

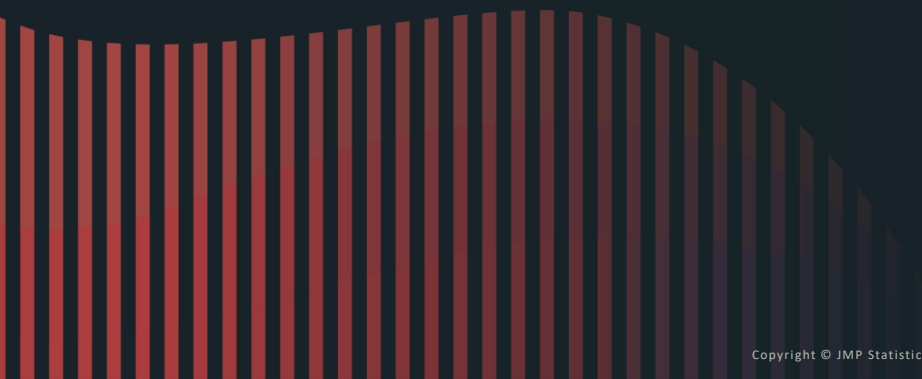
Functional Data Explorer for Spectral Data

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Sr. System Engineer, GTET

Agenda

- Introduction
- Application of functional data
- Application of Spectral data
- What is new in FDE in version 17
 - Data Preprocessing and data models
- Live Demonstration

Introduction



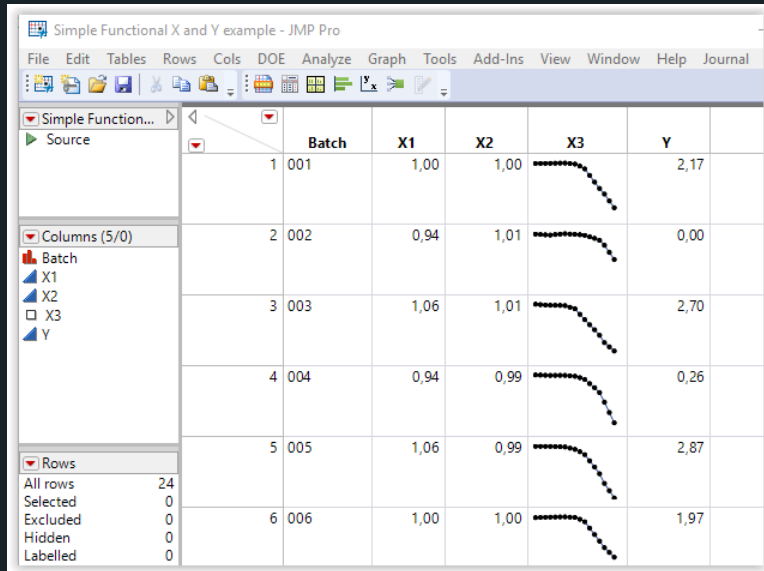
Traditional Data

Rectangular Data: 1 input data points affects 1 output data point

		Batch	X1	X2	Y
1	001		1.00	1.00	2.17
2	002		0.94	1.01	0.00
3	003		1.06	1.01	2.70
4	004		0.94	0.99	0.26
5	005		1.06	0.99	2.87
6	006		1.00	1.00	1.97

Functional Data

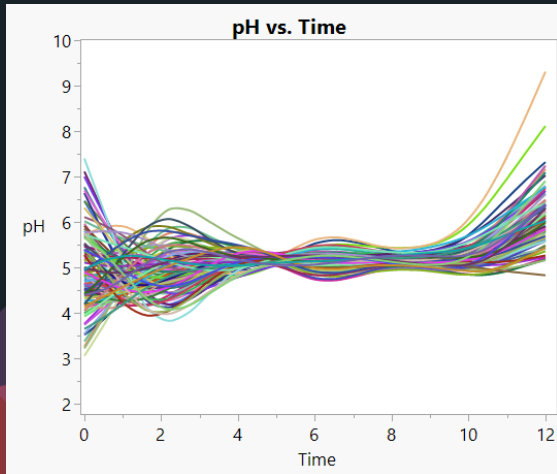
Measurements recorded over time



Where do you find functional data?

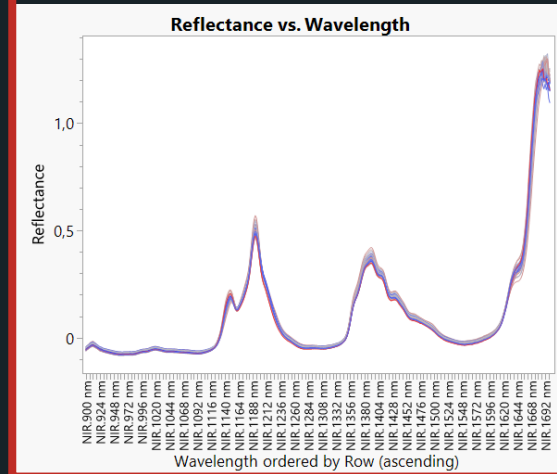
Sensor Data

Fermentation process



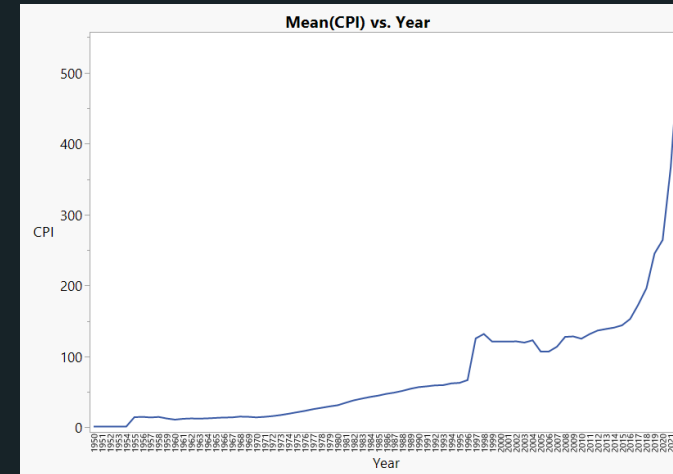
Spectral Data

NIR Spectroscopy



Time Series

Consumer Price Index



Spectral Data

Application

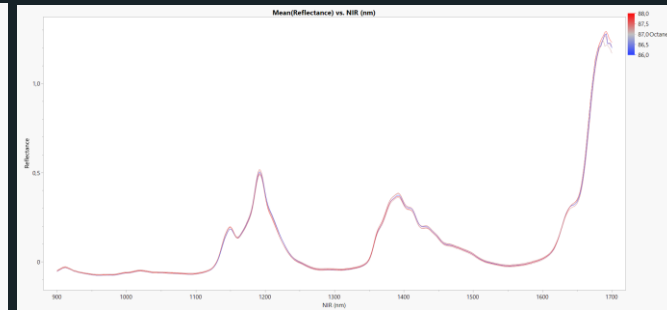
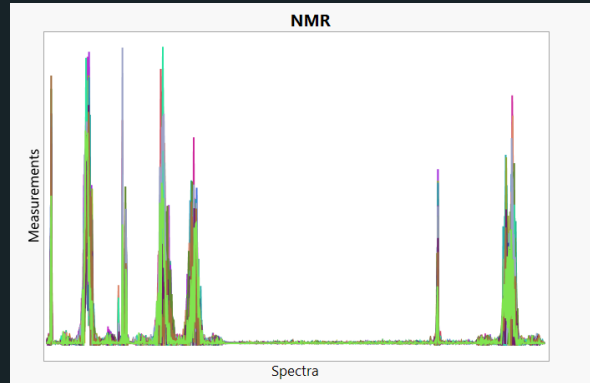
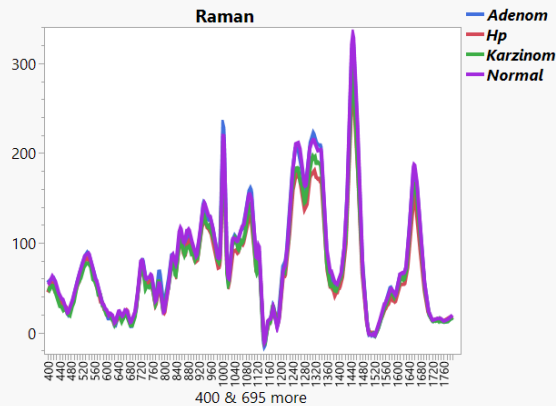
Valuable Information about Composition, Structure and Properties of materials

- **Chemical Analysis**
 - Concentration of chemical compounds in sample
- **Pharmaceuticals**
 - Analyze Drug formulation
 - Assess drug stability
 - Monitor quality of pharmaceutical products
- **Biology and Biochemistry**
 - Analyze metabolites in biological samples

