

WinePAT : Facing the Complexity of Grape Quality Management and Delivering an High-throughput Device

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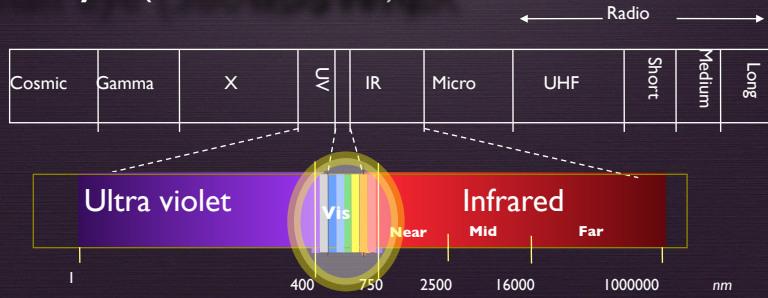
Objectives

1. Spectroscopy – Definitions
2. Spectroscopy – Holistic Measurement of Metabolism
3. Complexity and Information Processing
4. Spectroscopy Case Study : Hyperspectral monitoring



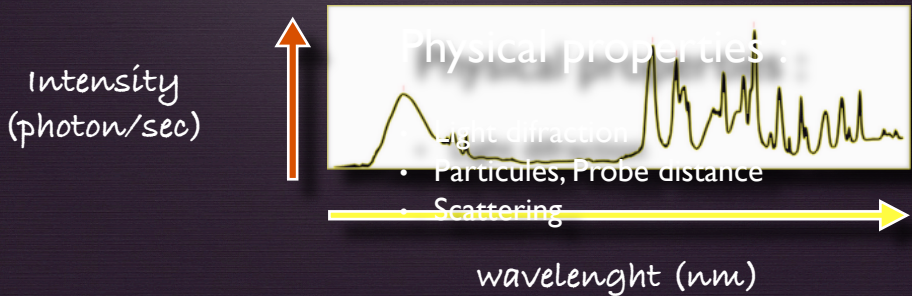
Electromagnetic Spectra

The visible portion of electromagnetic spectra is called light and can be detected by the human eye (380-750nm). The electromagnetic spectra is classified into types according to the frequency ...



Photonics : Molecular Information

Spectral Information :



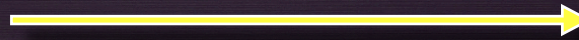
Photonics : Molecular Information

Spectral Information :

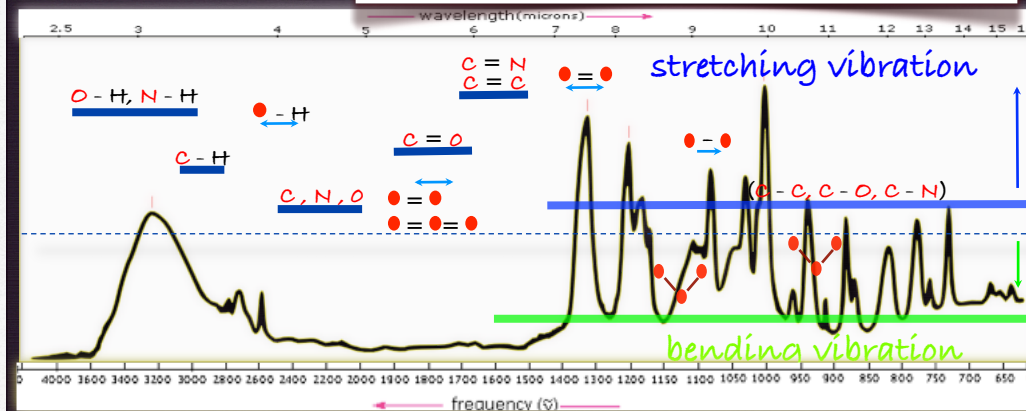
Chemical properties : “frequency changes”

