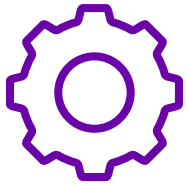
Adding Value with Spectroscopy Data in the PI System

Transferring 100 000 tags to ~100 without losing information

Johan Hultman

Process Intensification

SARTORIUS



Challenge

- The use of different types of spectral instrumentation have exploded in the Life Science, Food & Bev. industry and so has the amount of data associated with this.
- Many new types of applications are depending on the additional information that you can get out of complex, information rich spectra to complement the normal setup of standard process parameters.

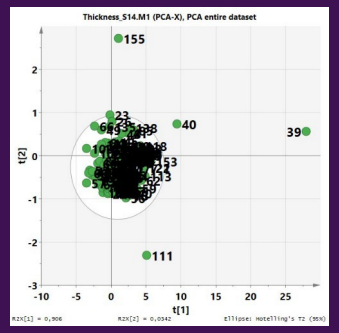
Solution

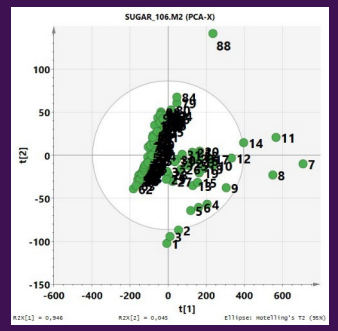
- We have now enabled the use of such information in our own production and together with partners developed tools to help drive Digital Transformation and Automation by using all the data, *compress or extract* the hidden information and made it easily accessible from partner applications like AVEVA PI or AVEVA Historian

Benefits

1. Easily use information from AI/ML prediction models in OSI PI system or the AVEVA™ Historian (Wonderware)
2. Use MVDA monitoring and diagnostic tools to improve our process models
3. Use and compress spectra without losing important information – edge analytics

AVEVA

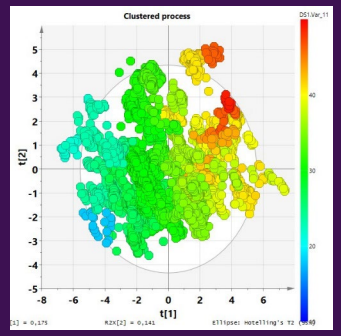


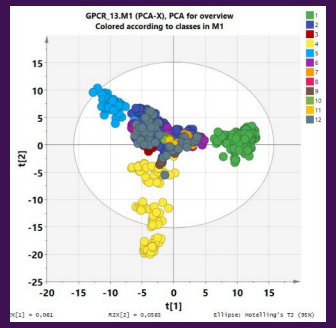


SPECTRAL DATA

AGENDA

For all industries





Sartorius intro

Business Challenge

Why Spectroscopy?

Typical Applications

Challenges

Spectral Data in PI

AVEVA

Sartorius

60+
Locations worldwide, headquartered in Göttingen, Germany

~16,000
Employees[1]

~€3.45bn
Sales revenue[1]

34.1%
EBITDA margin[1,2]

~€37.4bn
Sartorius AG market capitalization[3]; listed on the DAX and TecDAX

~33%
Sales revenue Americas

~41%
Sales revenue EMEA

~26%
Sales revenue Asia | Pacific

1 Preliminary figures as of December 31, 2021, 2 Underlying EBITDA 3 As of December 31, 2021

Data Analytics – Umetrics® Suite

Commitment to Solving Life Science Industry Challenges

- Reducing time to market
- Minimizing costs
- Safeguarding product quality

Long-Standing History in the Life Science Industry

- 30+ years of bioprocess analytics experience
- Life science domain expertise
- Diversified product and service offerings

Large Global Installation Base

- 10 000s of Umetrics® Suite installations globally
- Support teams positioned all around the world