Spectral Data

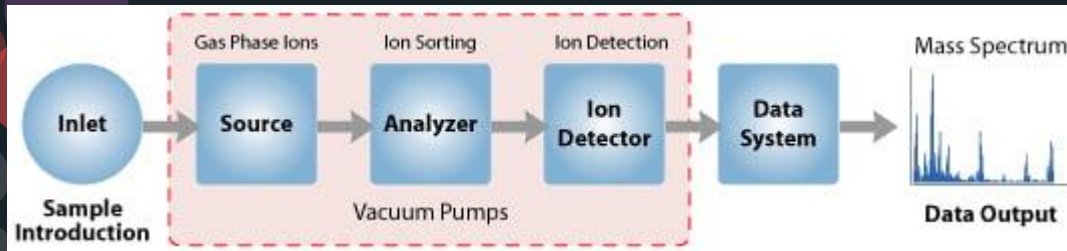
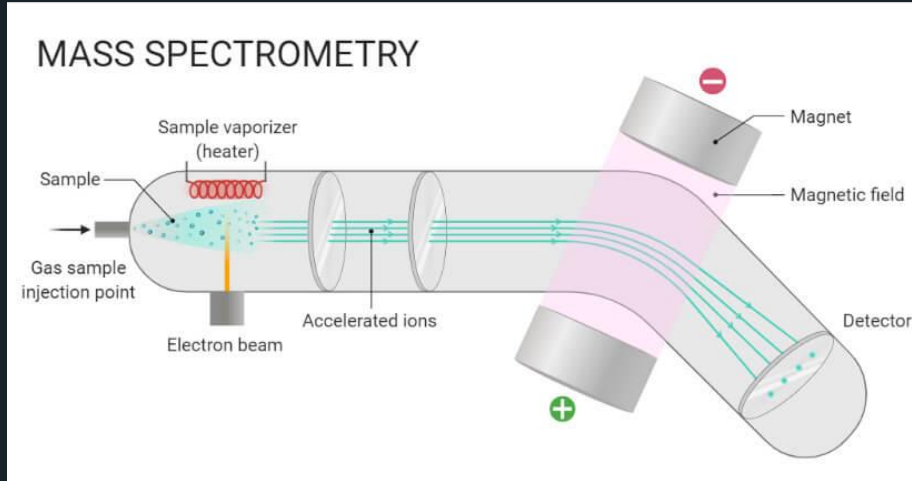
Spectroscopy

- Applications: Composition of materials, Detecting biomarkers
- Raman: lasers
- NIR: Infrared Lights
- NMR: magnets



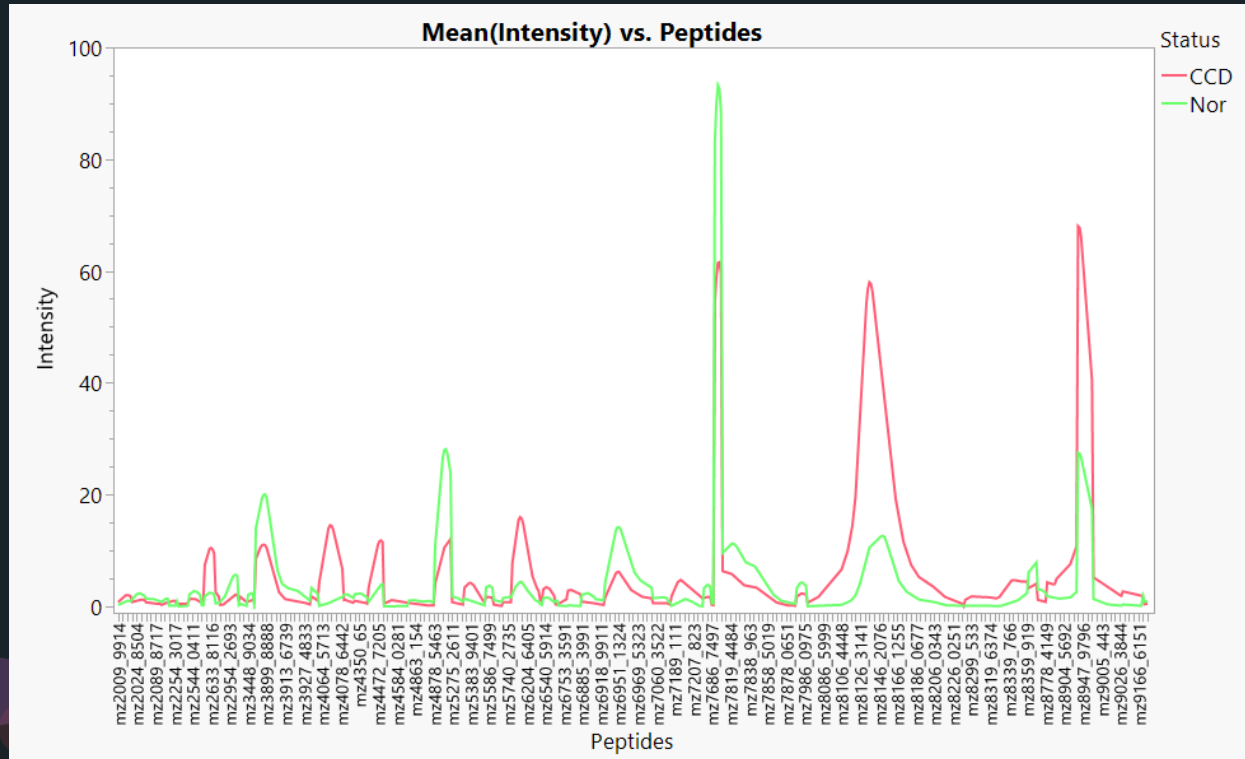
Spectral Data

Mass Spectrometry



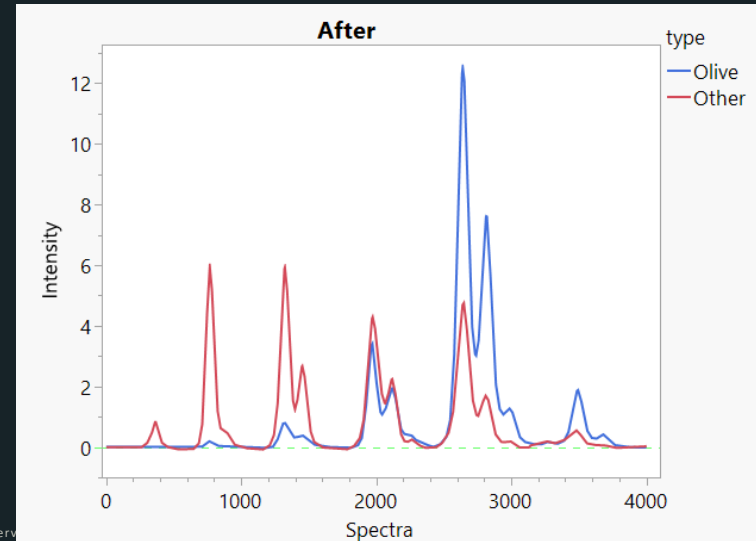
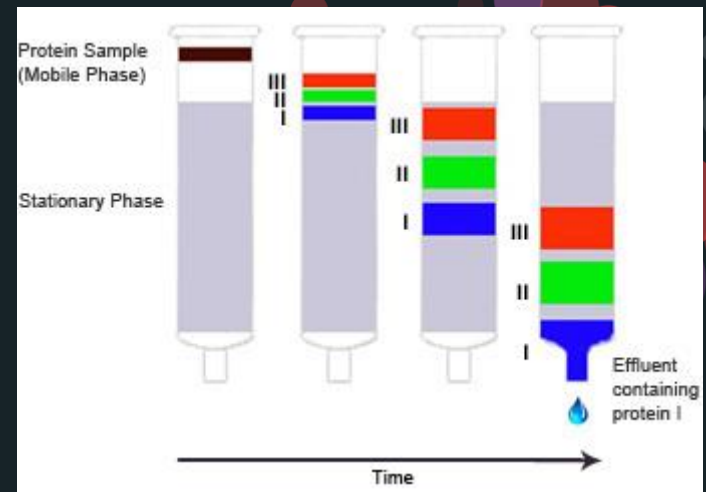
- Measures mass-to-charge ratio
- Used to construct proteomic spectrums
 - Peaks represent proteins
- One application is to compare differences between patients with and without cancer

Example of Mass Spectrometry data



Spectral Data Chromatography

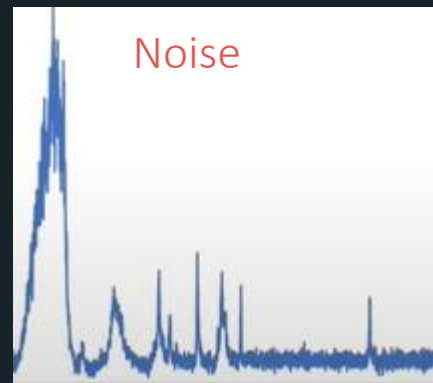
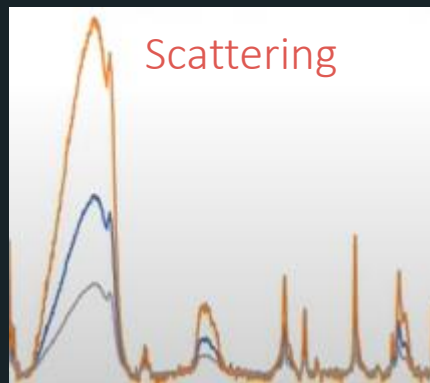
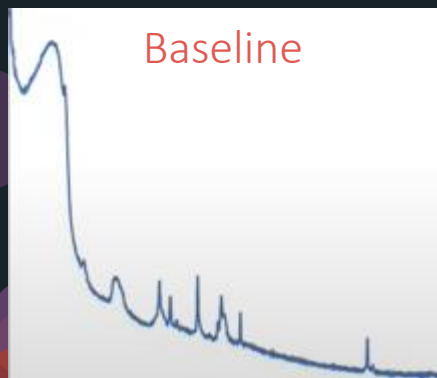
- Dissolve a chemical mixture over a material to quantify relative amounts of components
- Retention time quantifies the components in the mixture
- Example: identify olive-oil vs other vegetable oils.