- Absorption
- Fluorescence
- Resonance

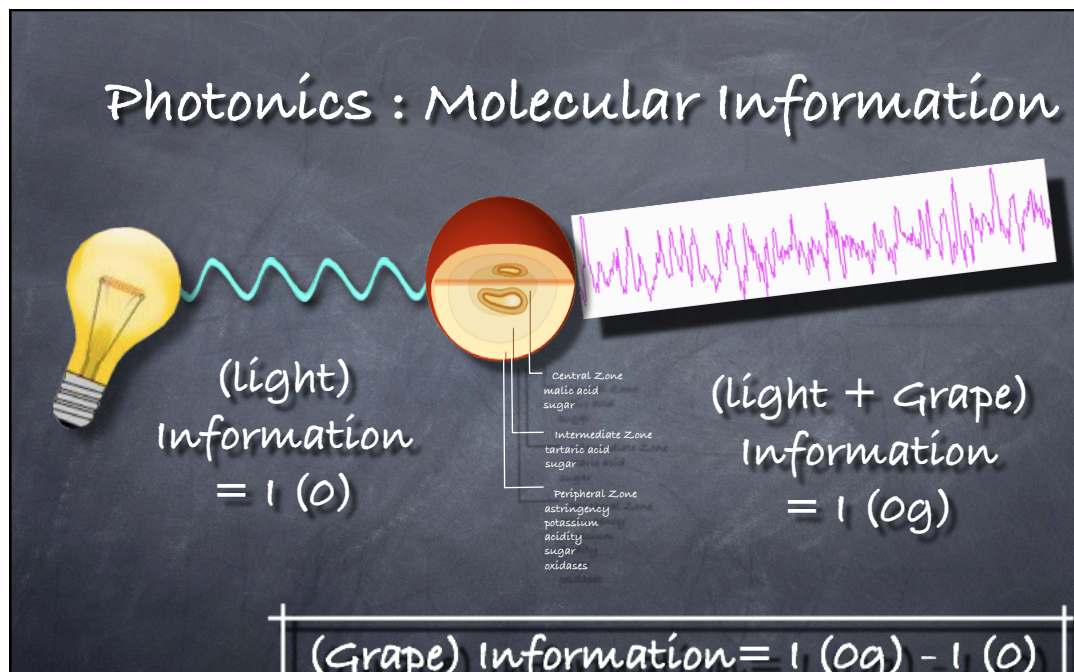
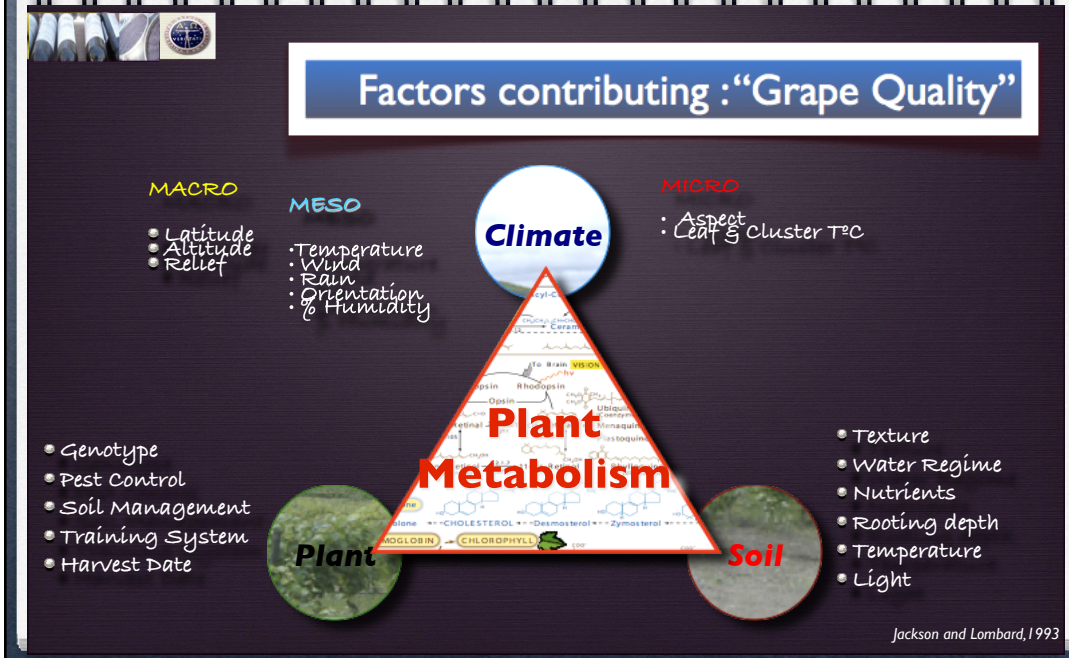
wavelength (nm)



Photonics : Molecular Information



The different features (peaks) in the spectra are result



Photonics : Molecular Information

Metabolic Information: Holistic

Complex Fingerprinting :

- Convoluted Information
- Advanced Computational Signal Processing, Feature and Pattern Recognition

Mediate Zone
sugar
acid

Peripheral Zone
astringency
potassium
acidity
sugar
oxidases

“Target Metabolites”

Selected Compounds ...

Glucose Fructose Malic Acid Tartaric Acid

beta-carotene Lutein Pheophytin A Pheophytin B

Aroma Precursors : Carotenoids

luteina flavoxantina

β,β-caroteno luteina 5,6-epóxido

neocromo zeaxantina

neoxantina β-criptoxantina

violaxantina equinenona

Why Carotenoids in grapes, musts and wines

WORK PROPOSAL

3 Direct conversion of Carotenoids into Norisoprenoids

Norisoprenoids Formation actual knowledge

Reevaluation of the presence of carotenoids in wine

Carotenoids (not reported in musts and wines) → **Glycosides precursors** (in musts) → **Norisoprenoids** (in wines)

Carotenoids in musts → **Norisoprenoids** (in wines)

Processes: Plant metabolism, Fermentation, Aging

Identification of the substances formed by degradation of the major carotenoids presents in musts and wines.

Measure of carotenoids levels and corresponding Norisoprenoids during pre- and vinification process.

Study of the evolution of remanent carotenoids in wine during aging.

actual knowledge of carotenoids in wine

Carotenoids (not reported in musts and wines) → **Glycosides precursors** (in musts) → **Norisoprenoids** (in wines)

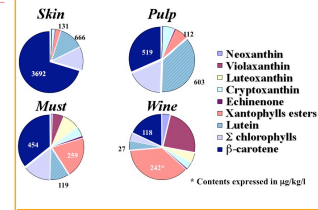
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GUEDES DE PINHO, SILVA FERREIRA, M. MENDES PINTO, GOMEZ BENITEZ, J e HOGG, T. Determination of carotenoid profiles in grapes, musts and fortified wines from Douro varieties of *Vitis vinifera*. J.Agric. Food Chem, 2001, 49, 11, 5484-5488.