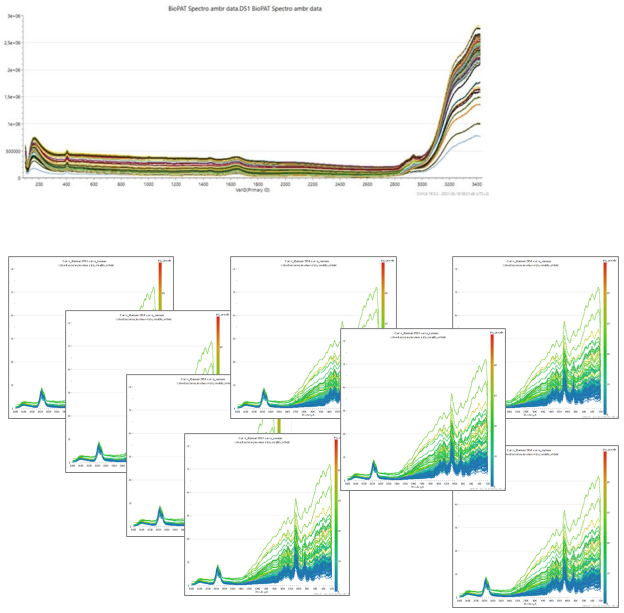
Proven Return on Investment (ROI)

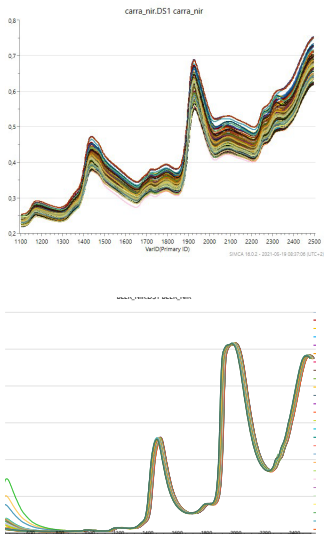
- Millions € saved
- Increased speed of operations
- Minimized risk of production failure

AVEVA

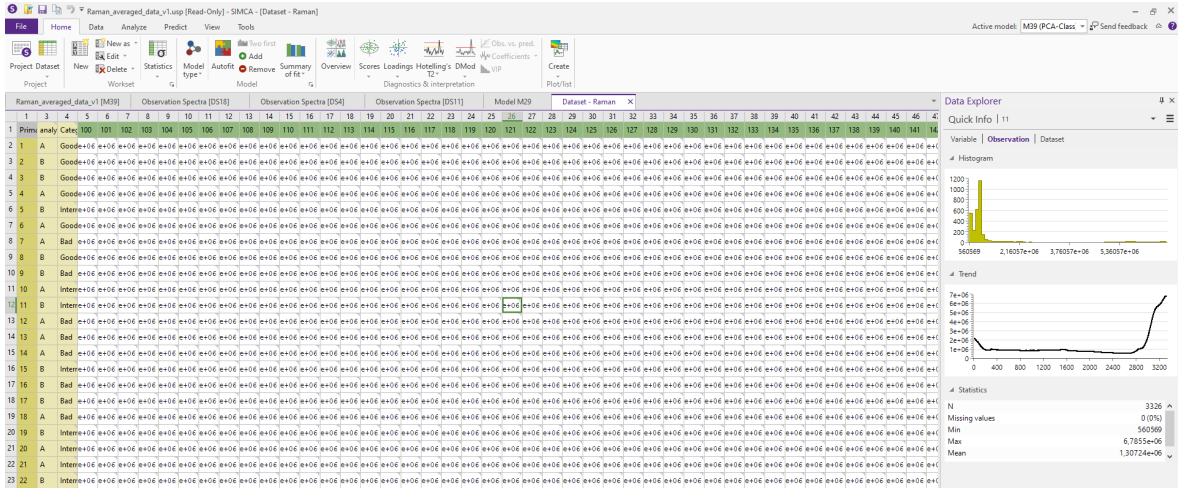
One of the Challenges with Spectral Data

