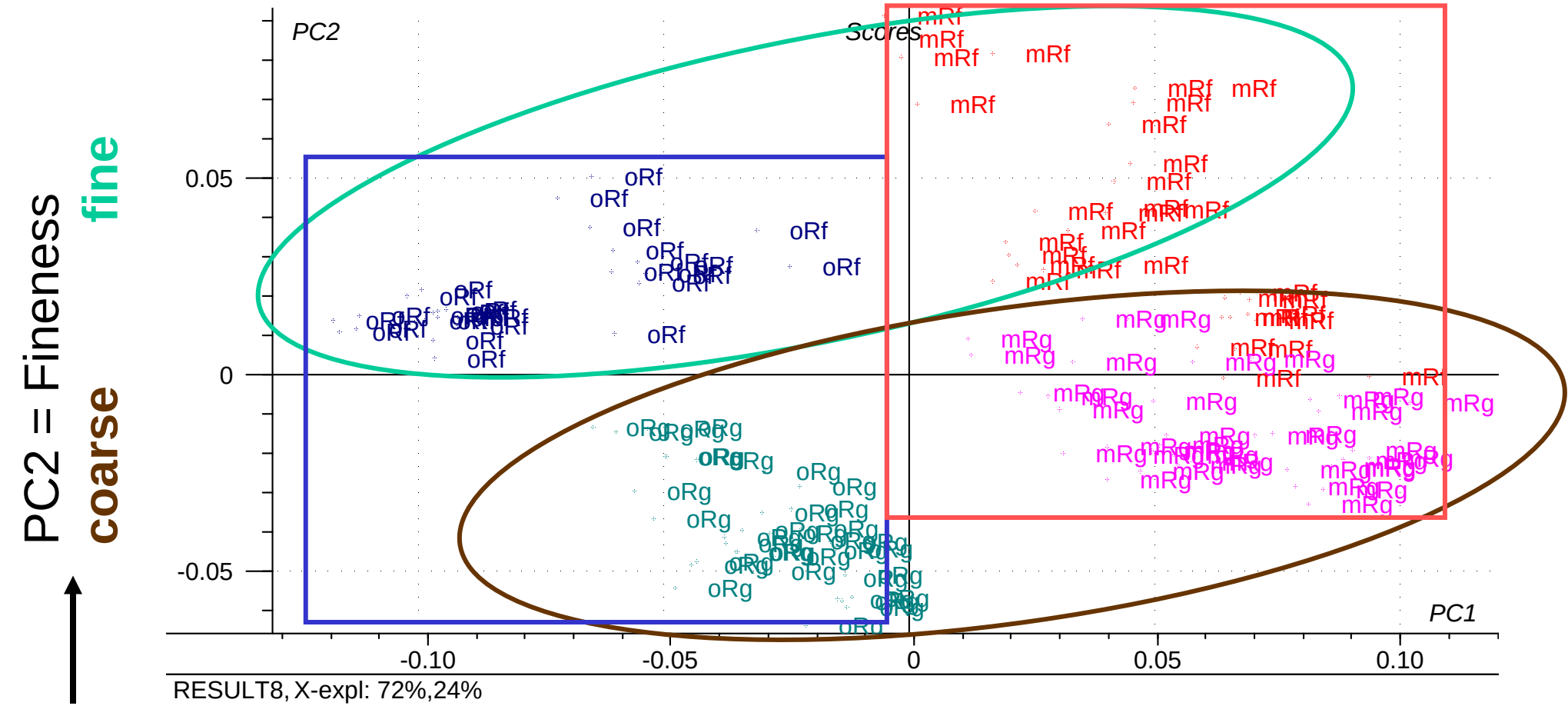


Spectra contain the following information:

- kind of wood
- fineness
- degradation of lignin

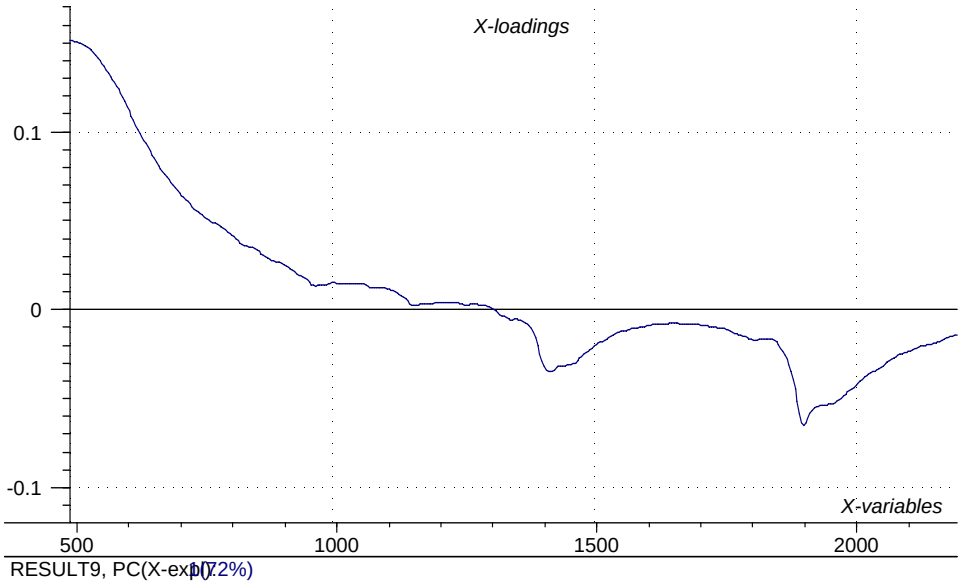
Information is hidden within complete wavelength range
Information overlaps – separation by PCA

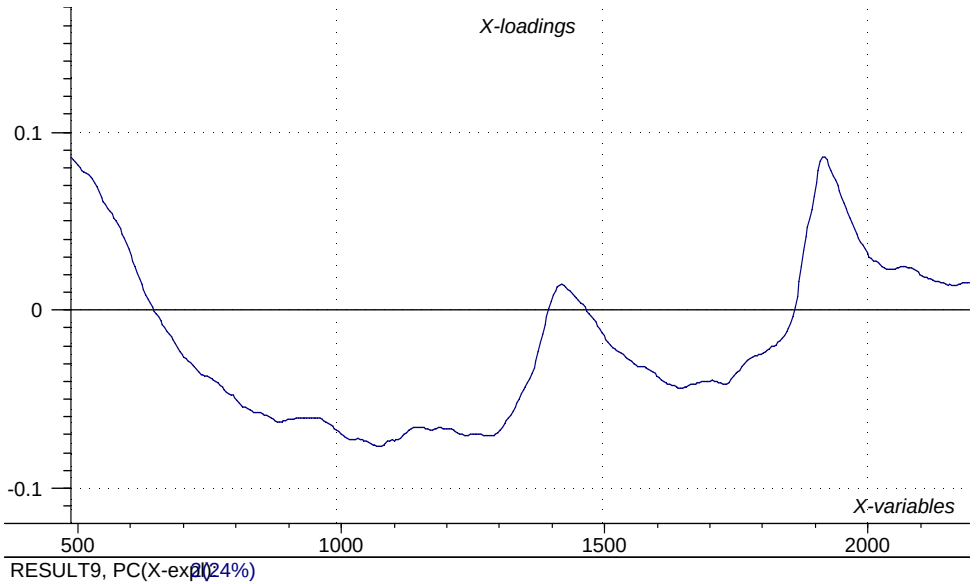
Principal Component Analysis
Separate the Overlapping Information