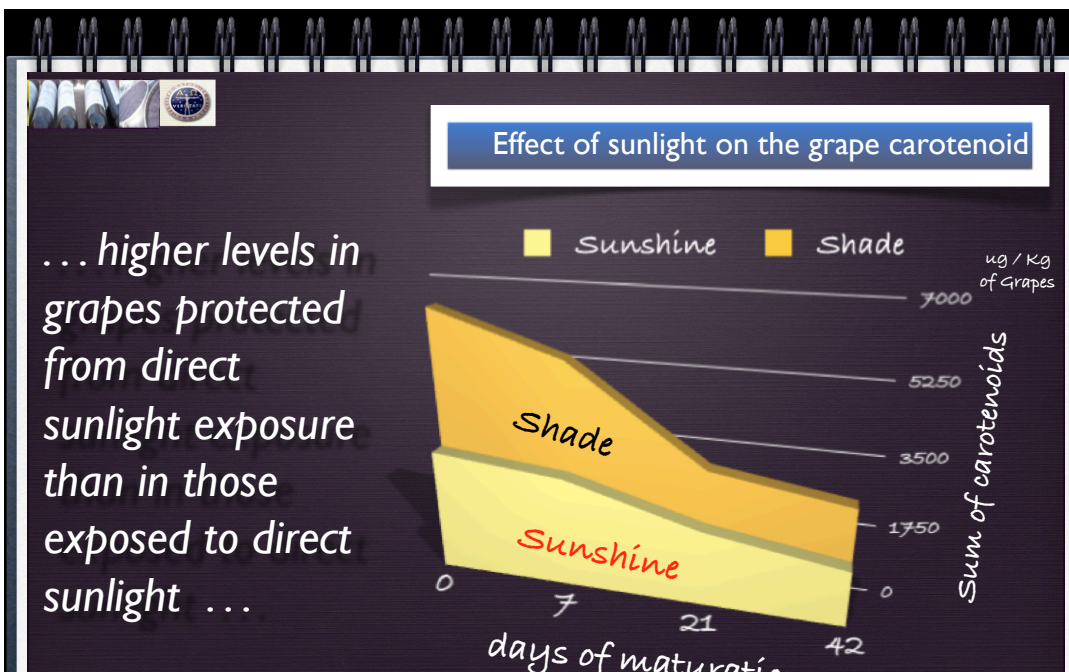
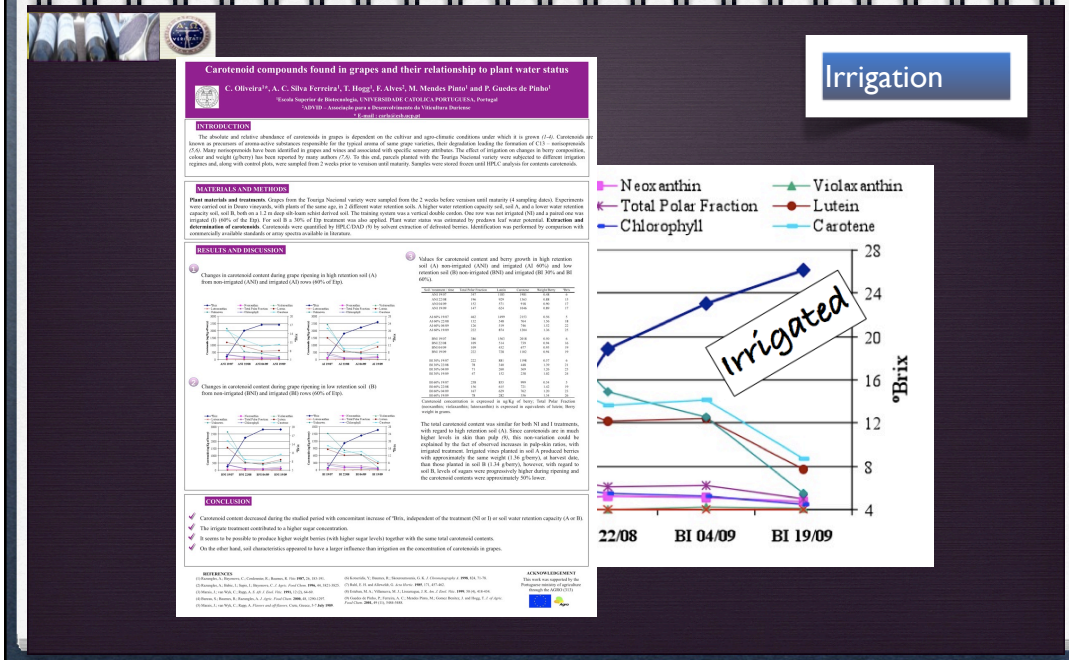
Why Carotenoids in grapes, musts and wines

"Pool" Metabólico

Carotenoids are mostly synthesized from the end products of the Calvin cycle. It is well known that carotenoid biosynthesis in plants is related to the degradation between "veraison" and metabolic processes of plant cells, which are dependent on climatic factors, agricultural compounds, which have been reported as odor compounds responsible for typical aromas of some grape varieties ...