Pre-processing Spectral Data

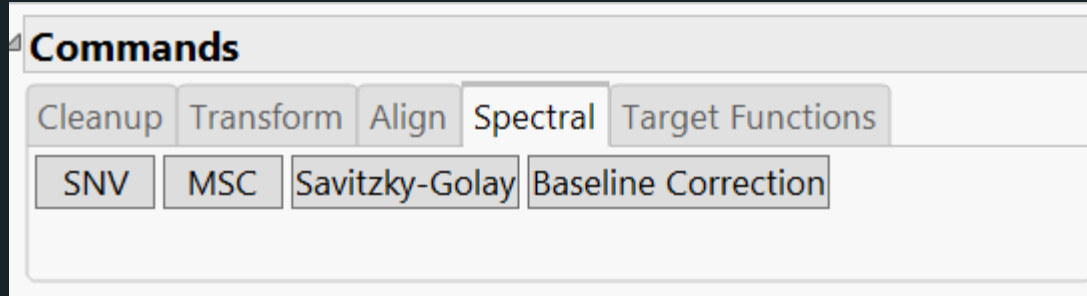
Challenges

- Raw data are not always clean for direct use
- Several preprocessing algorithms are already and new available in JMP Pro 17
- Typical problems



Pre-Processing Spectral Data

New in JMP Pro 17

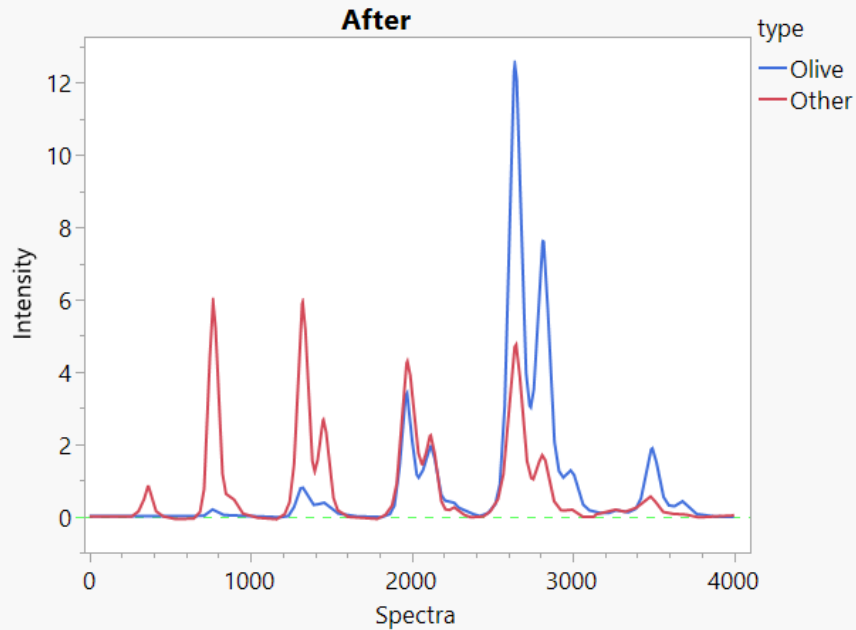
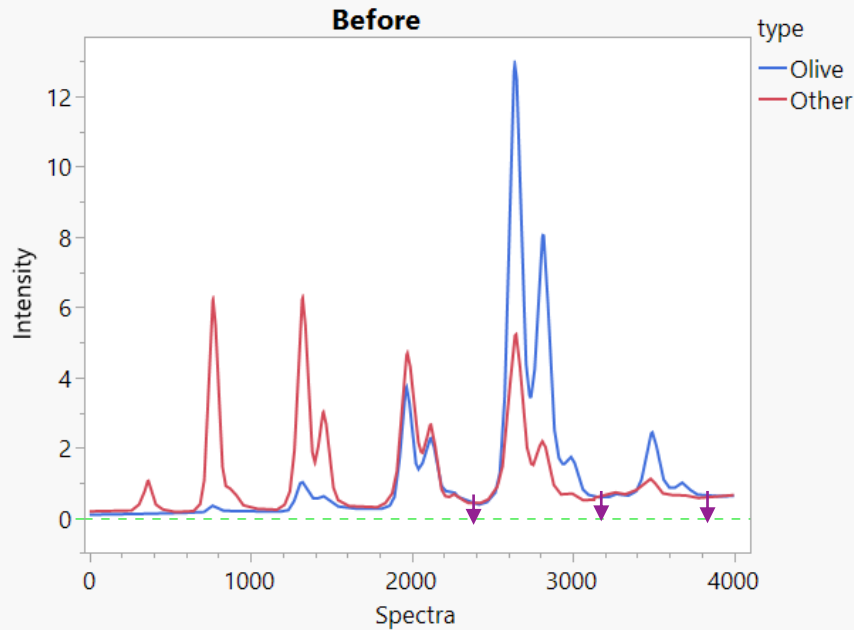


- Standard Normal Variate
- Multiplicative Scatter Correction
- Savitzky-Golay Filter
- Baseline Correction

Pre-Processing Spectral Data : Baseline

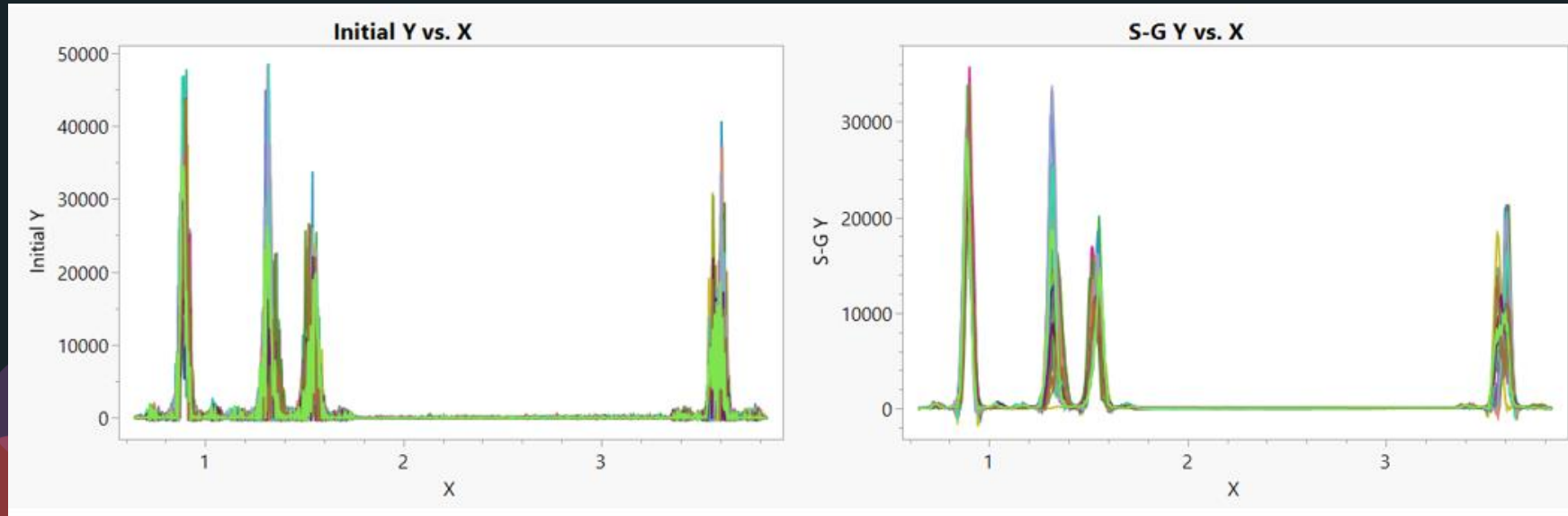
Baseline Correction

Data Preprocessing



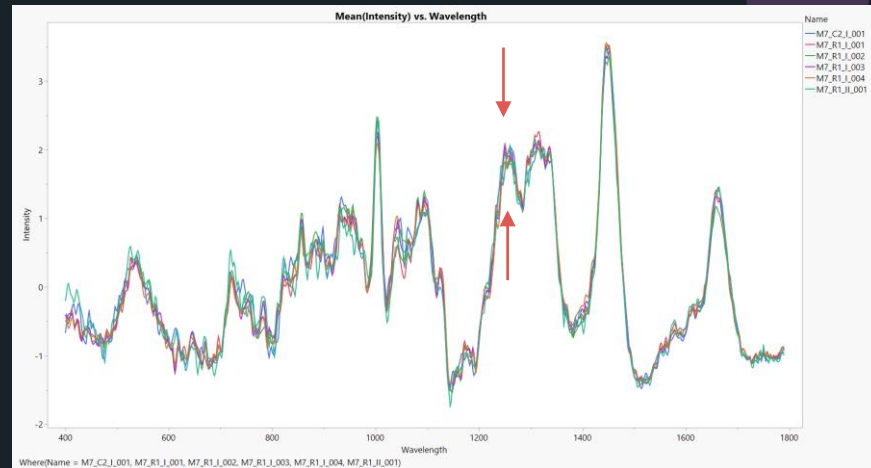
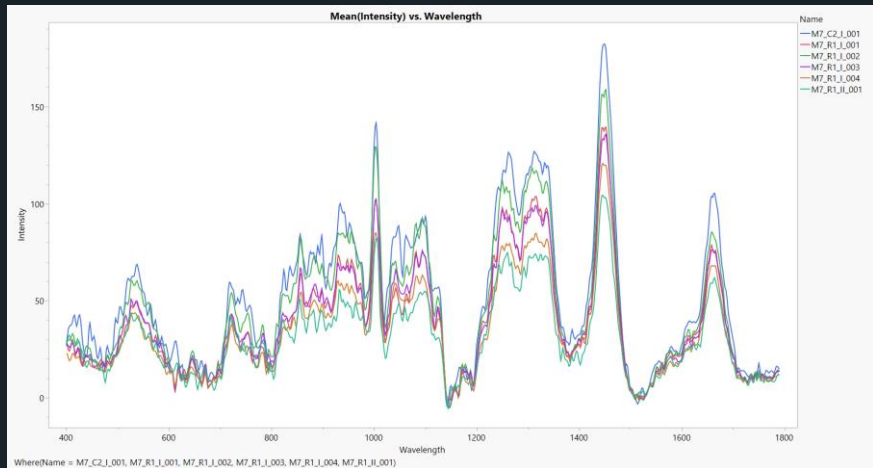
Pre-Processing Spectral Data: Baseline