- RAMAN ~ 2200
- NIR ~ 1400
- UV-VIS ~500





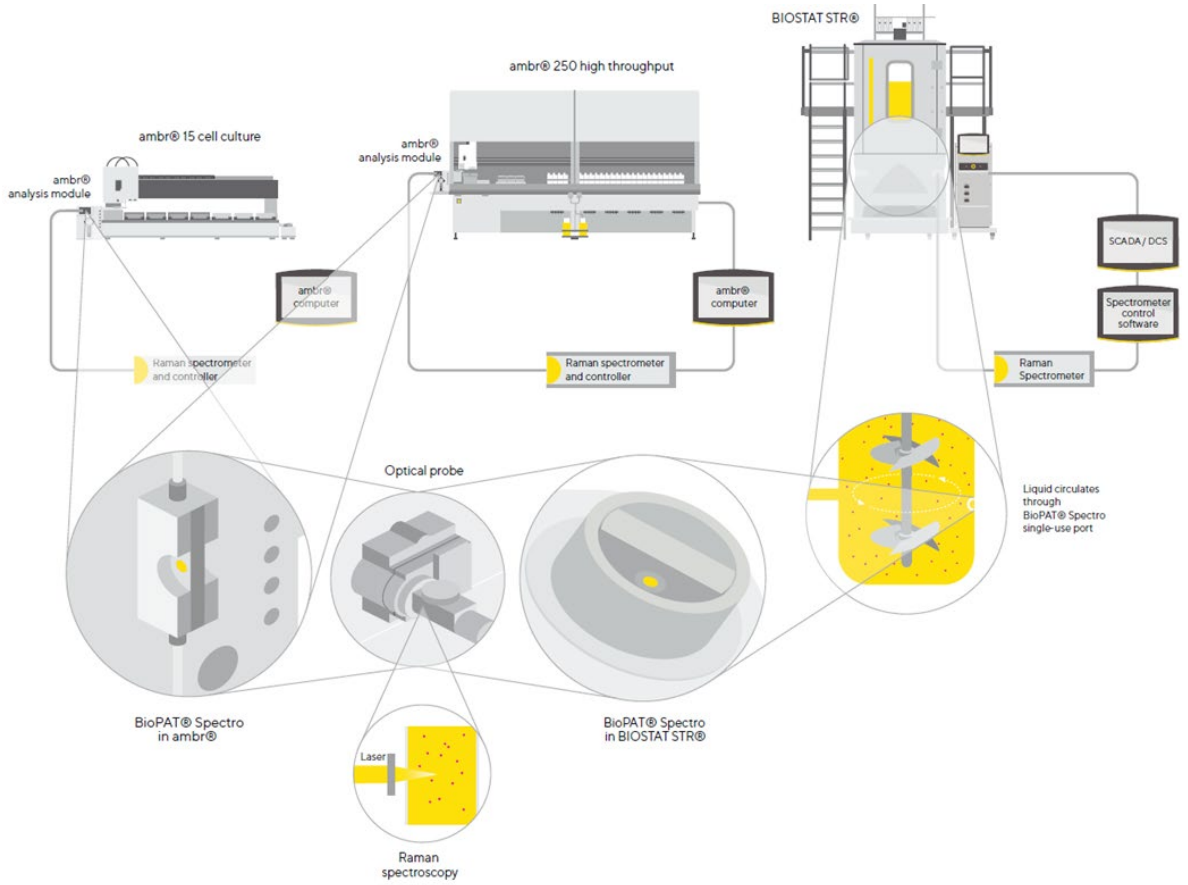
- Need Multivariate to use spectral data to its full potential
- Correlated data
- Normally use of MANY instruments



Business Challenge

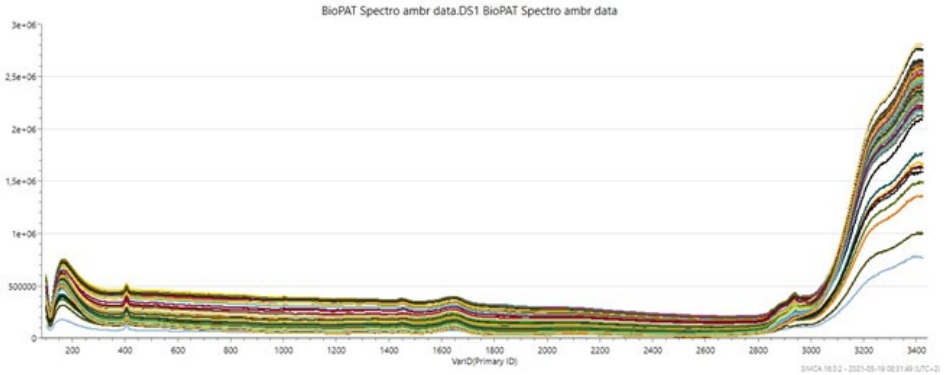
Using Spectral Data to its full potential