PC1 = kind of wood: **Spruce** **Spruce with bark**

Principal Component Analysis
Scores and Loadings for PC1 and PC2

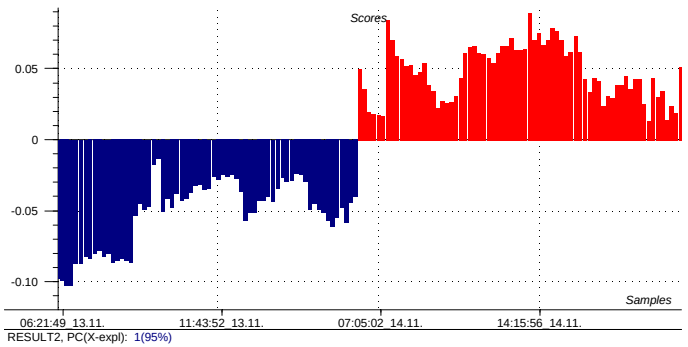




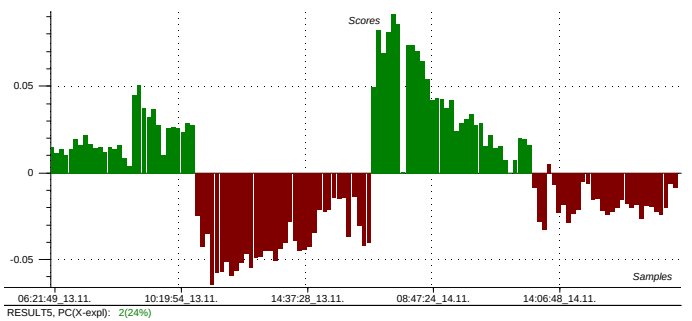
PC1: **Kind of wood**

Spruce with bark

Spruce



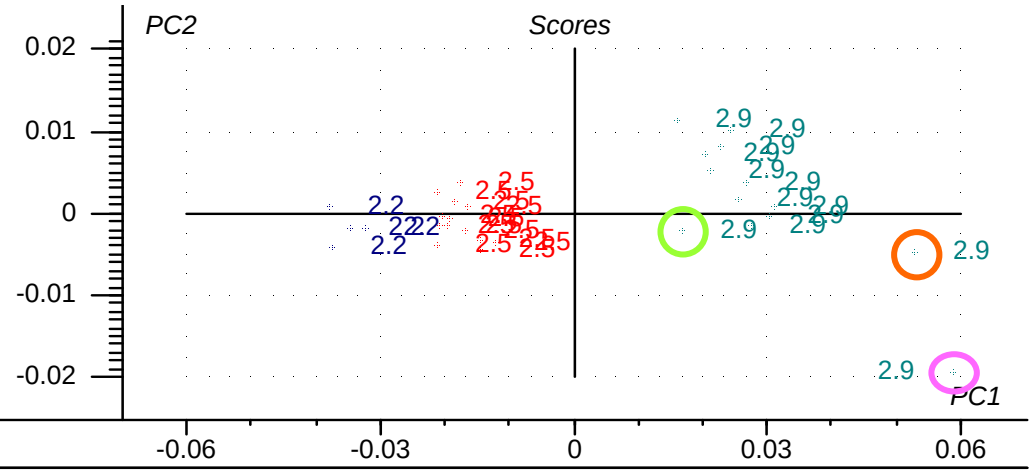
PC2: **Fineness**



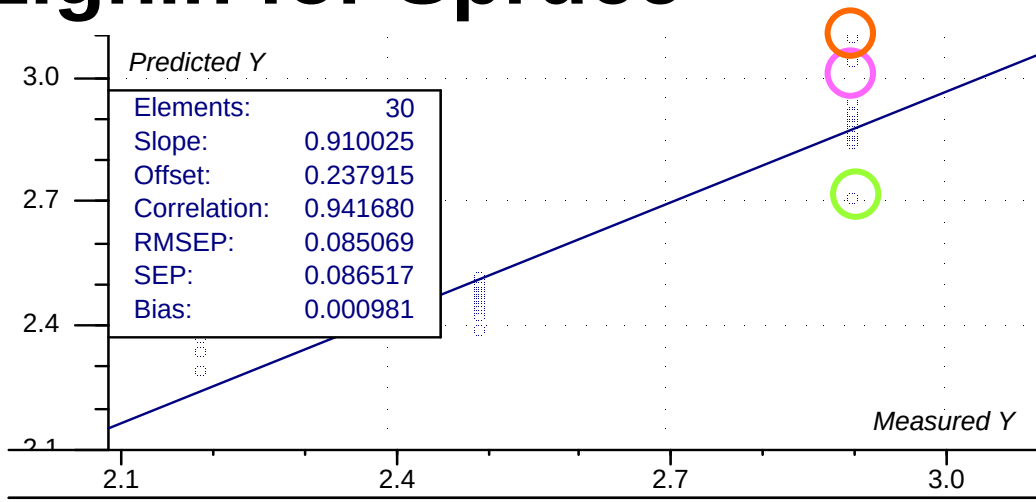
fine

coarse

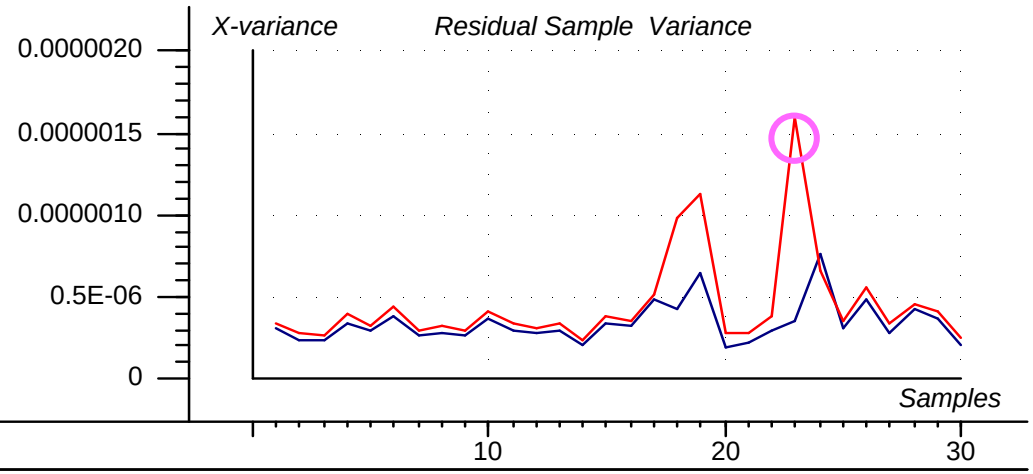
PLS Regression
Degradation of Lignin for Spruce