Altitude

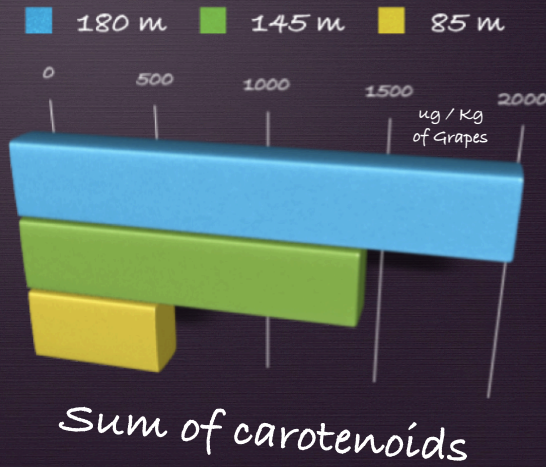
Xantofilas cíclicas



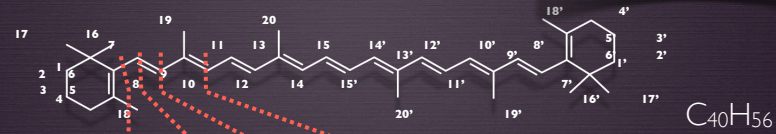


Effect of altitude on the grape carotenoid

... Altitude strongly affect climatic conditions due to it direct impact on T°C, humidity, and other environment factors that affect grape maturity ...



Norisoprenoids



non-Megastigma skeleton

Megastigma skeleton

2,2,6-Trimethylcyclohexanone
TCH

C9

β -cyclocitral

C10

DHC

C11

C13

Ionones

Damascones

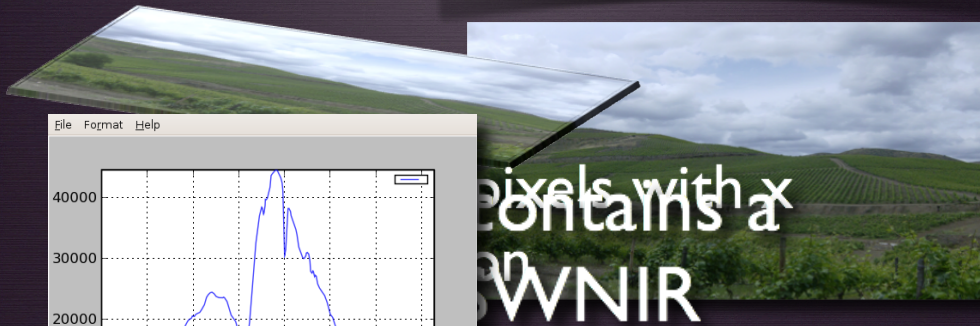


High Resolution vis-SWNIR Imaging

“Non Target Metabolites”



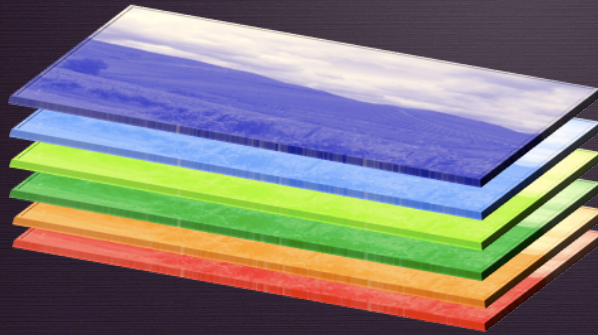
What is Hyperspectral Imaging?