- The use of different types of spectral instrumentation have exploded in the Life Science industry and so has the amount of data associated with this.
- One of the hurdles are how to store, use and prioritize the vast amount of data that this adds to the existing databased and process historians on-prem and in the cloud.
- Sartorius have for many years been driving and developing data analytics techniques to understand and use spectral data to its full potential.
- We have now also enabled the use of such information in our own production and together with partners developed tools to help drive Digital Transformation and Automation by using all the data, compress or extract the hidden information and made it easily accessible from partner applications like PI or AVEVA Historian

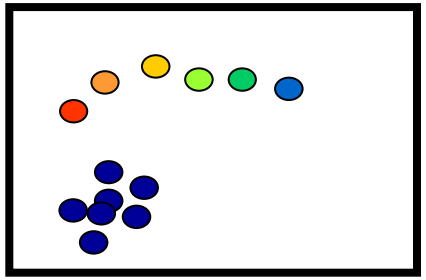
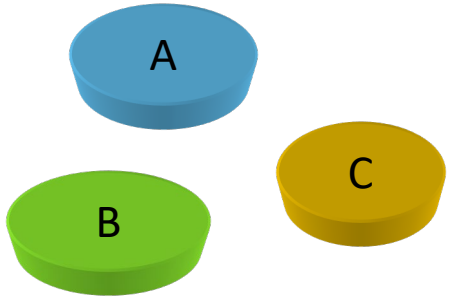
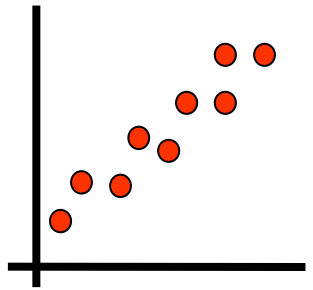


Why use Spectroscopy?

- To develop new rapid analytical methods
  - Based on multivariate (non-selective) spectroscopic sensors
  - UV, Vis , NIR, IR, Raman, Fluorescence
- For fast determination of quality
  - Concentration of constituents/ analytes of interest
  - Quality properties like viscosity, particle size, sensory descriptors etc.
  - Parameters that may be tedious and time-consuming to determine using conventional analyses
- Quality control in real-time
  - End-point detection
  - Process monitoring
  - Process Analytical Technology (PAT)



