Applied Chemometrics Research Group
Universitat Autònoma de Barcelona

Prediction of bean plants pathologies, and geographical origin by using NIR-Vis spectroscopy and chemometrics

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euss enginyeria

UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH
Escola Superior d'Agricultura de Barcelona

Fundació Miquel Agustí

The Council For Near-Infrared Spectroscopy CNIRS

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UAB Universitat Autònoma de Barcelona




Who am I?

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Escola Universitària Salesiana de Sarrià

and external researcher in Applied Chemometrics Group at Universitat Autònoma de Barcelona

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UAB
Universitat Autònoma de Barcelona

Where do I come from?

CATALUNYA a country that sees how the sun rises from the Mediterranean Sea

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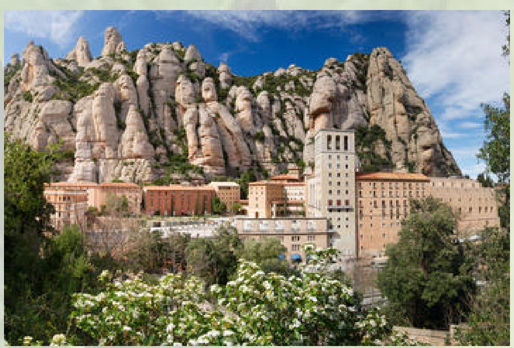
Where do I come from?

I come from CATALUNYA







Where do I come from?

CATALUNYA is country of ancestral traditions






Where do I come from?

CATALUNYA is a country of gastronomy.

Mongetes amb *botifarra*

One of the **CATALUNYA**'s most known recipes.

Best bean quality must be chosen

Phaseolus vulgaris L.

1. INTRODUCTION

1.INTRODUCTION

What kind of beans are we working with?

- Xana
- Cornel

What kind of beans are we working with?

Xana

It is an improved variety from the Asturian Fabes.

What kind of beans are we working with?

Xana

Used for cooking the super famous “Fabada Asturiana”

What kind of beans are we working with?

Cornel

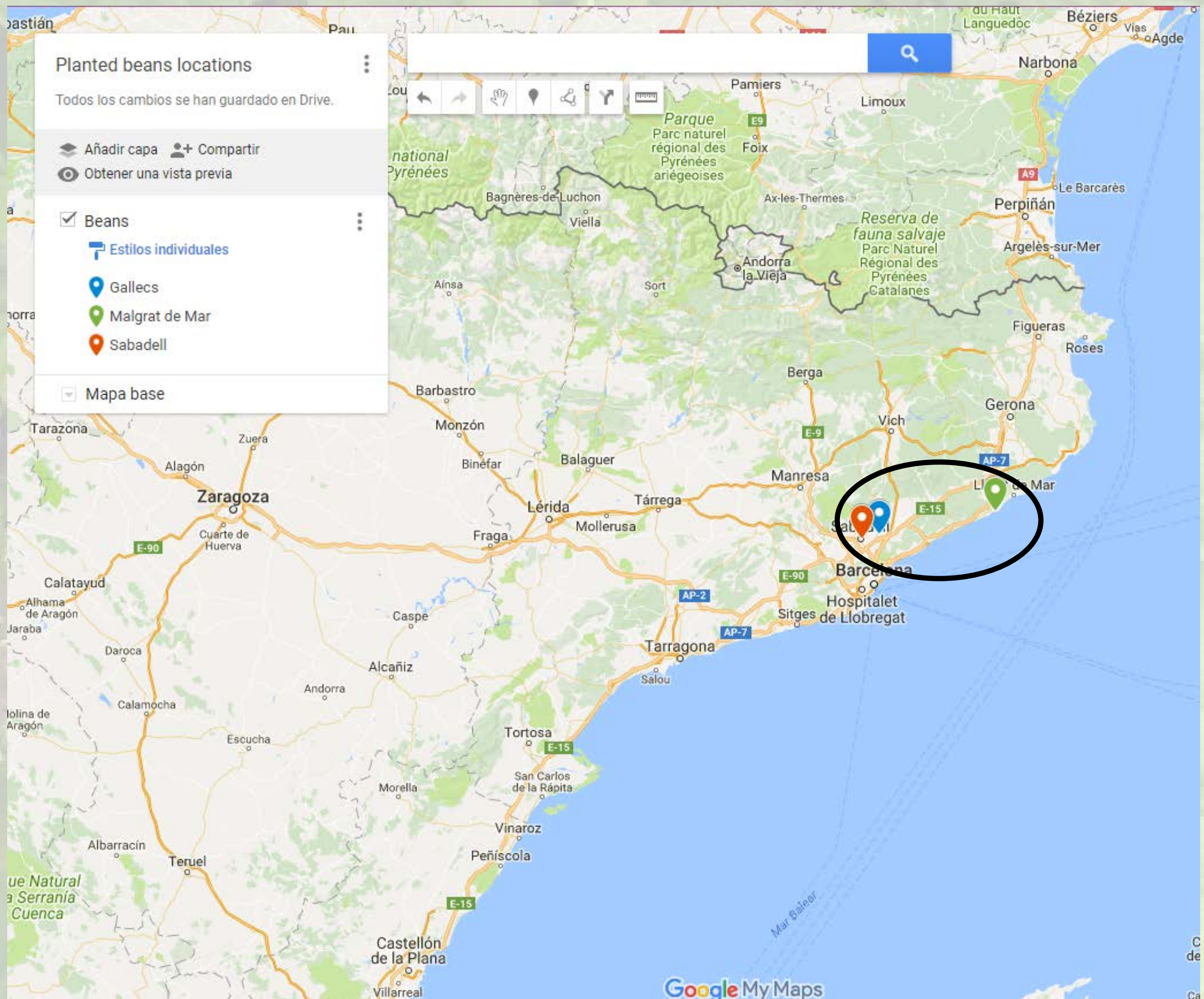
It is an improved variety from the American black beans.

