



Making sense of your data

*Donnez du sens à vos données*

We help you get the best from your data  
for a better product and process control

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Dr. Sylvie ROUSSEL, CEO



# Ondalys in short



**FOUNDED IN 2003**

- › **French Leader** in chemometrics
- › Located in Montpellier (34), **France**



## Customers

- › 50% Pharma-biotech
- › 25% Chemistry
- › 15% Food/Agri
- › 10% Optical Equipment



## Core business

- › Consulting / R&D  
    > **200 projects**
- › Training  
    > **1000 trainees**
- › Software retail  
    > **4 main chemometrics software**



## Chemometrics - Machine learning

- › Data mining
- › Spectroscopic calibrations
- › Model robustness
- › Sensor fusion
- › Process monitoring (MSPC, BSPC)
- › Design of Experiments (DoE / QbD)



## Multidisciplinary Team

- › Diverse application sectors
- › Instrumentation / Data
- › Machine Learning



## Software partners

 **EIGENVECTOR**  
RESEARCH INCORPORATED

 **MathWorks®**

 **StatEase®**

 **SARTORIUS**

 **aspentech**

# They trust us in various application sectors



Pharma – Biotech



Chemicals – Petro.



Agriculture – Food



Optical sensors – R&D



SANOFI



DEINOVE



Chemicals – Petro.



SOLVAY



TOTAL



Agriculture – Food



bertin  
TECHNOLOGIES



ARKEMA



# Instrumental data



## SPECTROSCOPY

- > Near Infrared (NIR)
- > Infrared (FTIR)
- > Raman
- > UV
- > Fluorescence...



## PROCESS PARAMETERS

- > In-line, on-line, at-line analyzers
- > Process parameters
- > Industrial IoT
- > In-line spectrometers



## IMAGING

- > Hyperspectral
- > Multispectral
- > RGB
- > UV, visible, NIR, Raman, ...



## PHYSICO-CHEMICAL

- > HPLC, GC
- > GC-MS
- > Physical measurements
- > ICP...



# A comprehensive service offer in Machine Learning

## Coaching

- > Expertise Transfer
- > Troubleshooting
- > Recommendation

## Training

- > Open-courses
- > In-house courses

## Model maintenance

- > Model Update
- > Inter-Instrument Transfer
- > Scale-up



## Software implementation

- > Sensor software
- > ML software
- > Open-source software

## Audit

- > On existing models and spectroscopic implementation

## Consulting

- > Acquisition optimization
- > Design of Experiments (DoE)
- > Quality-by-Design (QbD)

## Proof of concept

- > Machine Learning (ML) algorithm benchmarking
- > Data fusion
- > Process monitoring (PAT)

## Model development

- > Calibration robustness
- > Model Validation



Making sense of your data

# Customer Success Cases

# Proof of Concept (PoC) for discrimination based on micro-spectrometer



## Pectic composition of grape musts

- > Dosage of pectin in the grape musts
- > Concentration of pectolytic enzymes to add for juice clarification?



## Fast decision-aid tool based on (NIR) near-infrared portable spectrometer

- > SVM discrimination (pectin / no pectin) : 3 % of error
- > Tests during pectolytic process

**Classification Rate (CR) = 97.1% → Error = 2.9%**

Balanced Classification Rate (BCR) = 95% → Error = 5.0%

	% correct classification	
	CV	Test set #1
T0 – T0bis (pectin)	100%	100%
T1 (pectin)	100%	100%
TF (no pectin)	100%	100%
TQ (no pectin)	75%	50%
BCR	97.5%	95.0%
CR	98.5%	97.1%

# Proof of Concept (PoC) for product composition prediction



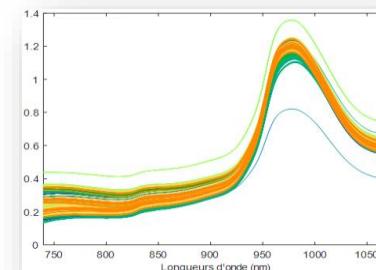
## Grape must data sets

- > 6 pectolytic enzyme suppliers
- > 2 pectin types x 2 concentrations
- > Measurements during pectolytic process
- > 2 classes : Pectin / No pectin