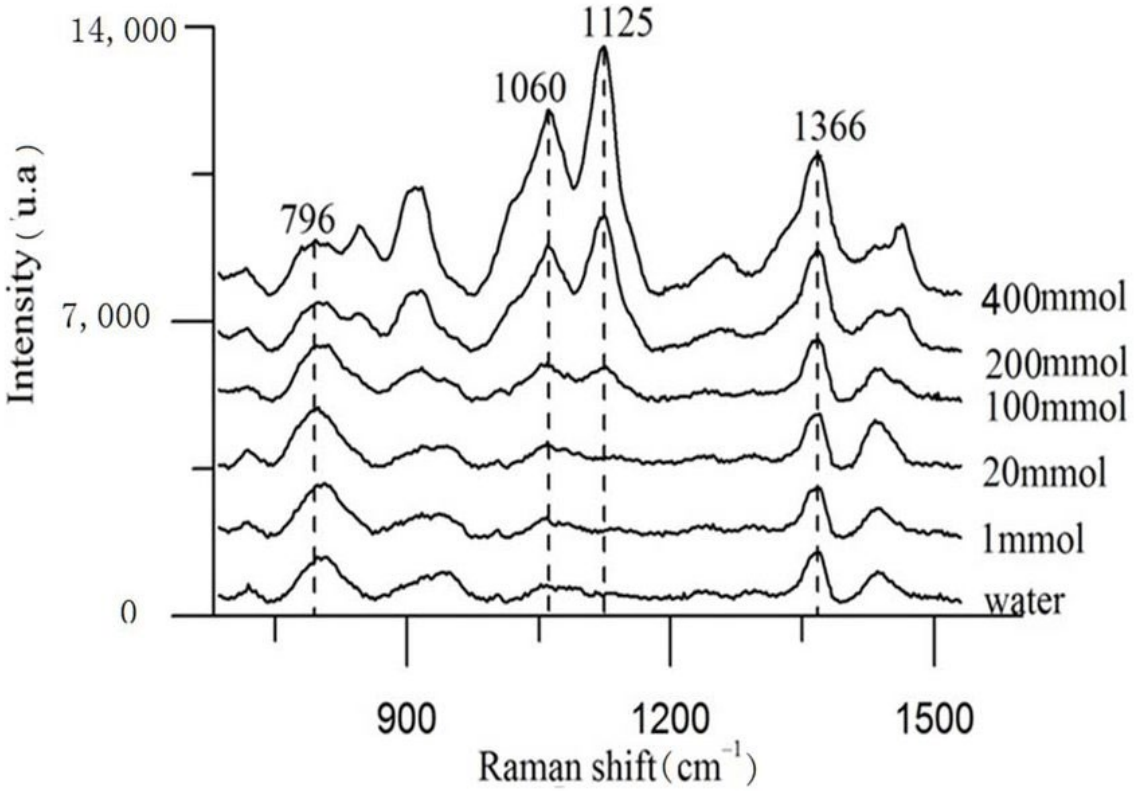
Typical Spectroscopy Applications

Overview	Classification	Regression
Process monitoring Assessing biological variation Trends in quality 	Classification of raw materials / foodstuffs Authenticity / counterfeit Genomics / Proteomics / Metabolomics i.e. Control vs Treated 	Material properties Calibration models PAT models– moisture/ particle size / actives Sensory information Process Quality prediction Batch Modelling Process Modelling 
PCA	**PCA-Class/ PLS-DA / OPLS-DA**	**OPLS/PLS**

Spectroscopy Basics

- Spectroscopy is used to measure **molecular vibrations and energy levels** in a molecule.
  - Each molecule has a unique fingerprint when stimulated with light
  - For example, glucose absorbs light at different wavelengths and levels than fructose and galactose
- Light-based techniques examine absorption, transmission, or emission across multiple wavelengths
  - Wavenumber unit is frequently used for easier numbers
- Peak heights and areas are directly correlated with concentration of molecules – easy quantitation…
  - Beer's Law from high school chemistry
- But what about in a mixture?