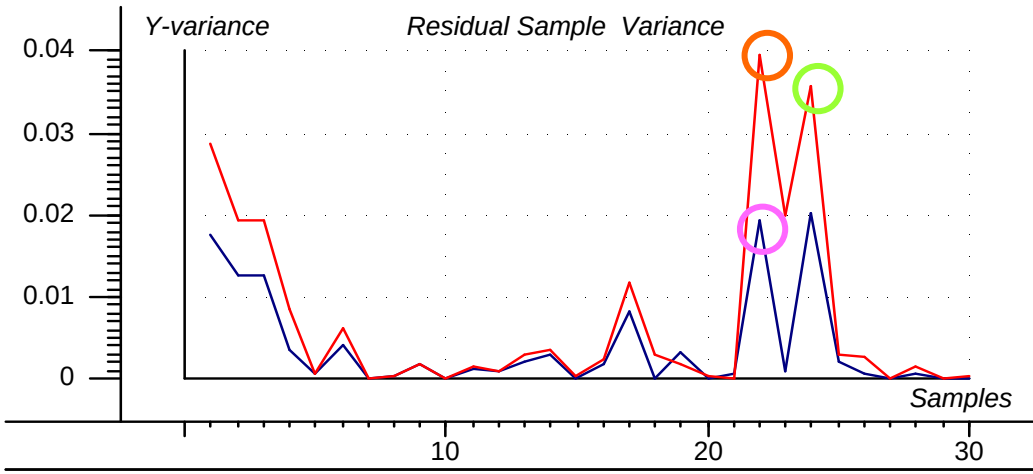
RESULT16, X-expl: 80%,5% Y-expl: 88%,6%



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

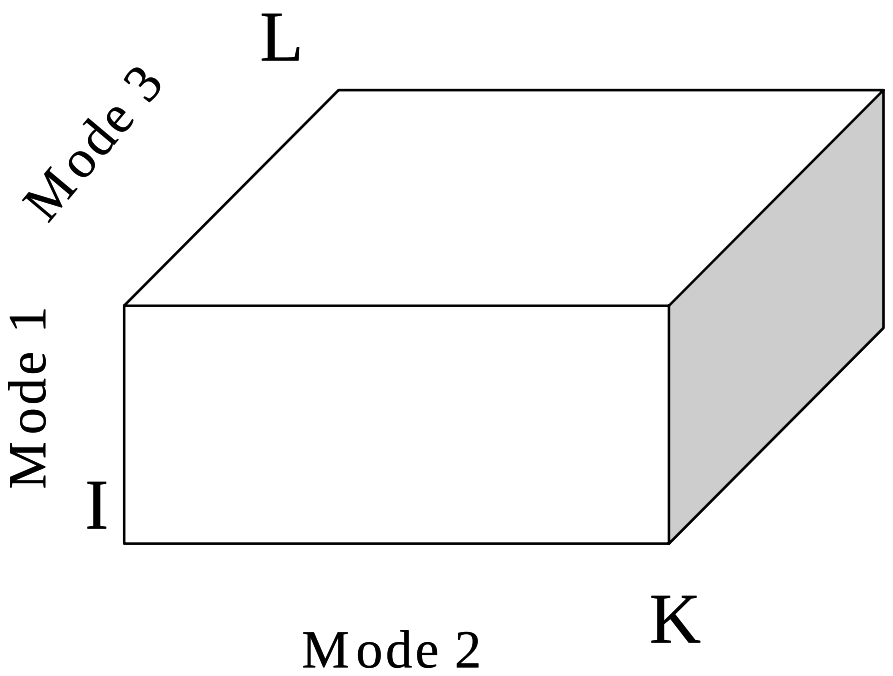


RESULT16, PC: 2 2



RESULT16, PC: 2 2

Analysing Three-Way Data



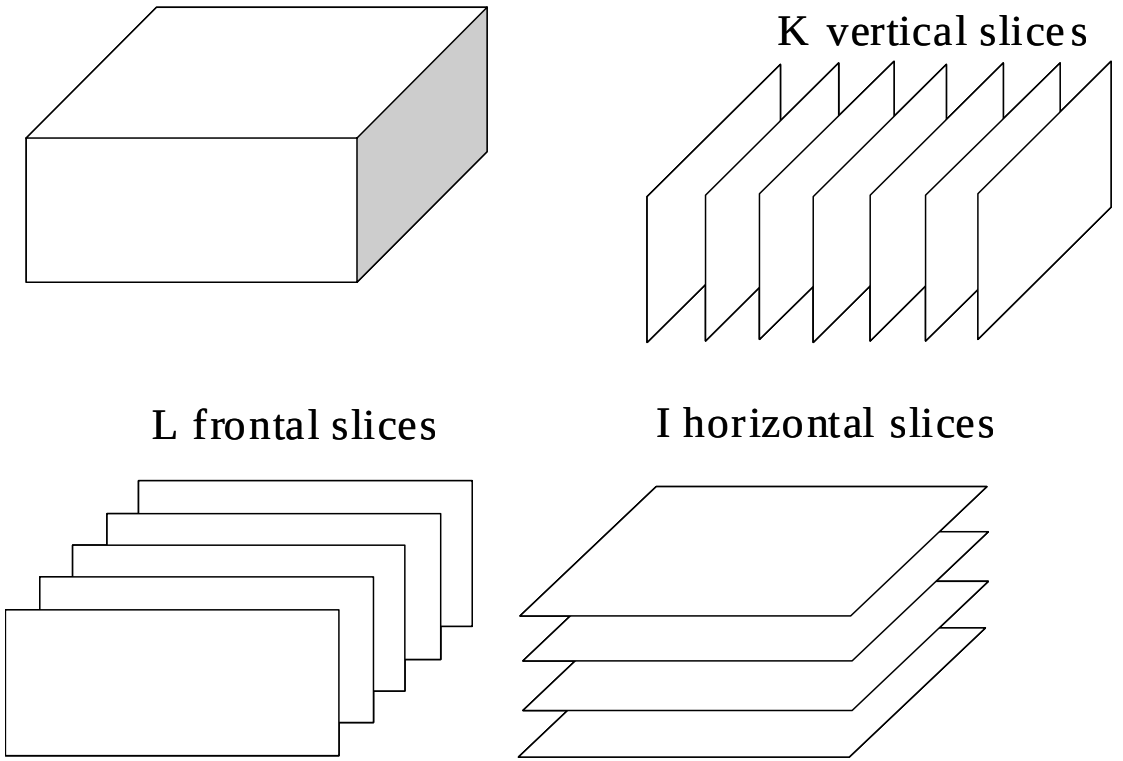