## Micro Near-Infrared (NIR) Spectroscopy

- > NIR spectrometer : SCIO™
- > Wavelengths : [740-1070nm], 35gr

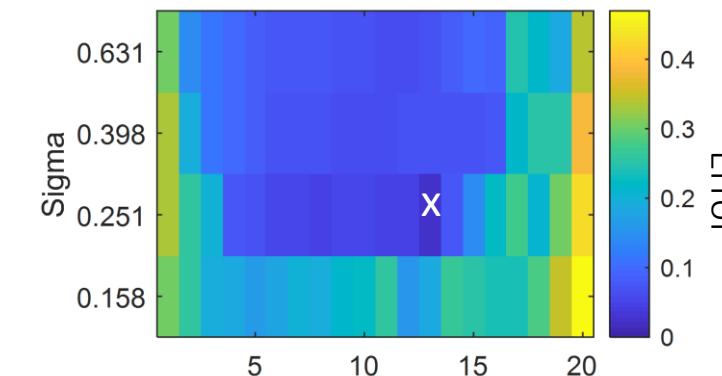


## Machine Learning Methods

- > Support Vector Machines (SVM)
- > 2 class-discrimination (Pectin / no Pectin)
- > Spectral preprocessing and compression



## SVM optimization grid search



# Training sessions

Ondalys provides you with a tailored program according to :

## Chemometrics / Machine Learning methods

- > **Exploratory analysis**  
→ PCA, ICA, MCR, Clustering, ...
- > **Quantitative model optimization**  
→ PLS, LWR, SVR, RF, ANN, ...
- > **Classification / Pattern Recognition**  
→ PLS-DA, SIMCA, SVM, RF, ANN, ...
- > **Calibration transfer**
- > **Sensor fusion / Multi-block analysis**
- > **Process monitoring** (MSPC, BSPC)
- > **Experimental design** (DoE, QbD)



SPECTROSCOPY



PROCESS PARAMETERS



IMAGING



PHYSICO-CHEMICAL



Pharma – Biotech



Chemicals – Petro



Agriculture – Food



Optical sensors

# Our training partners and software packages



## Calibration software



MathWorks



SIMCA<sup>®</sup>



## Online implementation

SIMCA-online



## Design-of-Experiment (DoE)

DESIGNEXPERT  
VERSION 13



MODDE<sup>®</sup>



## Training institutes



SARTORIUS

StatEase.

aspentech

ondalys

# Upcoming open-course training sessions (S2 2022)

## > Analyse de données spectroscopiques

- 27 au 29 Septembre 2022 - Paris
- 4 au 6 Octobre 2022 - Lyon
- 15 au 17 Novembre 2022 - Paris
- 6 au 8 Décembre 2022 - Montpellier

## > Analyse de données multivariées

- 20 & 21 Septembre 2022 - Montpellier
- 2 & 3 Novembre 2022 - Montpellier

## > Analyse de données sous Python

- Spectroscopiques du 11 au 13 Octobre 2022 - Montpellier
- Utilisation de scripts Python le 25 Octobre 2022 - Montpellier

## > Support Vector Machines SVM

- 22 Novembre 2022 - Paris

## > Supervision de procédés

- 7 et 8 Juin 2022 - Strasbourg
- 3& 4 Novembre 2022 - Lyon

## > Plans d'expériences

- 4 & 5 Octobre 2022 - Montpellier



# THANK YOU FOR YOUR ATTENTION



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## Disponibles sur notre stand

- > Livre blanc sur la comparaison des méthodes de ML
- Poster µspectromètre / SVM
- Planning des formations S2 2022
- > Logiciels de chimiométrie
- > Offre d'emploi
- > L'équipe Ondalys ☺ !
  - > Sandra AUBERT
  - > Cécile FONTANGE
  - > Sylvie ROUSSEL