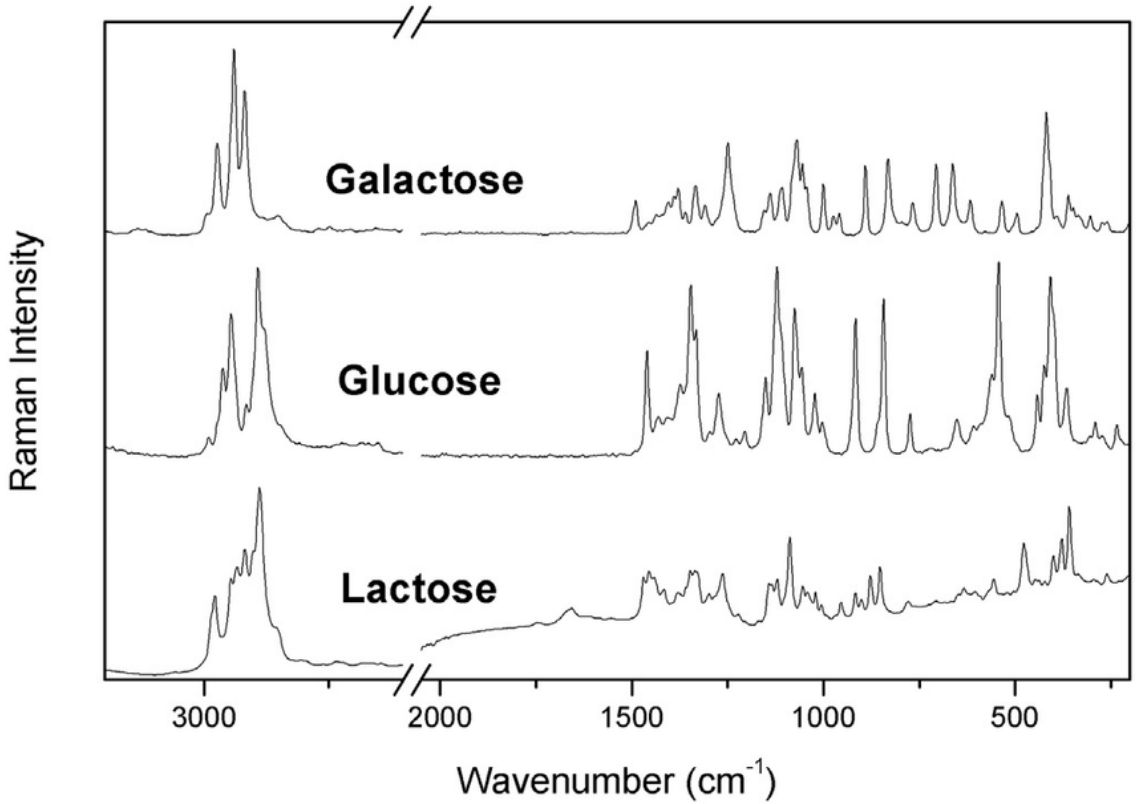
Raman spectra of aqueous glucose



DOI: 10.1371/journal.pone.0048127.g002

Spectroscopy of a Mixture

- In a mixture, peaks are likely to overlap.
  - In simple mixtures, maybe one wavelength per constituent can be identified
    - Though no ability to detect contamination
- In complex mixtures, we use multivariate analysis to “unmix” the fingerprints that are present in an acquired spectrum
- Even more critical in aqueous mixtures, where the solvent effectively smooths out all sharp vibrational features
  - Solvent absorbs and dilutes much of the vibrational energy / signal of the analytes



DOI: 10.1016/j.foodres.2017.08.043

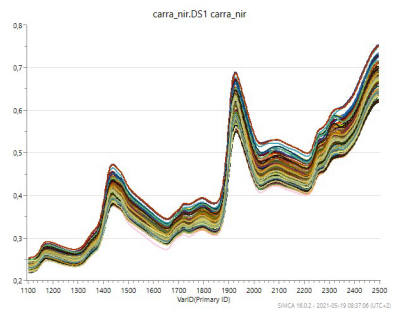
Advantages and Disadvantages of Spectroscopy

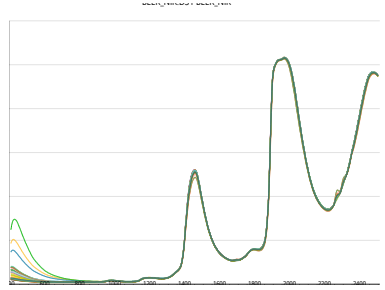
Advantages

- Spectroscopy measurements require minimal preparation before measurement
  - Pre-filtration is occasionally needed
- Non-destructive, minimal maintenance
- Rapid measurements allow for fast decision-making and early detection of problems
- Multi-channel measurements allows for measurements of complex mixtures
  - Multiple wavelength measures in single spectrum
- Sensitive to process changes – can be great!

Disadvantages

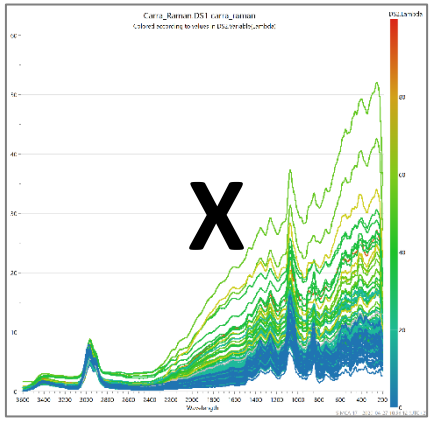
- Light-based methods that are susceptible to light interference, fluorescence, and temperature changes
- Requires advanced data analysis methods to model
  - Why we're here today!
- Less accurate than reference methods
- Sensitive to process changes – can be bad!





Spectra compression for use in SIMCA-online/Studio/PI

Spectra



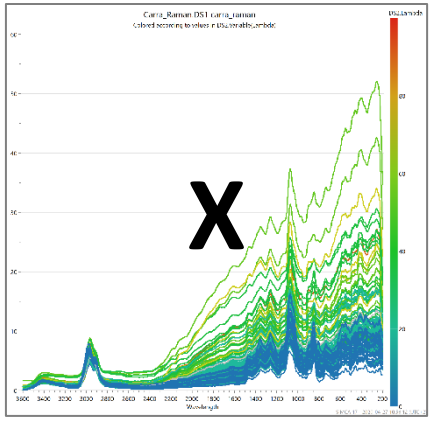
PLS
OPLS

Predictions

Glucose	Lactacte
2.740	2.740
2.010	2.010
3.750	3.750
3.750	3.750
3.690	3.690
3.690	3.690
3.690	3.690
3.690	3.690
5.230	5.230