What kind of beans are we working with?

Cornel

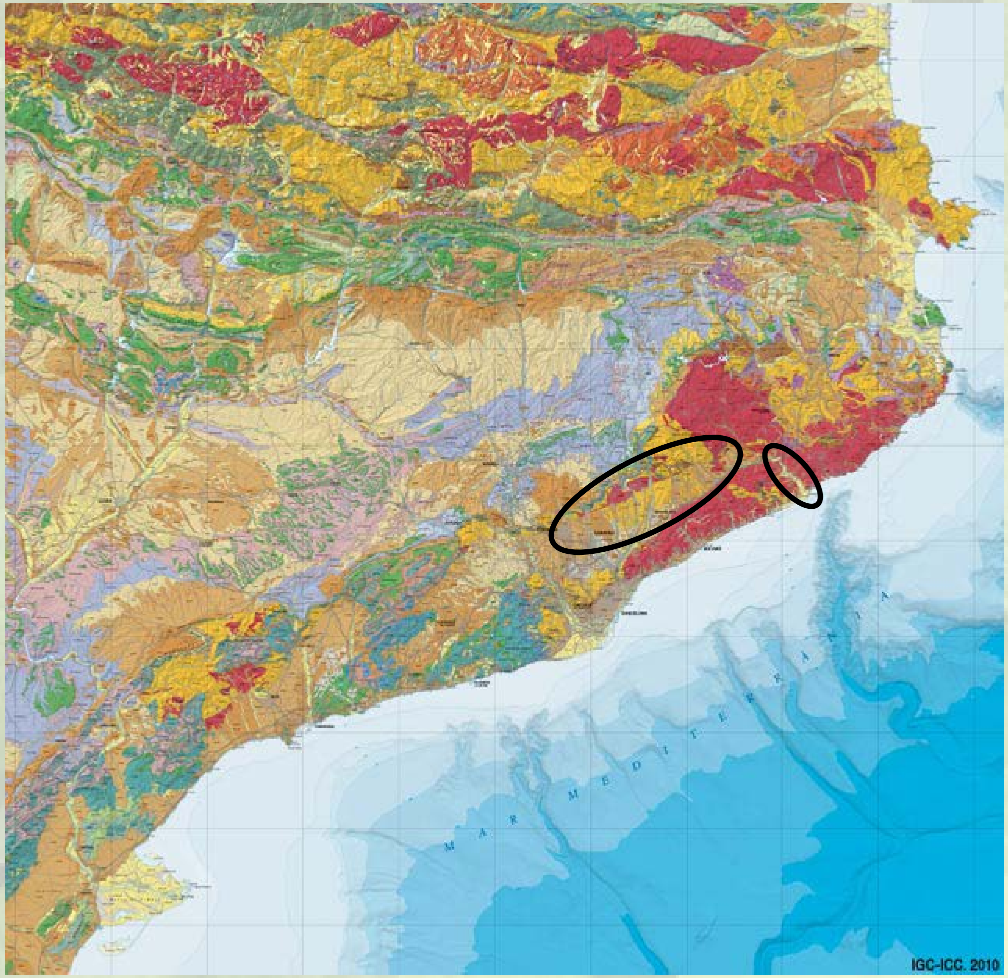
Used for cooking the super famous Mexican recipe “Rice and beans”.

Where are the beans planted?