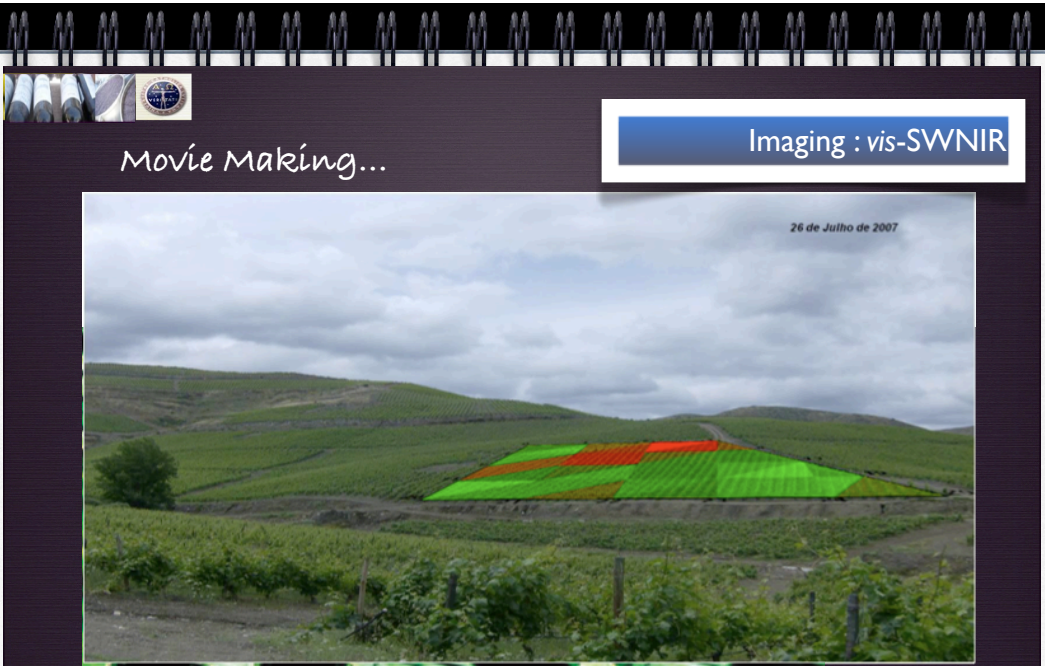
pixels with a
SWNIR



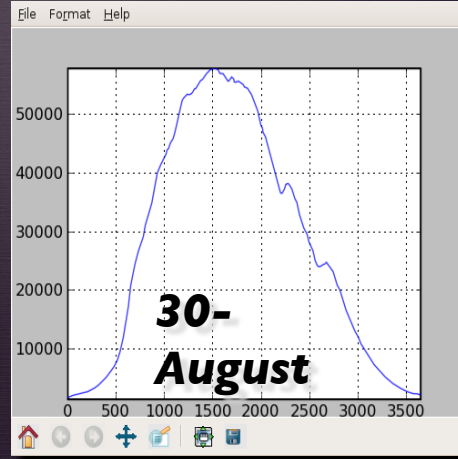
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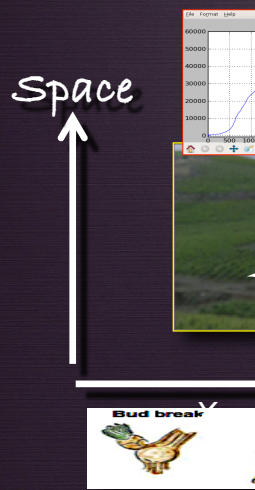
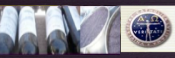
- Spatial Information for each time,
- Time Course Resolution,
- Each point of the field is a spectra,
- Allows high discrimination,
- Maturation Monitoring...



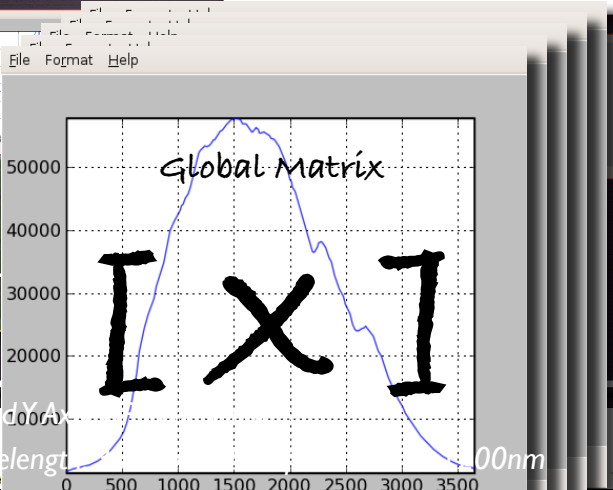
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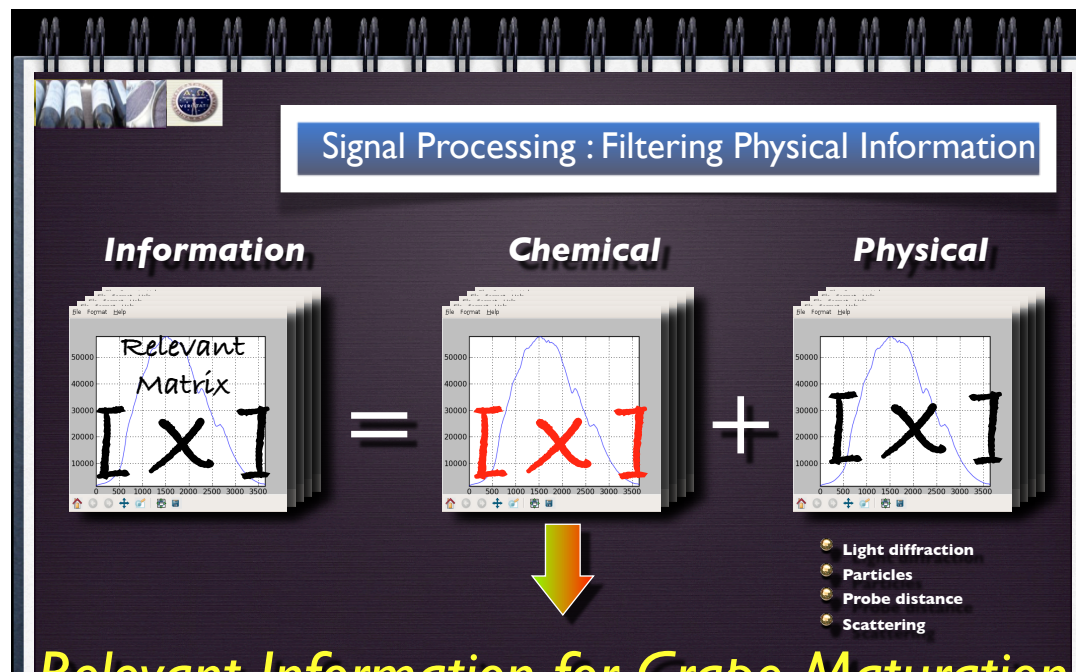
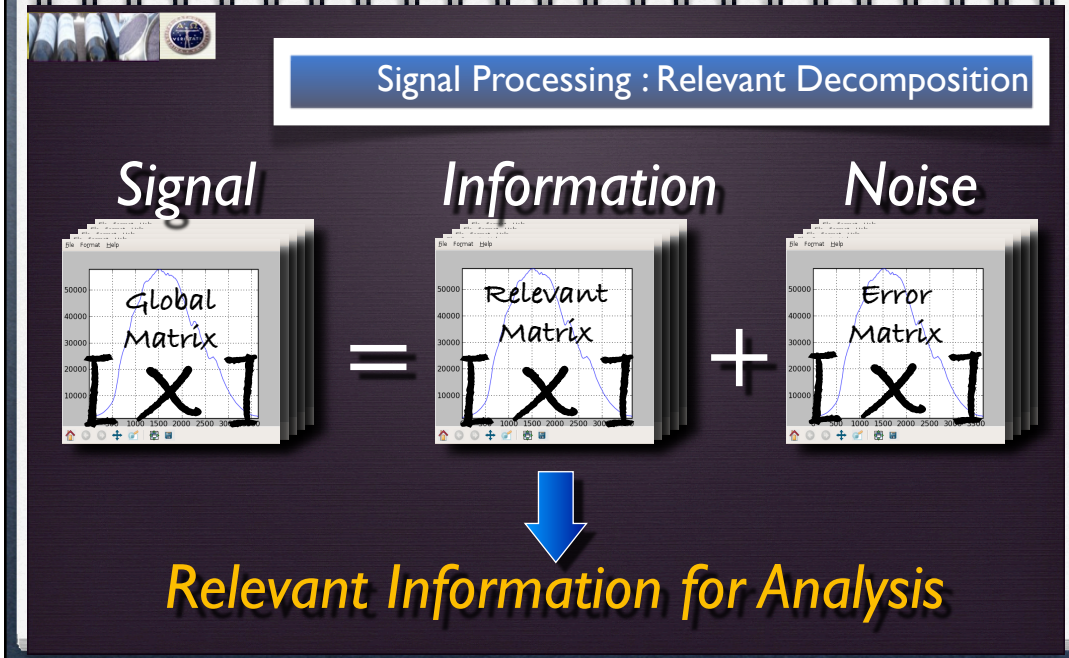
Grape Berry Ripening



