

# Varietal discrimination of Extra Virgin Olive Oils – “terroir” effect

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4€/L

VS

20€/L



Quality

Traceability



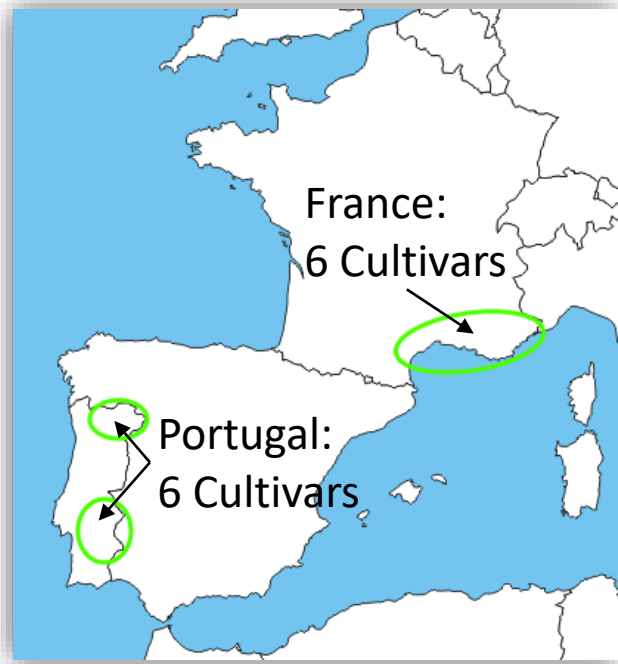
Olive variety / ripeness

Climate / soil

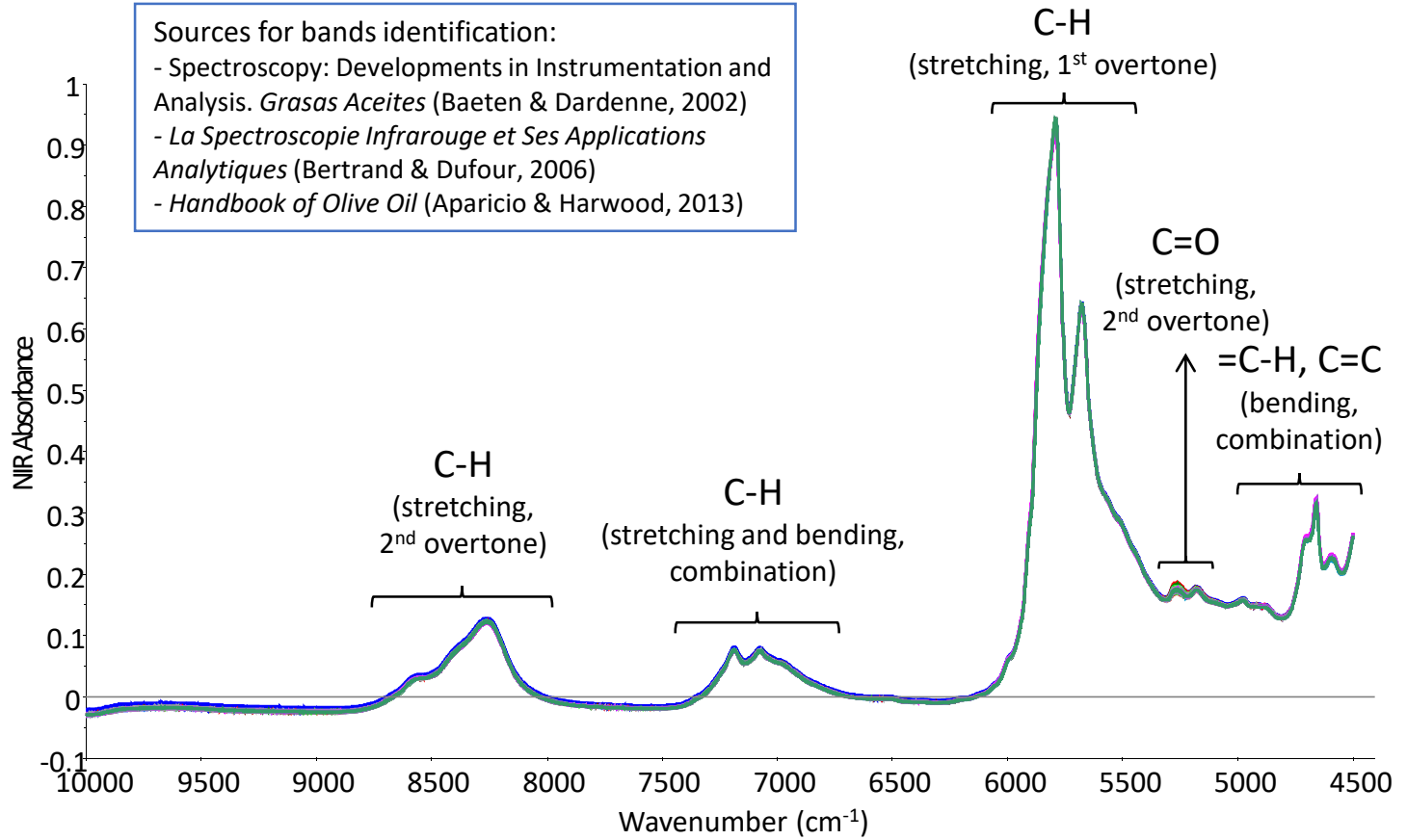
Agricultural practice

Extraction method



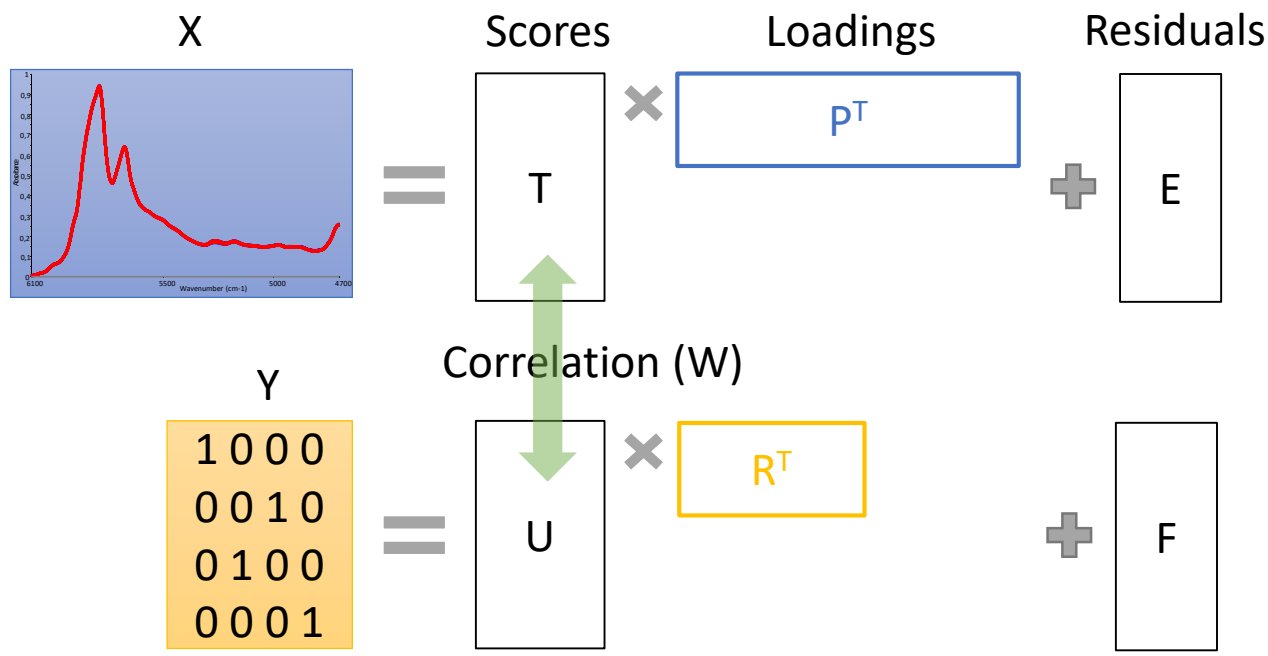


Sources for bands identification:  
 - Spectroscopy: Developments in Instrumentation and Analysis. *Grasas Aceites* (Baeten & Dardenne, 2002)  
 - *La Spectroscopie Infrarouge et Ses Applications Analytiques* (Bertrand & Dufour, 2006)  
 - *Handbook of Olive Oil* (Aparicio & Harwood, 2013)



- 🔍 133 EVOO samples, 1 production year
- 🔍 Near Infrared Spectroscopy: Thermo Nicolet Antaris II, 2 spectra / sample, transmission acquisition: range 10 000 to 4 500  $\text{cm}^{-1}$ , resolution 4  $\text{cm}^{-1}$ , accumulation 16 scans
- 🔍 Chemometrics: The Unscrambler X 10.4, various pre-treatments (Detrend, SNV, SG 1<sup>st</sup> derivative, EMSC), Principal Component Analysis, Partial Least Squares 1 - Discriminant Analysis regression model