Baseline: Savitzky-Golay (SG) Filter



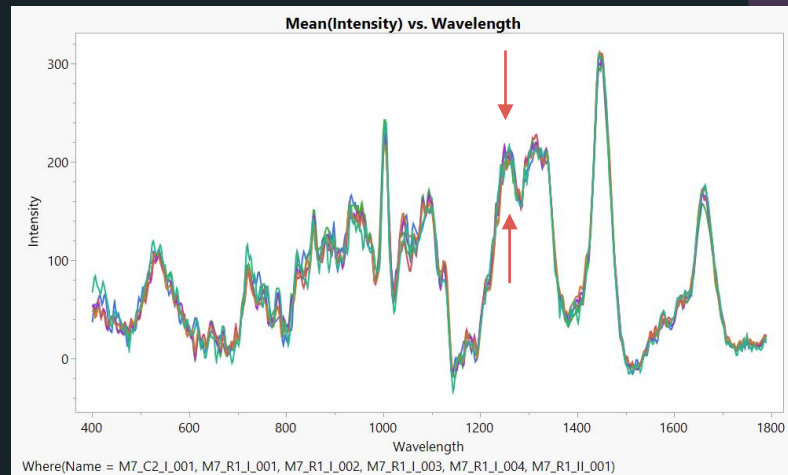
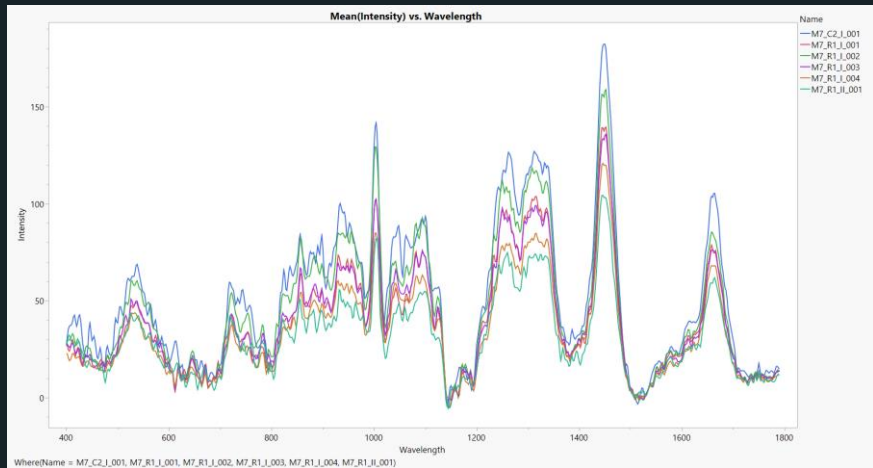
Pre-Processing Spectral Data: Scattering

Standard Normal Variate (SNV)



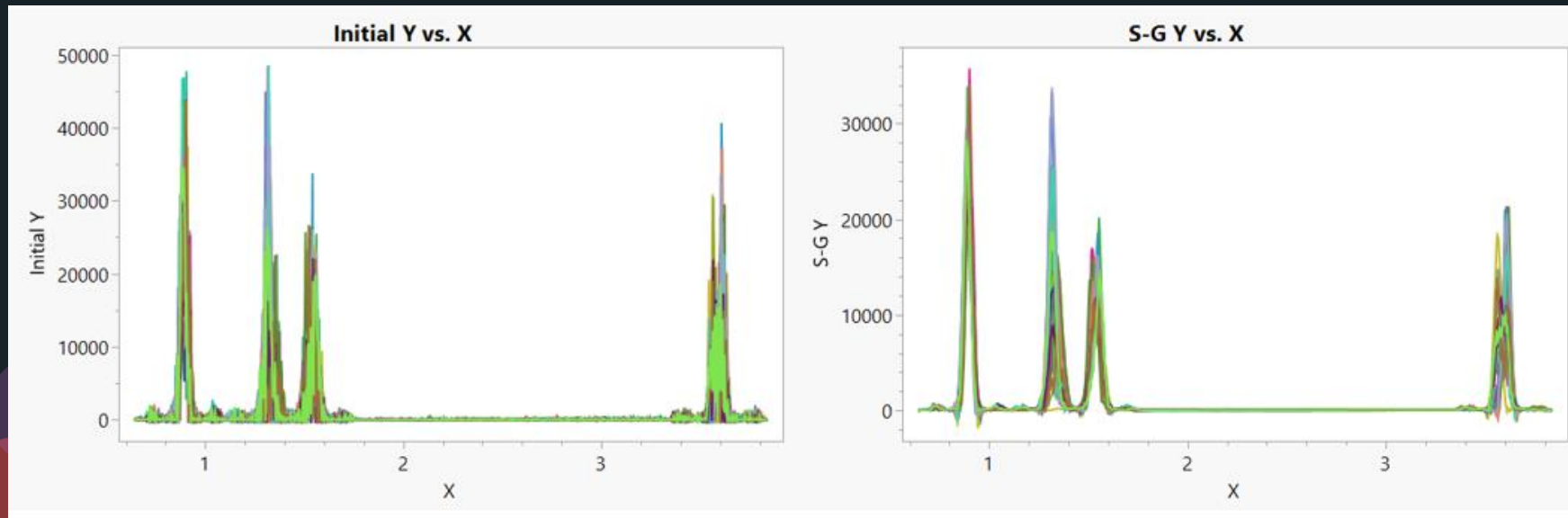
Pre-Processing Spectral Data: Scattering

Multiplicative Scatter Correction (MSC)



Pre-Processing Spectral Data: Noise

Savitzky-Golay (SG) Filter

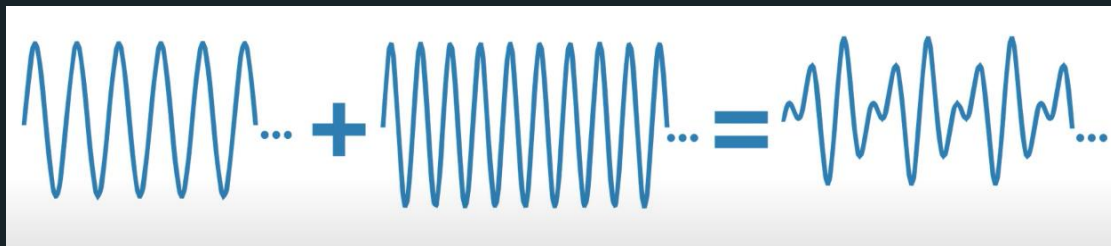
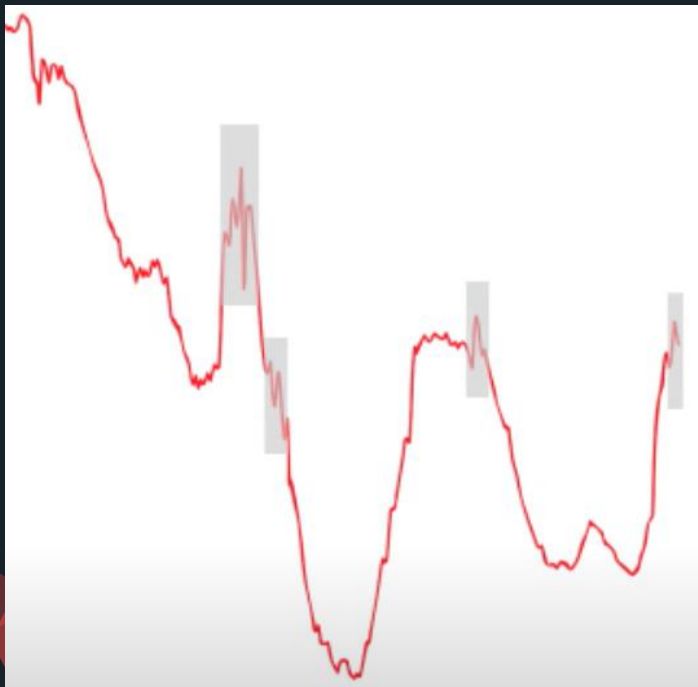


Data Models

- B-Spline:
 - A piecewise polynomial curve, and the knots are the points where the pieces meet
 - For non-periodic data
- P-Splines Basis
 - A piecewise polynomial penalized B-Spline and the knots are the points where the pieces meet
 - Help overfitting noisy data
- Fourier:
 - For periodic (oscillatory) data
- Wavelets (new in JMP Pro 17) ...