Space
↑

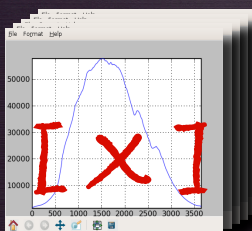


→
time




Signal Processing

Chemical



Convolution

Blind Signal Decomposition
SVD



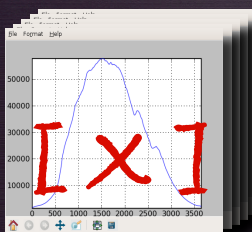
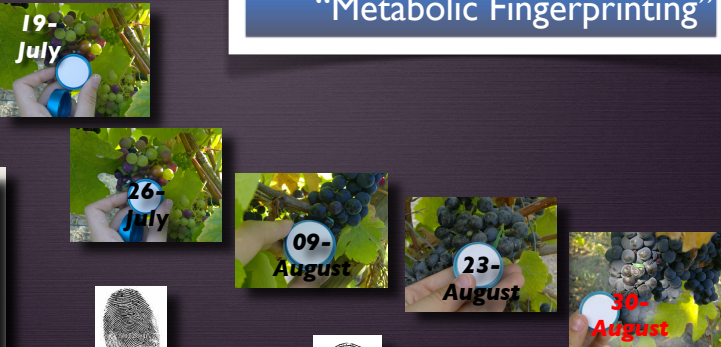
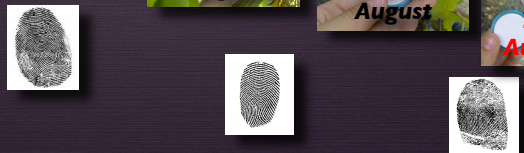
Metabolic Fingerprint

Deconvolution

Supervised Signal Decomposition
PLS

"Metabolic Fingerprinting"