Y

Spectra

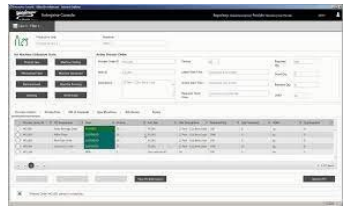


PLS
OPLS

Compressions

T1	T2	DmodX
2.740	2.740	2.740
2.010	2.010	2.010
3.750	3.750	3.750
3.750	3.750	3.750
3.690	3.690	3.690
3.690	3.690	3.690
3.690	3.690	3.690
3.690	3.690	3.690
5.230	5.230	5.230

Y

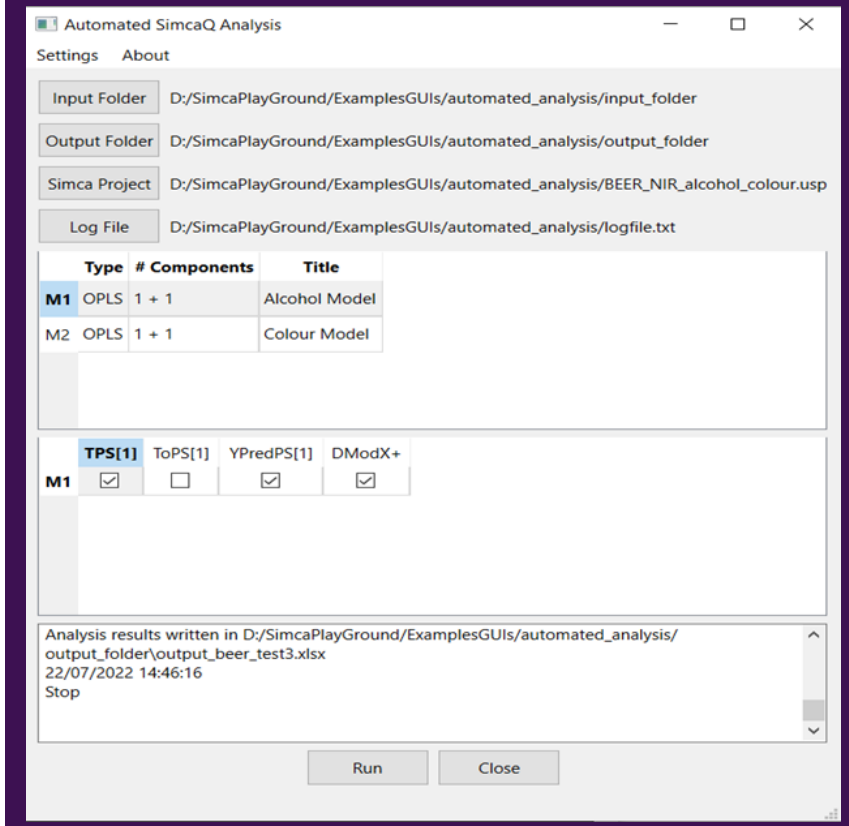


Implementation Details

Using SIMCA-Q as the compression tool

- NEW tool to complement the current portfolio and enable a better use of spectral information.
  - Quick
  - Light footprint
  - Flexible
  - Next release will have multiple models