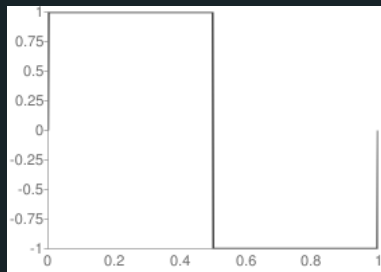
Data Models

From Fourier transformation to Wavelets

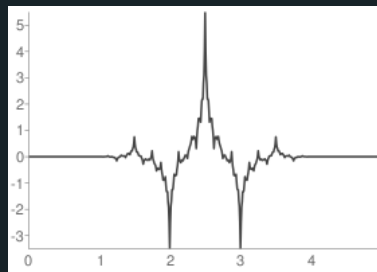


Data Models

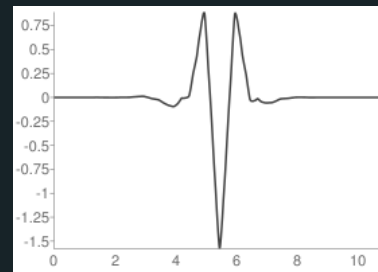
Wavelets



Haar



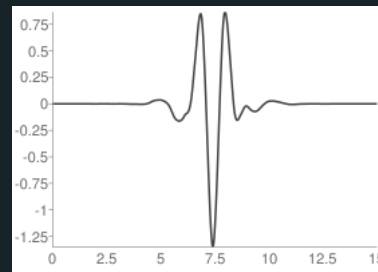
Biorthogonal



Coiflet



Daubechies



Symlet

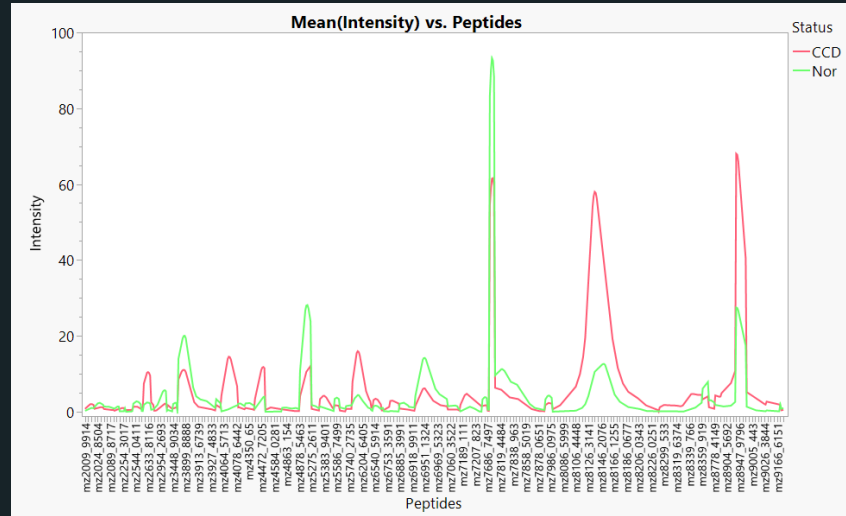
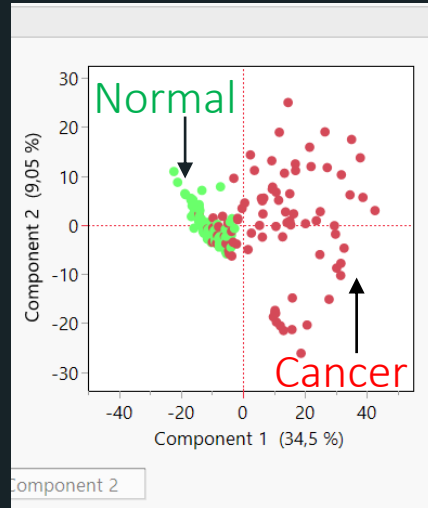
Example 1:

Mass Spectrometry: Prostate Cancer

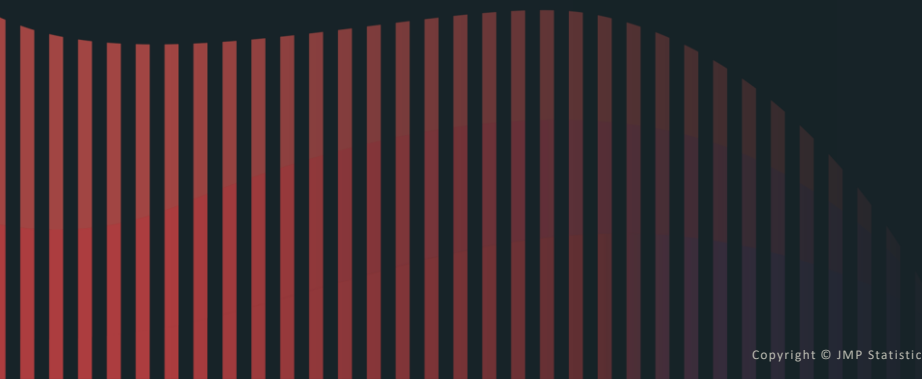
Characterizing changes in protein expression

Mass Spectrometry data

Functional data explorer example



Let's demo!



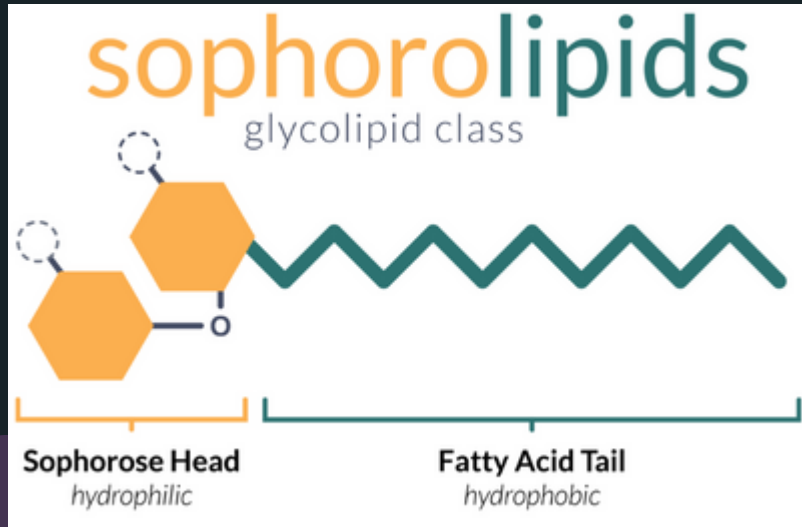
Example 2:

HPLC: Sophorolipids biosurfactants

Condition Optimization for peak separation

Background

Sophorolipids biosurfactants

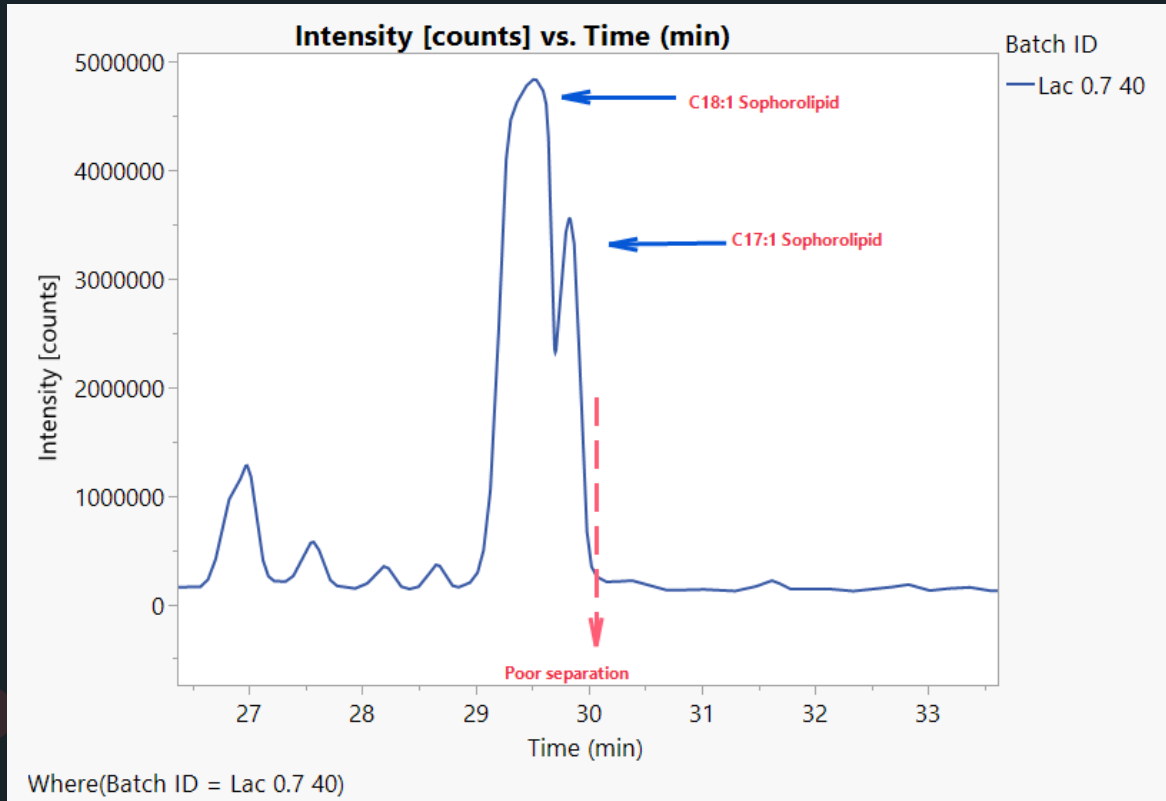


- Produced in non-pathogenic Yeast species
- Anti-microbial action against gram-positive and gram-negative microorganisms
- High Biodegradable properties
- Attractive in food and health industries
- Structural forms exhibit different biological and physicochemical properties
- Challenge in separating these different compounds