Two different types of modes are distinguished:

- 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



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

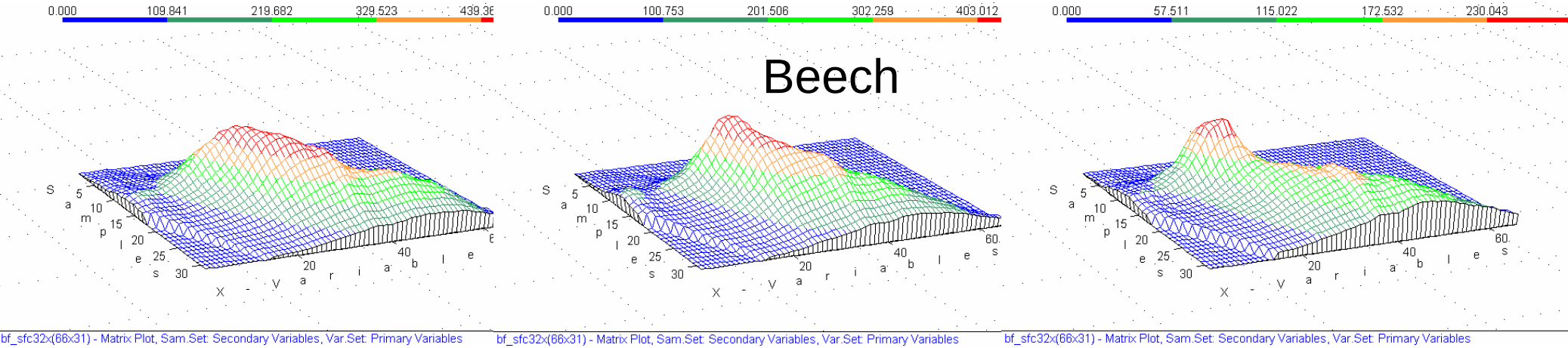
Three-way Data Example: Fluorescence Excitation Emission Spectra