Chemical

19-July

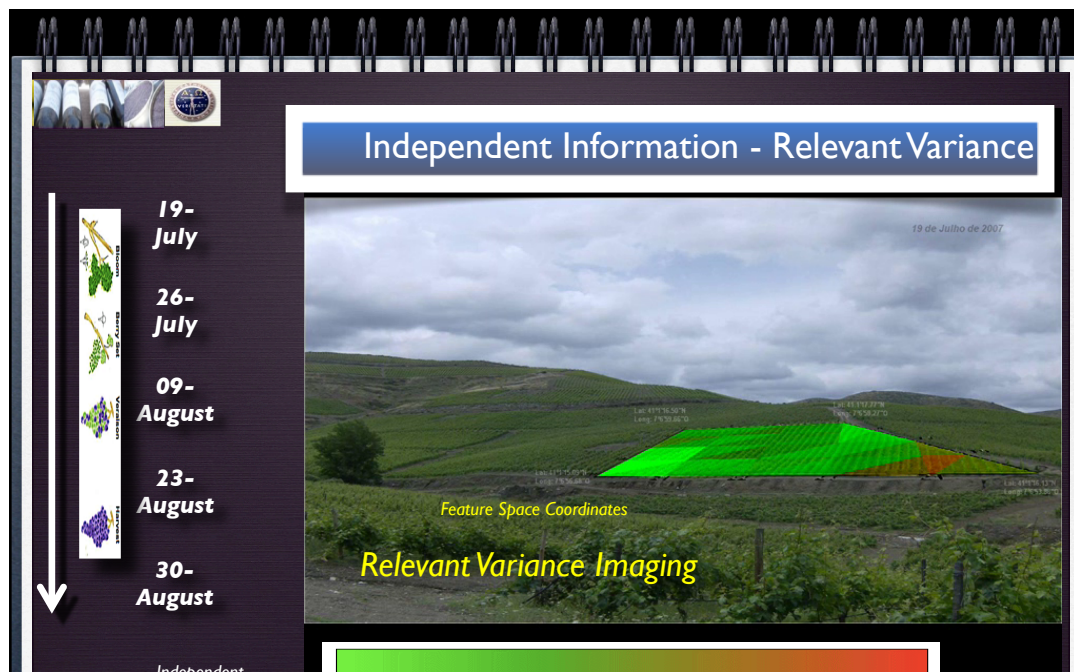
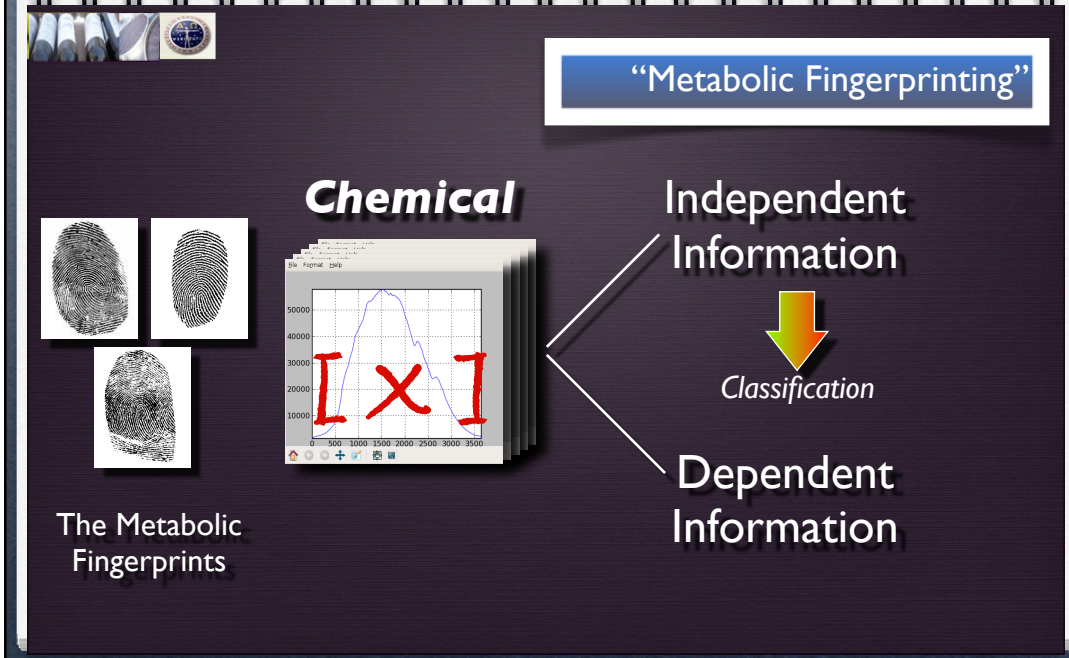
26-July

09-August

23-August

30-August

What Relevant Information Discriminates between the "metabolic fingerprints" ?



Correlation Spectra & Chemical Composition

Relevant Metabolites:

- Glucose
- Organic Acids
- Lutein
- beta - Carotenes
- Chlorophyll
- Pheophytins
- Antocyanins
- "Combined fraction"