<https://community.jmp.com/t5/Technical-Reference-Library/C71-Using-Functional-DoE-to-optimise-analytics-high-performance/tac-p/611042>

Sophorolipids biosurfactants

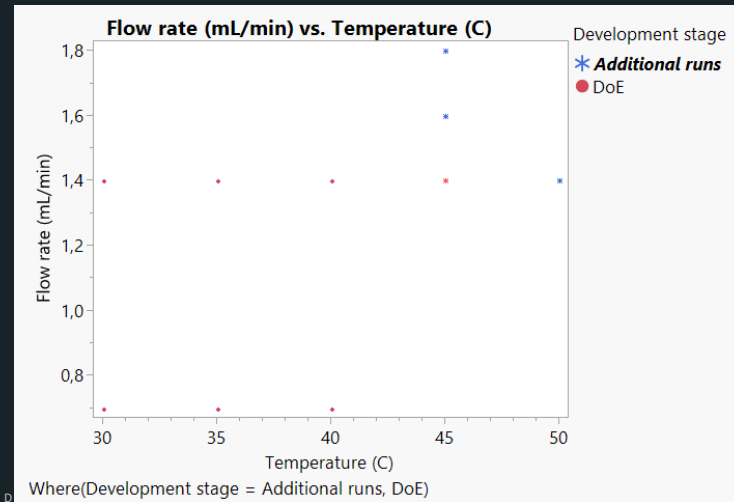
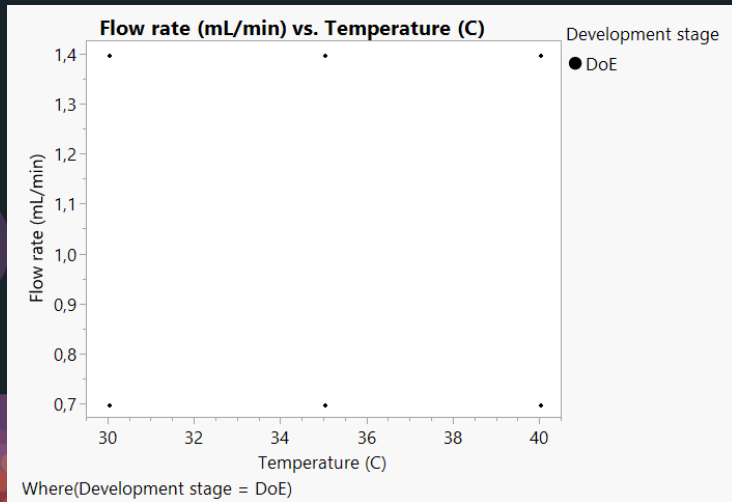
HPLC Poor separation



Sophorolipids biosurfactants

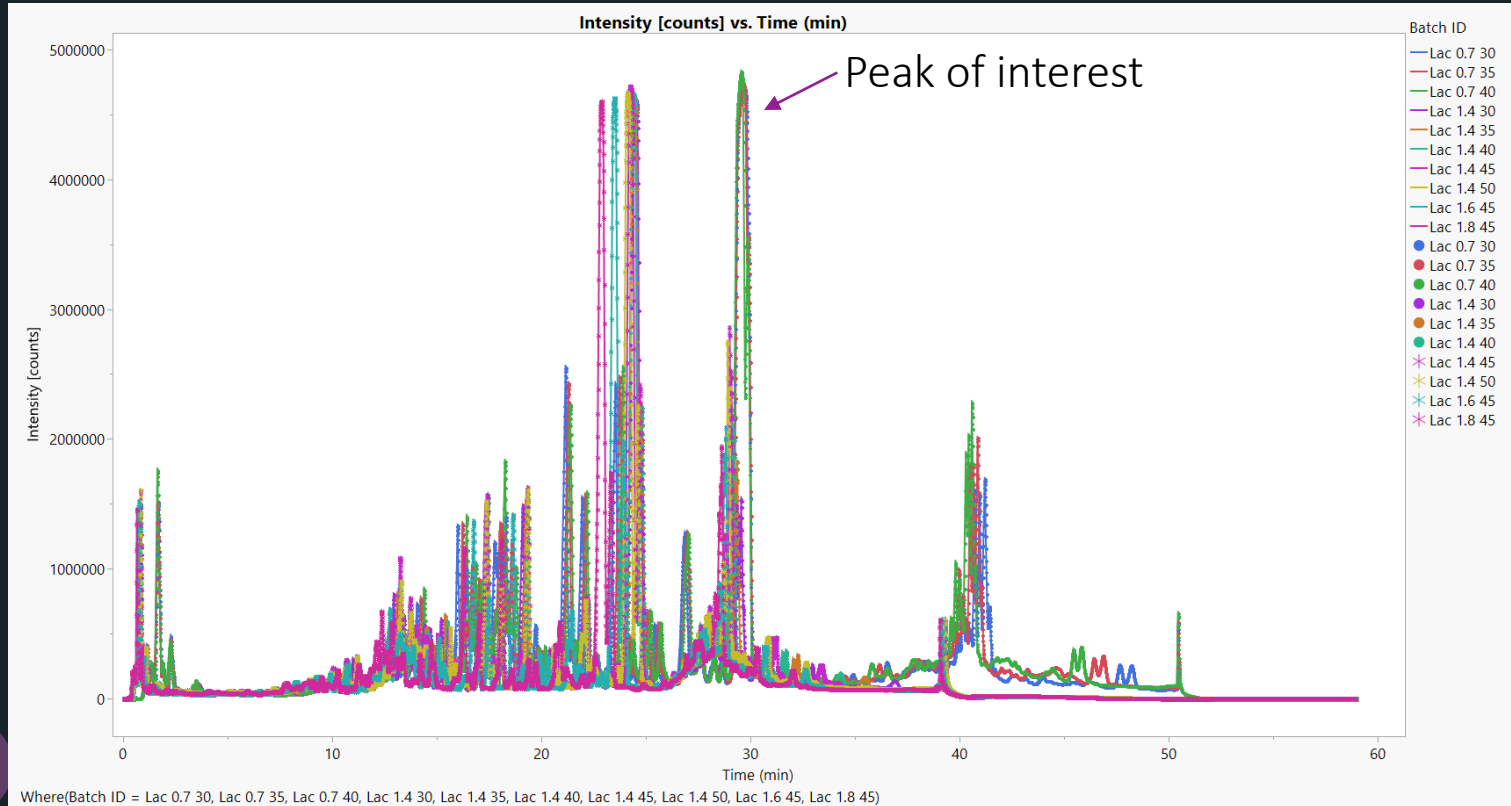
Initial and additional DOE

- To optimise the HPLC settings in order to effectively separate the C18:1 and C17:1 peaks
- Ensure that the peaks are sensitive (no major loss in peak height) and specific (no broad peaks)

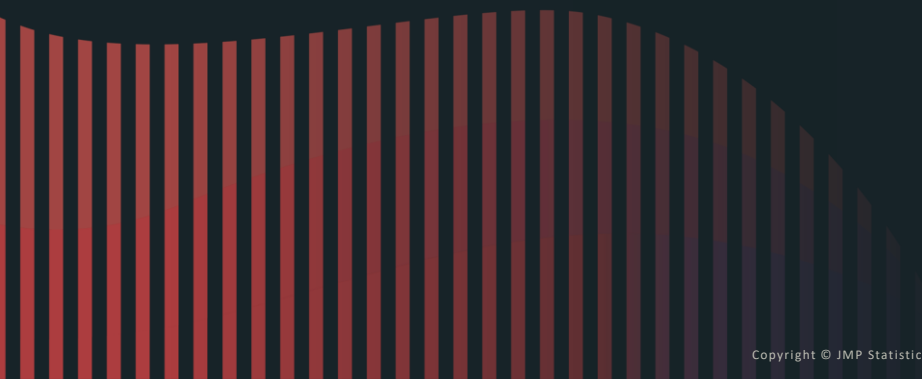


Sophorolipids biosurfactants

HPLC output

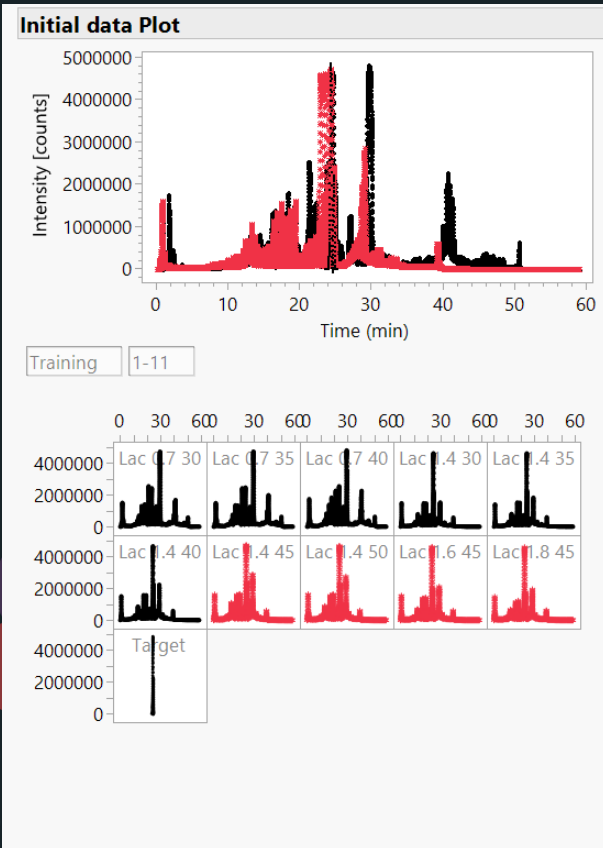


Let's demo!