EVOO: Extra Virgin Olive Oil – SNV: Standard Normal Variates – SG: Savitzky-Golay – EMSC: Extended Multiplicative Scatter Correction



$$Y_{predicted} = X W (P^T W)^{-1} R^T$$

- Samples with theoretical value = 1
- 🟢 True positive if  $Y_{pred} > 0.6$
  - 🔴 False negative if  $Y_{pred} < 0.5$
  - 🟡 Uncertain if  $Y_{pred} \in [0.5 ; 0.6]$
- Samples with theoretical value = 0
- 🟢 True negative if  $Y_{pred} < 0.4$
  - 🔴 False positive if  $Y_{pred} > 0.5$
  - 🟡 Uncertain if  $Y_{pred} \in [0.4 ; 0.5]$

Quality criteria of the model :

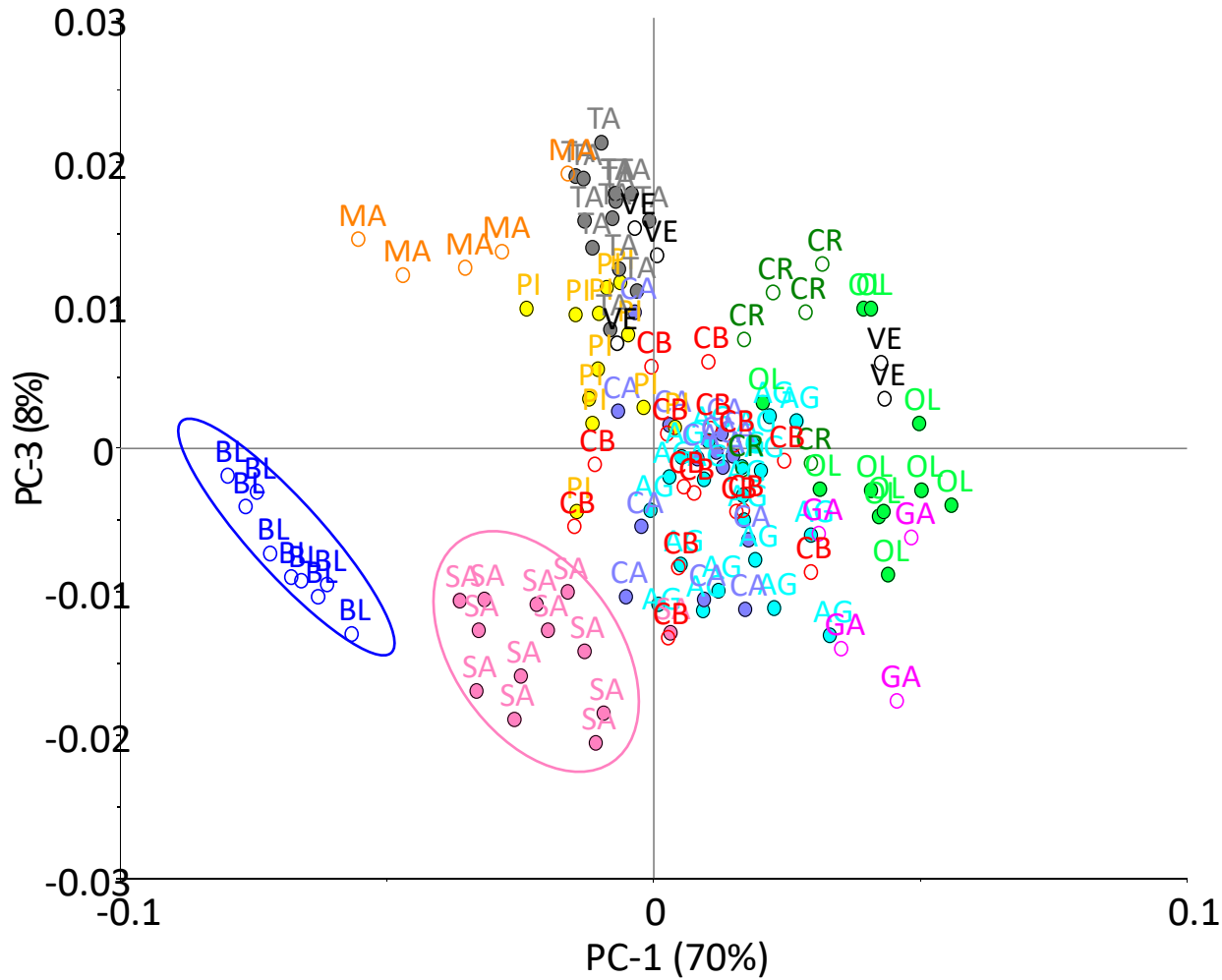
$$\% \text{ correct} = \frac{\text{true positive} + \text{true negative}}{\text{true positive} + \text{true negative} + \text{false positive} + \text{false negative} + \text{uncertain}} \times 100$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (Y_{Reference} - Y_{Predicted})^2}{n}}$$