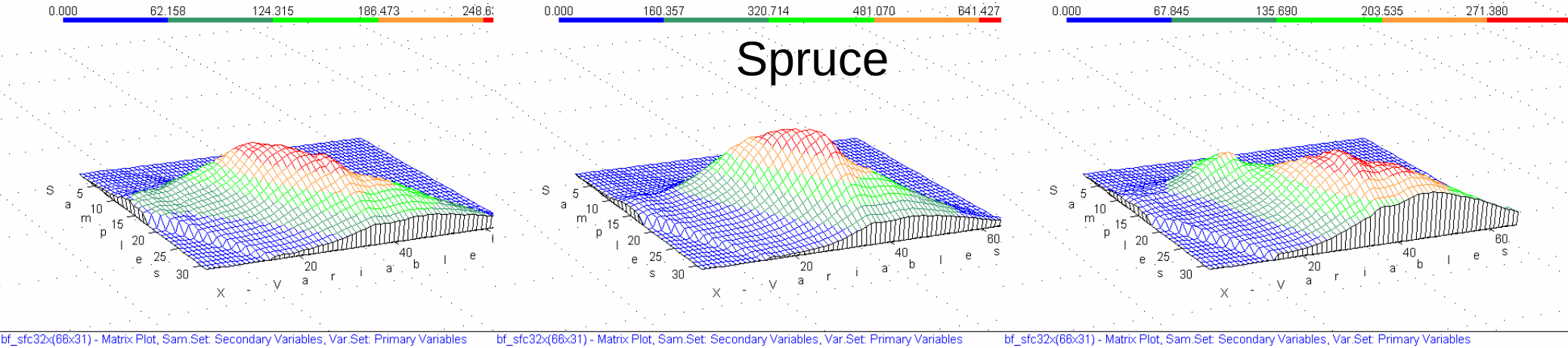
- **Samples**: 32 fibres from steam treated and ground woodchips

- **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).

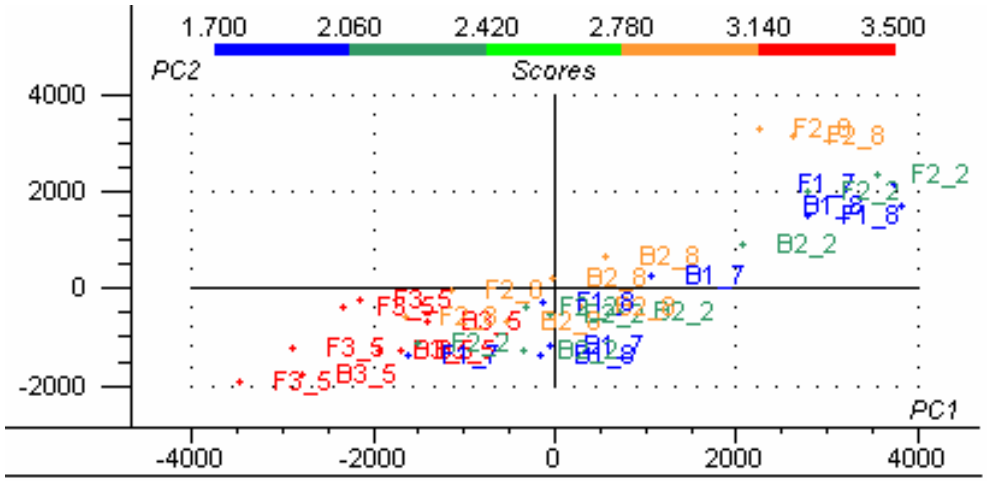
Three-way Data Example: Fluorescence Excitation Emission Spectra