Sophorolipids biosurfactants

Functional Data Explorer

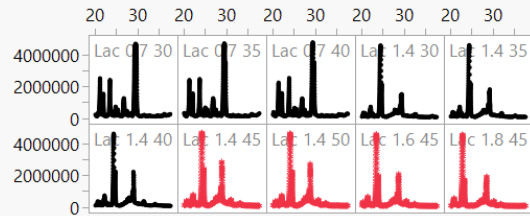
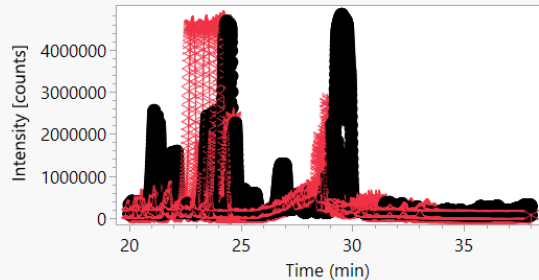


- Data cleanup process:
 - Target function: Target
 - Filter X (20 – 34)
 - Align Maximum
 - Filter X (-1 – 1)
 - Reduce Grid

Sophorolipids biosurfactants

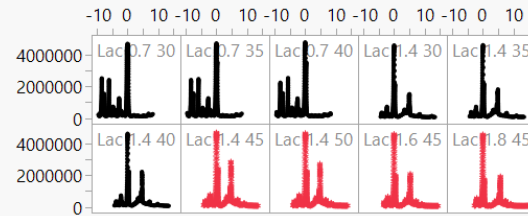
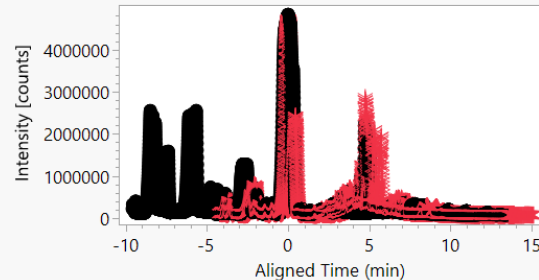
Data Cleanup

Filter X Plot



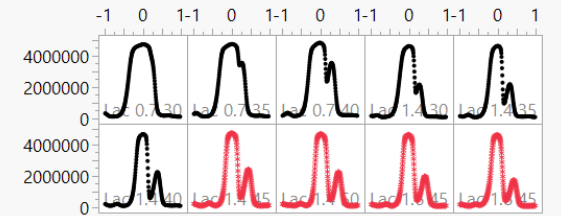
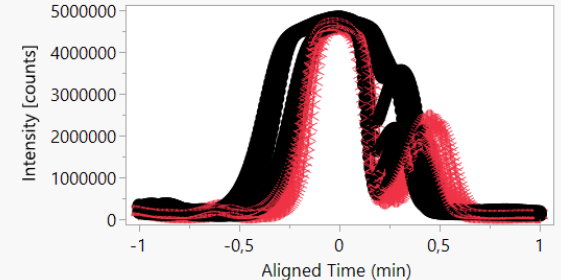
Filter X (20 – 34)

Align Maximum Plot



Align Maximum

Filter X Plot

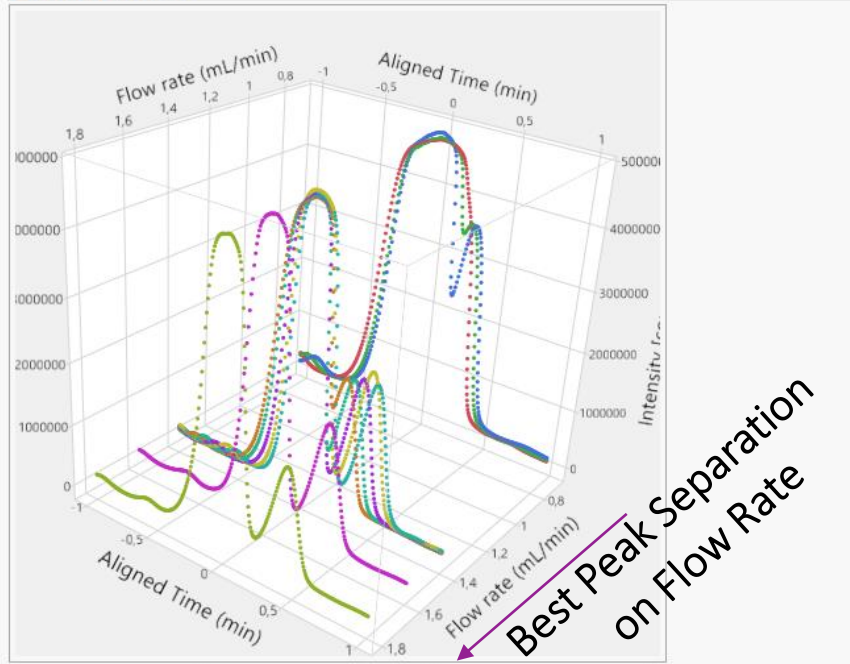


Filter X (-1 – 1)

Sophorolipids biosurfactants

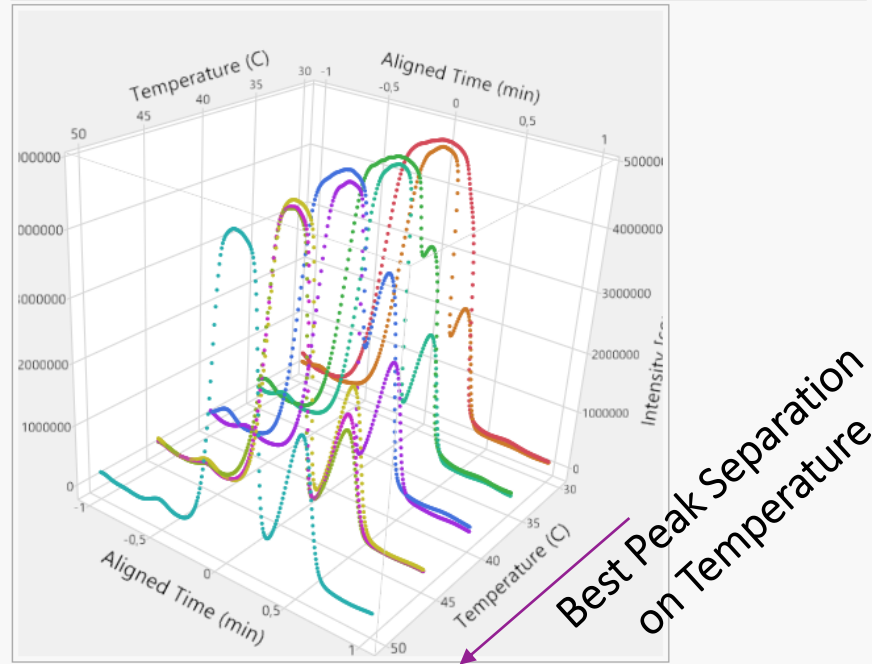
Data Visualisation after data cleanup

Scatterplot 3D



Data Columns | Aligned Time (min) | Intensity [counts] | Flow rate (mL/min)

Scatterplot 3D



Data Columns | Aligned Time (min) | Intensity [counts] | Temperature (C)

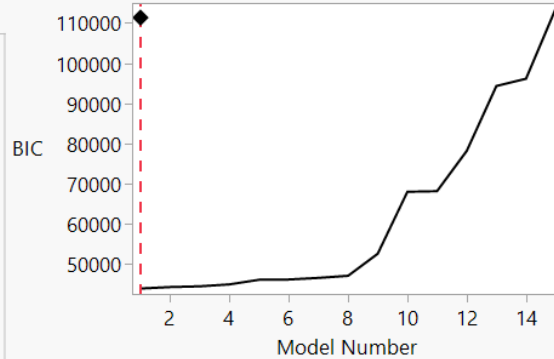
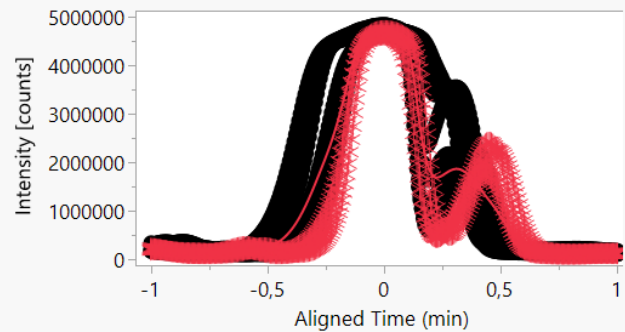
Sophorolipids biosurfactants

Wavelets model

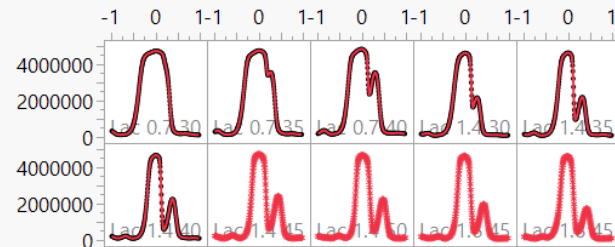
Wavelets on Reduce Grid (301)