$$\text{sensitivity} = \frac{\text{true positive}}{\text{expected positive}}$$

$$\text{specificity} = \frac{\text{true negative}}{\text{expected negative}}$$

### PCA Score plot after EMSC on NIR spectra (6100-4700 cm<sup>-1</sup>)

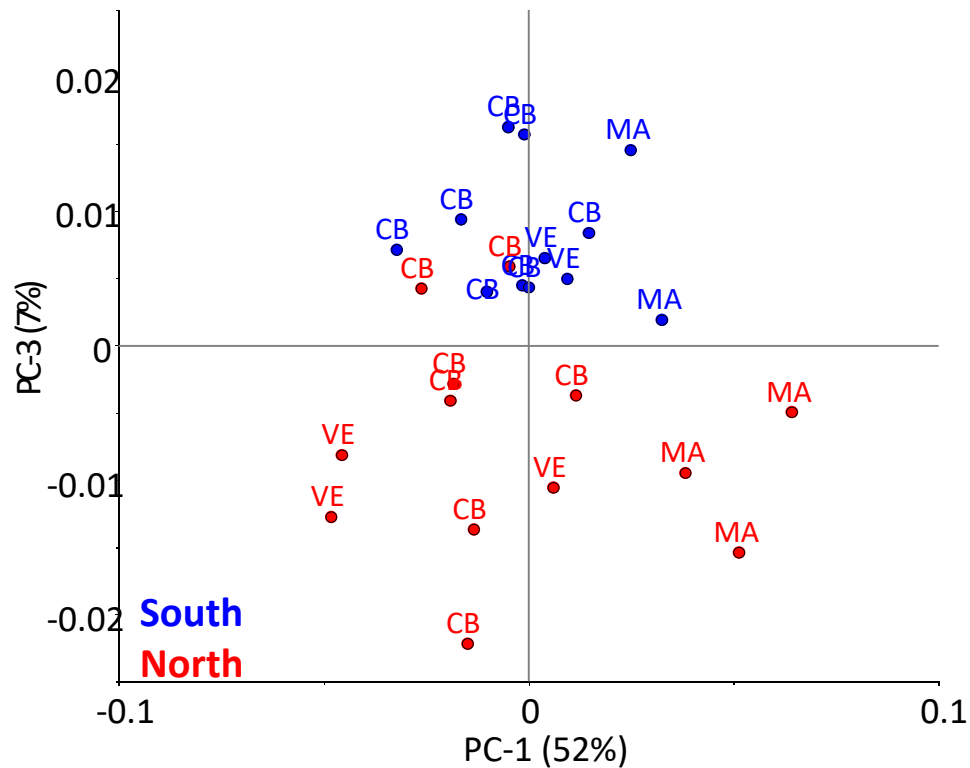


- PLS1-DA after EMSC on NIR spectra (6100-4700 cm<sup>-1</sup>)
- 84 samples for Calibration (C), 49 samples for Prediction (P)
- RMSEP: 0.11 to 0.32, 6 to 9 factors