- Will start POC with a number of customers

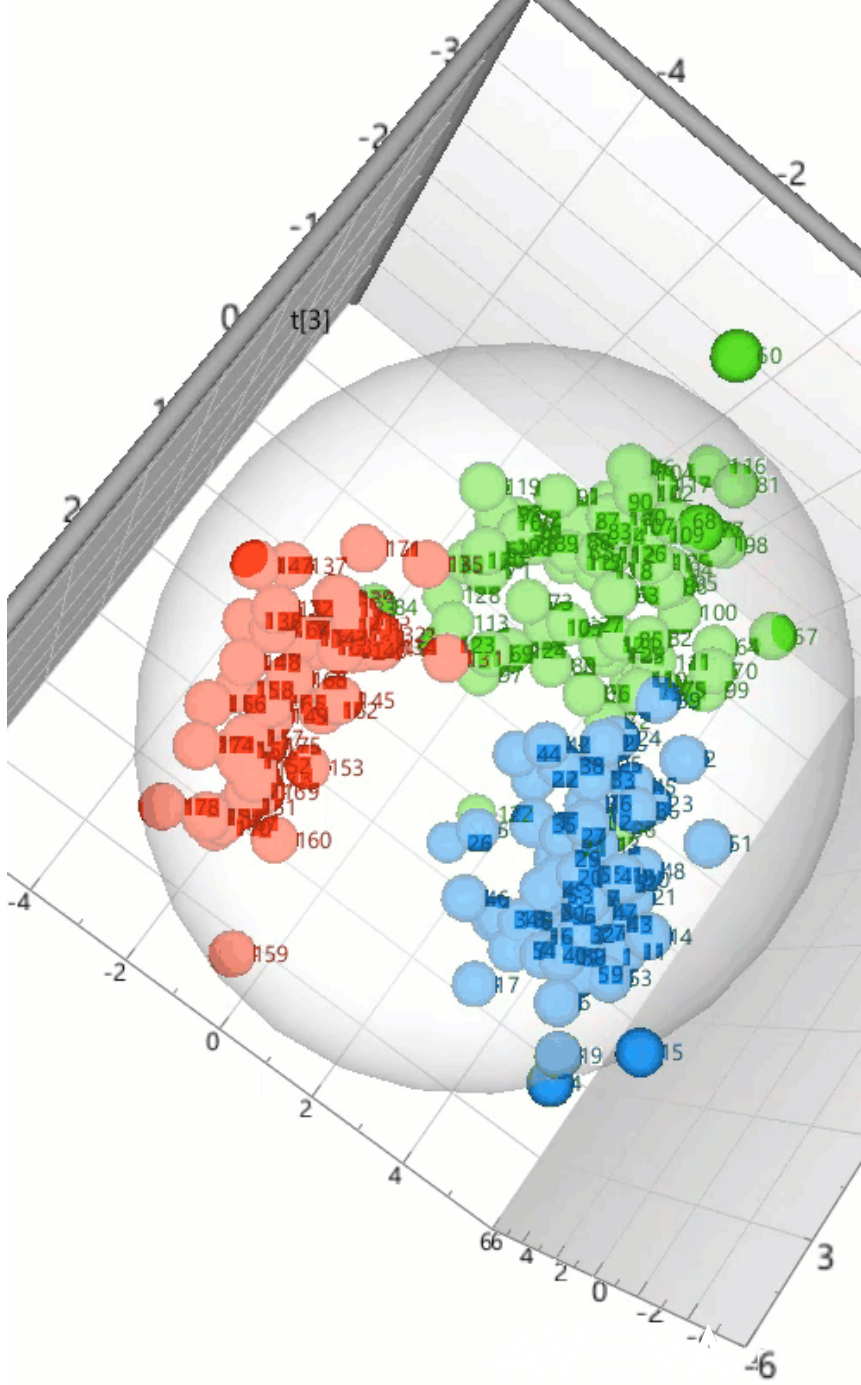


Impact of implementation

- Internal:
  - Real-time predictions
  - Compressed data
  - Easier use of predictions + diagnostics
- External:
  - End-users can direct use Spectral data into their own applications
  - Partnering with Software and Automation suppliers to enhance their solution for spectral handling in an easy way.

3 things to remember

1. Easily use and deploy predictive information from AI/ML models
2. Use MVDA monitoring and diagnostic tools to improve our models in batch and continuous processes
3. Spectral data can be used direct into any other application
   a) Predictions
   b) Compressing tool



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Questions?

Please wait for the microphone.

State your name and company.

Please remember to…

Navigate to this session in the mobile app to complete the survey.

Thank you!

AVEVA

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Over 20,000 enterprises in over 100 countries rely on AVEVA to help them deliver life's essentials: safe and reliable energy, food, medicines, infrastructure and more. By connecting people with trusted information and AI-enriched insights, AVEVA enables teams to engineer efficiently and optimize operations, driving growth and sustainability.

Named as one of the world's most innovative companies, AVEVA supports customers with open solutions and the expertise of more than 6,400 employees, 5,000 partners and 5,700 certified developers. With operations around the globe, we are headquartered in Cambridge, UK and listed on the London Stock Exchange's FTSE 100.

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