Model Selection

Data Coefficients

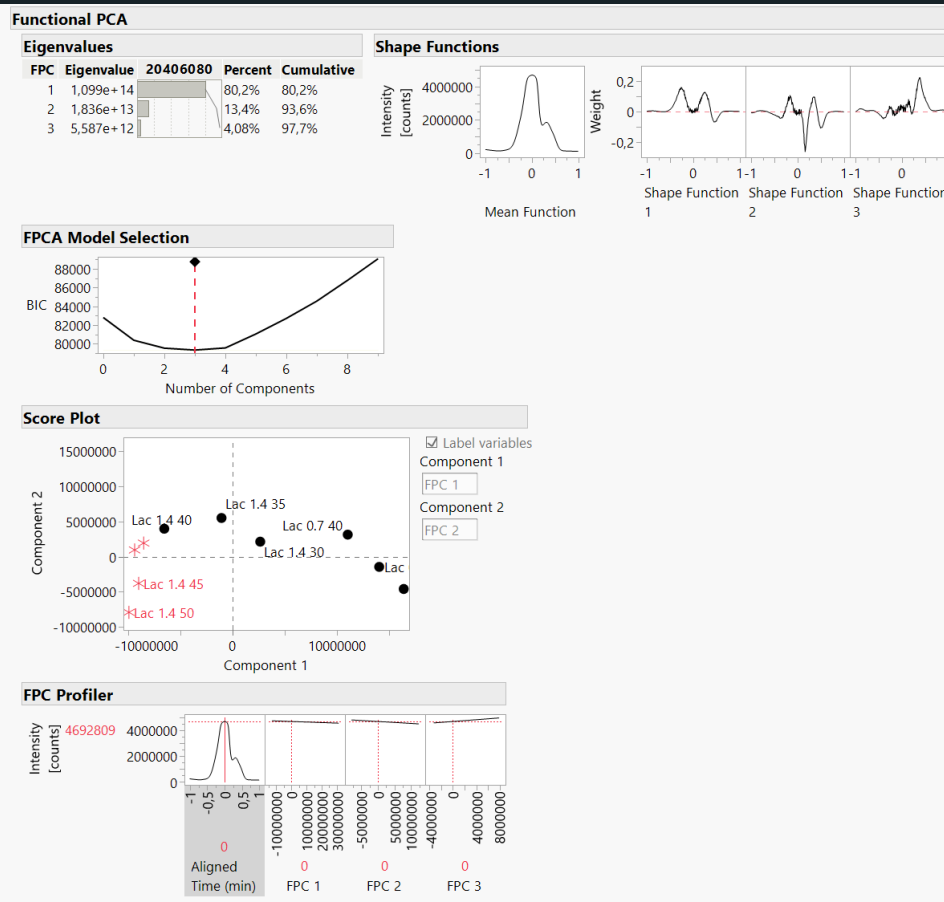


Training 1-10

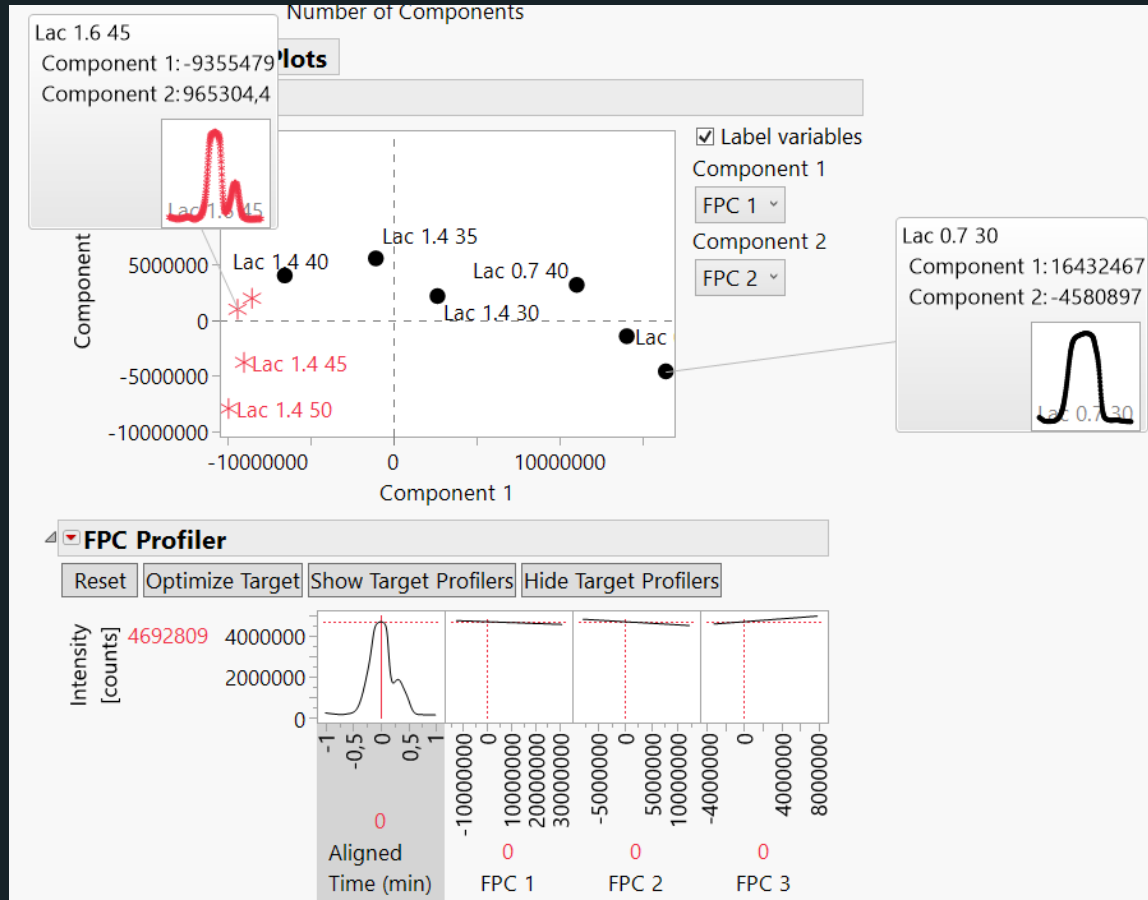


Model	Wavelet	AICc	BIC	GCV
1	Daubechies 10	160869	43914,89	8,143e+8
2	Symlet 20	148428,5	44267,85	9,03e+8
3	Coiflet 5	121635,5	44456,11	9,416e+8
4	Symlet 10	138391,7	44934,36	1,116e+9
5	Coiflet 3	160736	46084,57	1,67e+9
6	Daubechies 20	565213,2	46155,46	2,58e+9
7	Symlet 6	169597,8	46545,85	1,965e+9

Sophorolipids biosurfactants

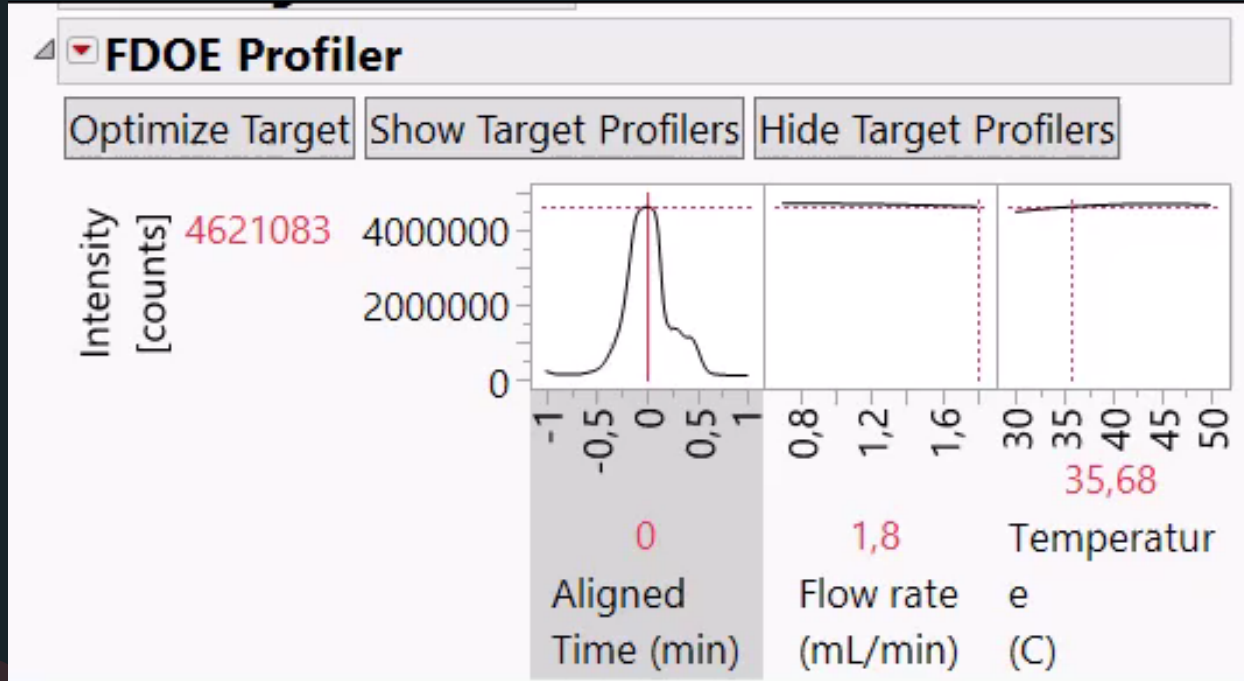


Sophorolipids biosurfactants



Sophorolipids biosurfactants

Functional DOE



THANK YOU!



[jmp.com](https://www.jmp.com)