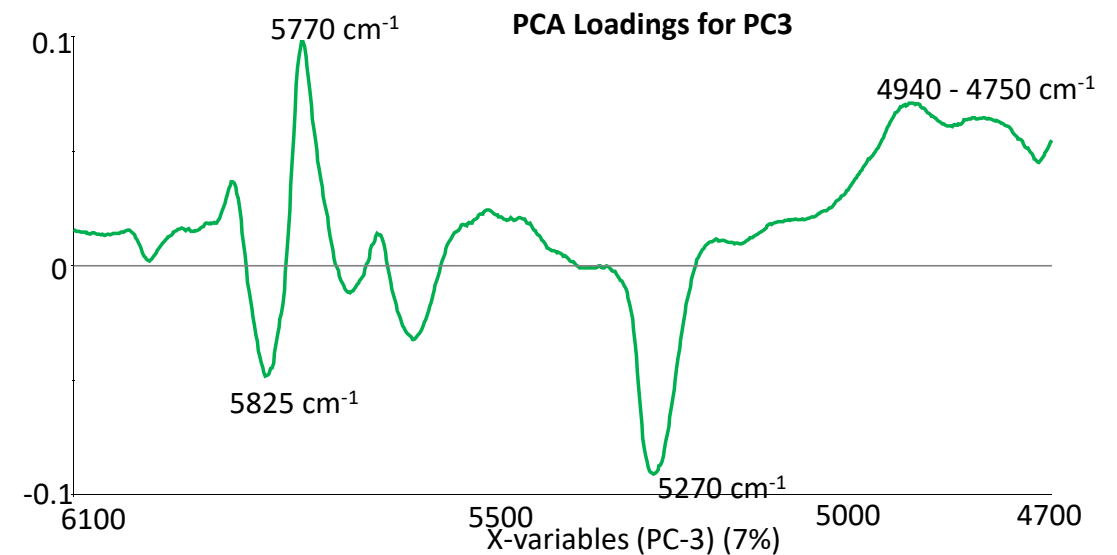
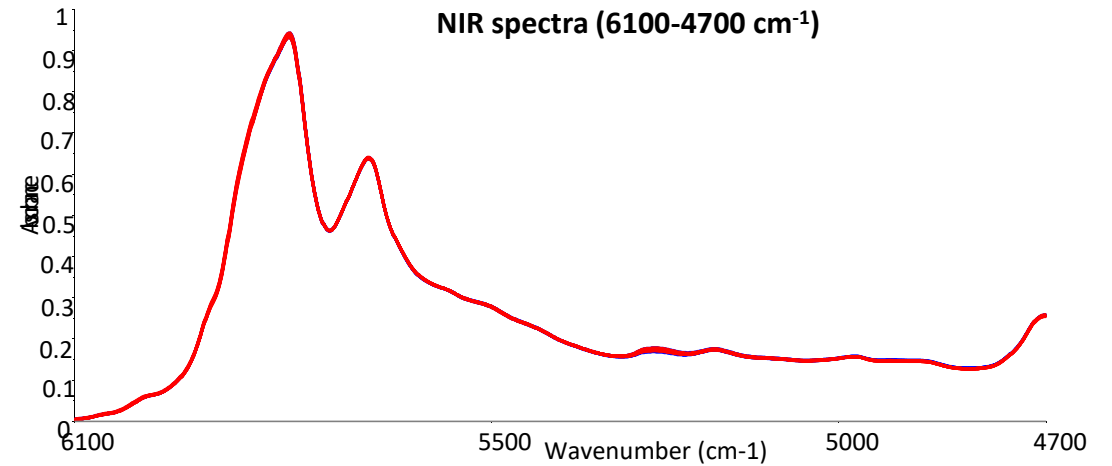
PLS1-DA Model	% Correct	% Uncertain	Sensitivity	Specificity
<b>BL</b> (C: 6, P: 3)	100.0%	0.0%	100.0%	100.0%
<b>OL</b> (C: 8, P: 4)	98.0%	2.0%	100.0%	97.8%
<b>TA</b> (C: 10, P: 5)	98.0%	2.0%	80.0%	100.0%
<b>SA</b> (C: 8, P: 6)	93.9%	2.0%	66.7%	97.7%
<b>AG</b> (C: 14, P: 7)	91.8%	0.0%	100.0%	90.5%
<b>CA</b> (C: 9, P: 5)	89.8%	4.1%	20.0%	97.7%
<b>PI</b> (C: 8, P: 5)	87.8%	2.0%	0.0%	97.7%
<b>CB</b> (C: 9, P: 6)	85.7%	8.2%	33.3%	93.0%
<b>CR</b> (C: 4, P: 2)				
<b>GA</b> (C: 2, P: 2)				
<b>MA</b> (C: 3, P: 2)				
<b>VE</b> (C: 3, P: 2)				
<b>Average</b>	<b>93.1%</b>	<b>2.6%</b>	<b>62.5%</b>	<b>96.8%</b>

- French Cultivars: **AG** (Aglandau), **CA** (Cailletier), **OL** (Olivière), **PI** (Picholine), **SA** (Salonenque), **TA** (Tanche)
- Portuguese Cultivars: **BL** (Blanqueta), **CB** (Cobrançosa), **CR** (Cordovil), **GA** (Galega), **MA** (Madural), **VE** (Verdeal)

PCA Score plot for Portuguese regions on NIR spectra (6100-4700 cm<sup>-1</sup>)



PLS1-DA Model	% Correct	% Uncertain	Sensitivity	Specificity	Factors	RMSEP
<b>North vs South</b> (C: 16, P: 9)	88.9%	11.1%	80.0%	100.0%	3	0.23



### Conclusion and perspectives:

- 🌿 Possible discrimination of EVOO samples depending on Cultivars and Region of origin : “terroir” effect?
- 🌿 More samples to be analysed / several other analytical techniques / chemometrics on concatenated data