Metabolic Composition

Chemical

The Metabolic Fingerprints

Correlation Spectra & Chemical Composition

Glucose

Fructose

Malic Acid

Tartaric Acid

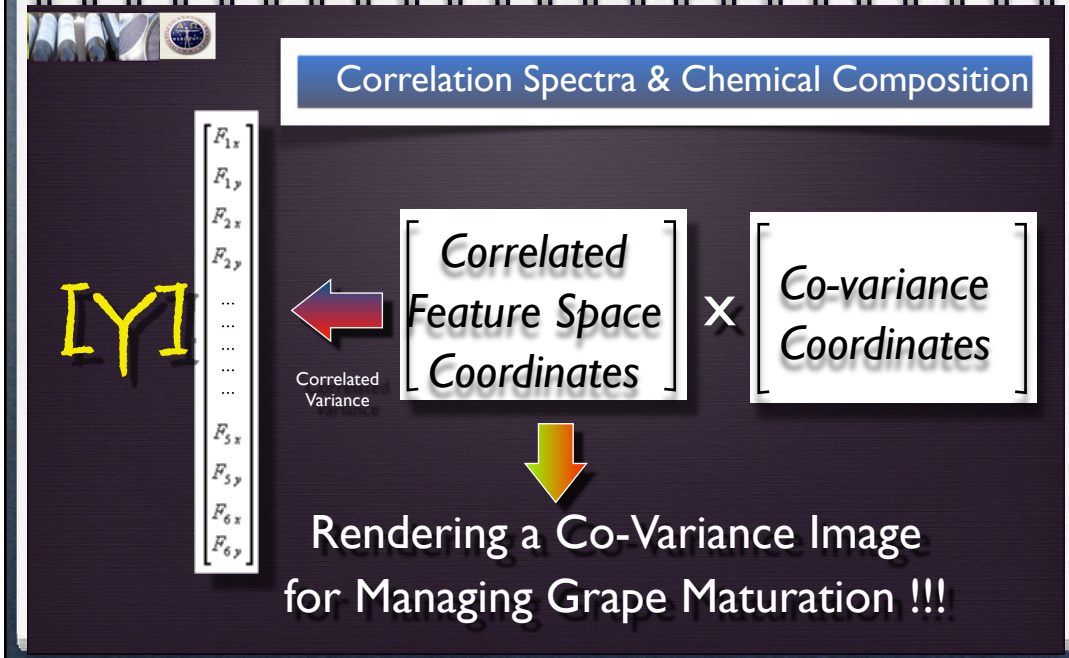
Lutein

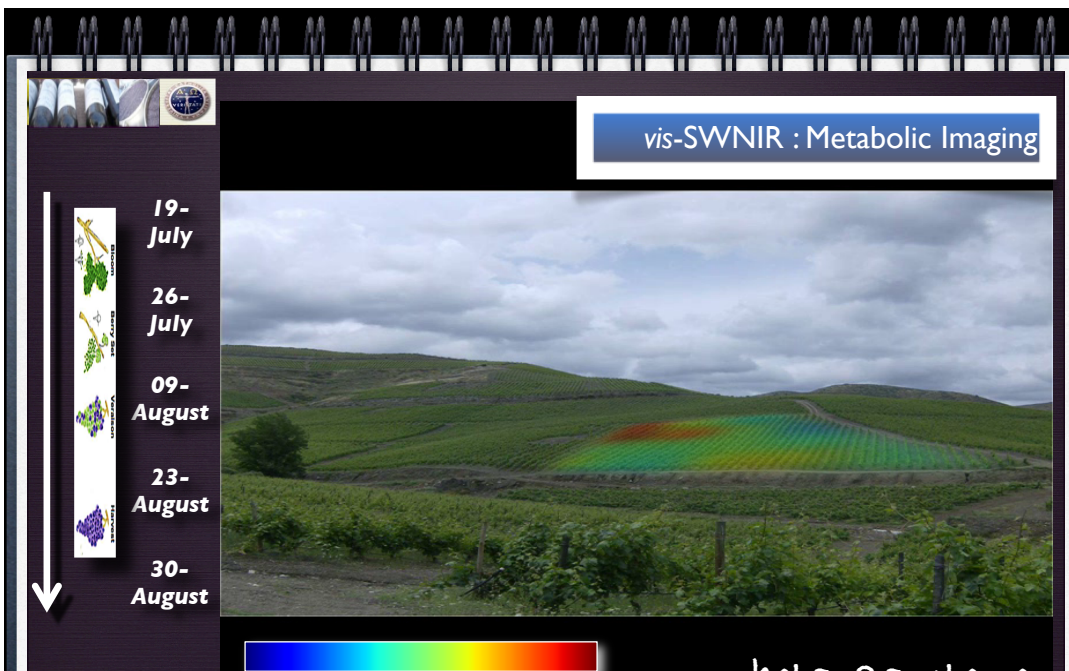
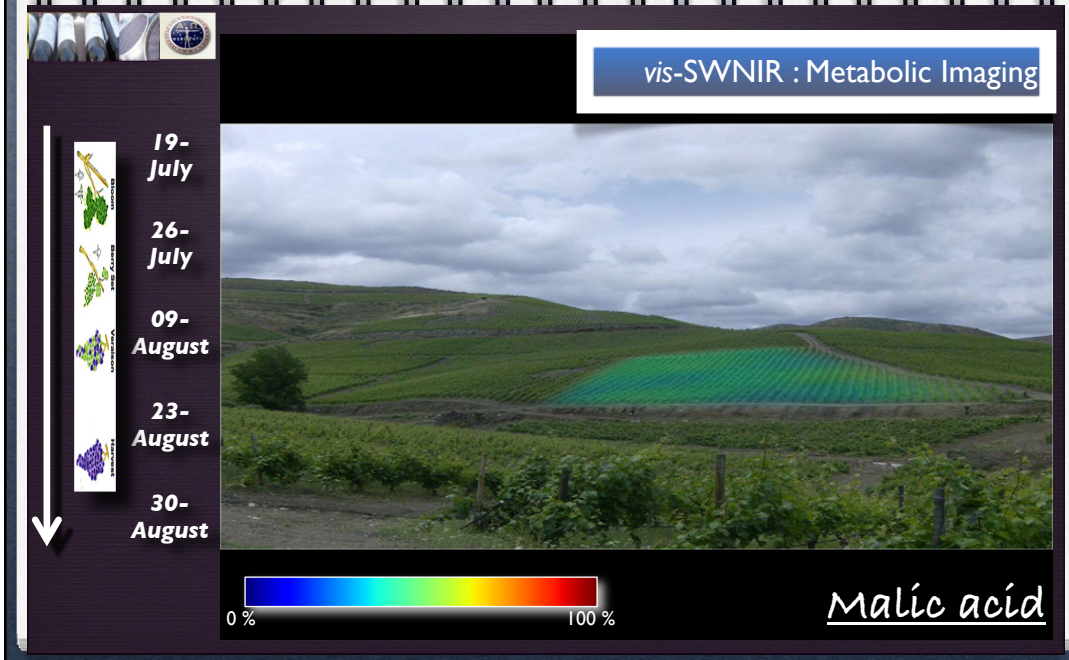
beta-carotene

Pheophytin A

Pheophytin B

ALS models







-
- Conclusion
- Non destructive Spectroscopy techniques coupled with signal processing are ideal tools for management of “grape quality” ;
 - Non targeted approach enables the “glass to vineyard” sensory perspective ;
 - 3. Hyperspectral monitoring allows optimization and consistence in final wine quality.