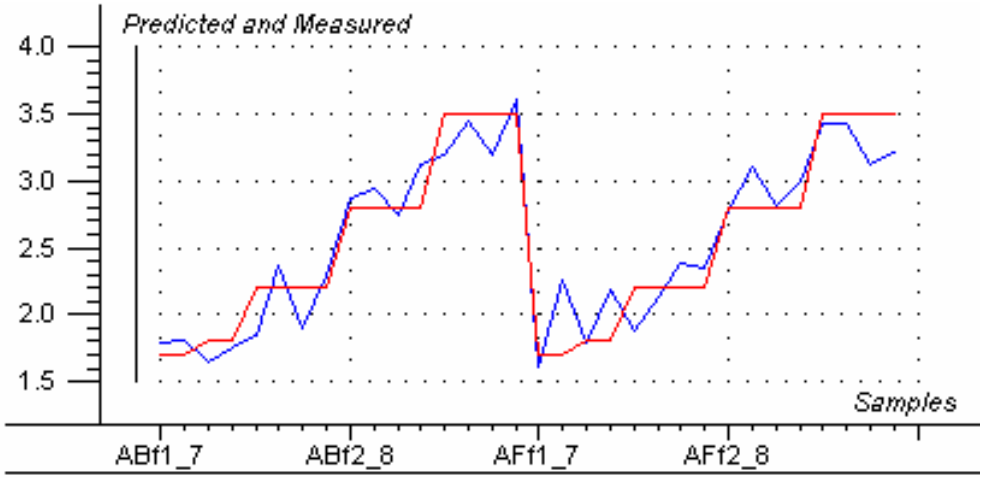


Treatment: low middle severe

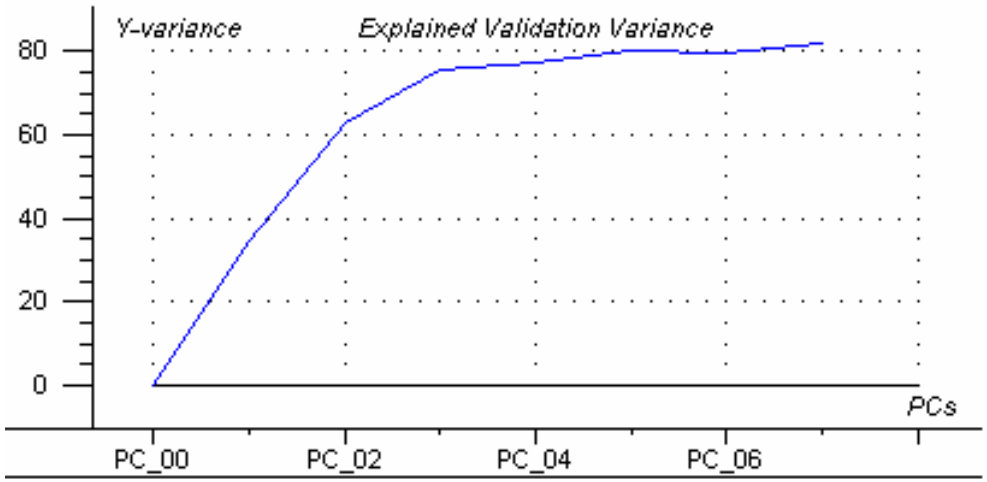
Fluorescence Excitation Emission Spectra Results of N-PLSR



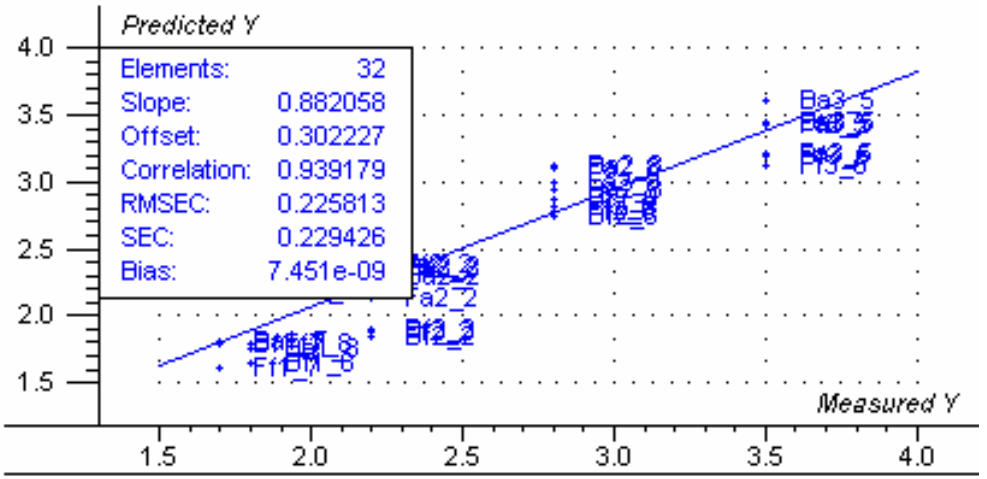
RESULT4, X-expl: 58%,19% Y-expl: 40%,26%



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

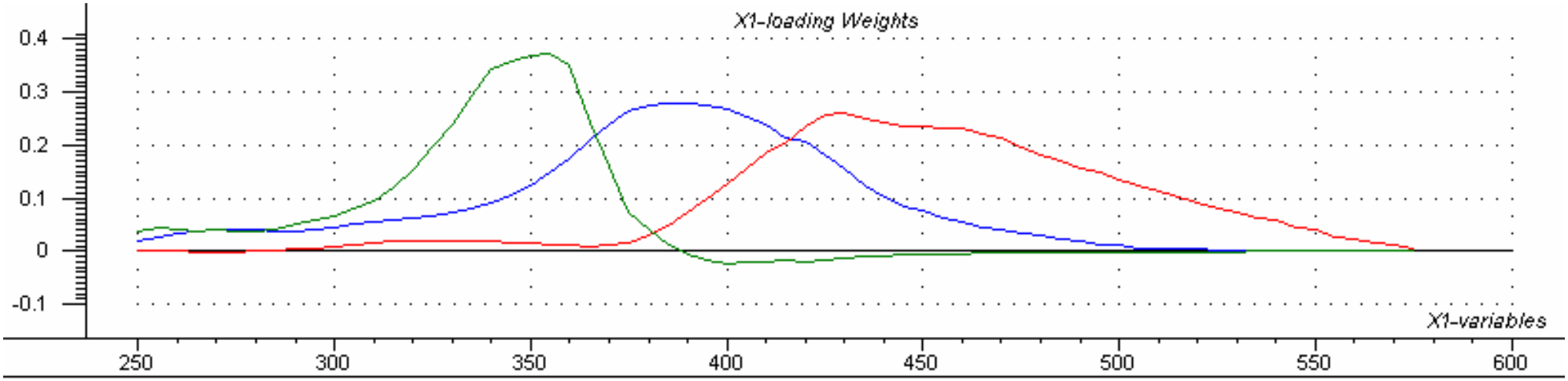


RESULT4, Variable: *v.Total*

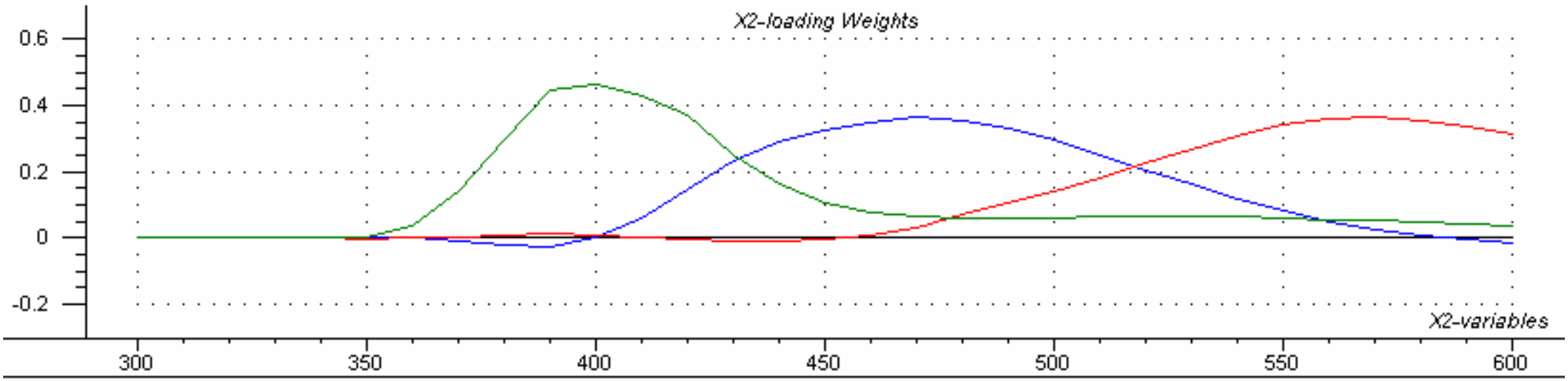


RESULT4, (Y-var, PC): (Severity,5)

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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