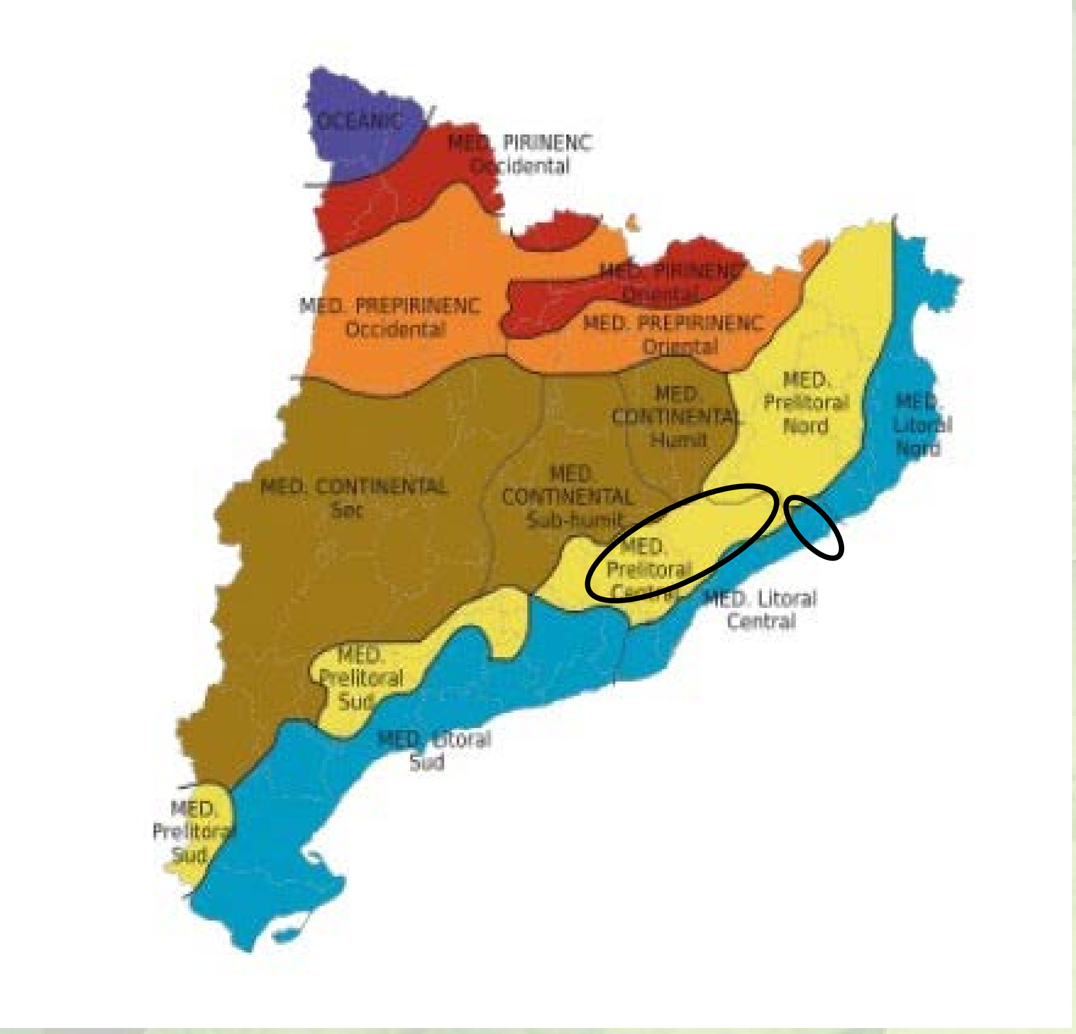


Geographic environment

- Soil rich in Calcium



Climate


OCEANIC
MED. PIRINENC Occidental
MED. PIRINENC Oriental
MED. PREPIRINENC Occidental
MED. PREPIRINENC Oriental
MED. CONTINENTAL Humit
MED. Prelitoral Nord
MED. Litoral Nord
MED. CONTINENTAL Sec
MED. CONTINENTAL Sub-humit
MED. Prelitoral Central
MED. Litoral Central
MED. Prelitoral Sud
MED. Litoral Sud
MED. Prelitoral Sud

Climatic differences between Sabadell Gallecs and Malgrat

	Sabadell Gallecs	Malgrat
Climate	Central Prelitoral Mediterranean	Central Litoral Mediterranean
Annual precipitation	600-650 mm	550-800mm
Storm risk	Moderate in summer, fall and	High because of its orography
Precipitation peaks	Fall- Spring	Fall- Spring
Winters	Cold: 6-8ºC average temperature	Cool: 8-11º average temperature
Under 0ºC temperatures	From November to March	No under 0ºC temperatures
Summers	Hot: 25-27ºC average temperature	Warm: 22-23ºC average temperature
Annual thermal amplitude	Moderate	Moderate

Bean's diseases

- Bacteria: *Pseudomonas sp*.

- Fungus and oomicets which attack the seed and the root: ***Pythium sp***, *Fusarium sp, Rhizoctonia sp, Verticillum sp.*

- Fungus and oomicets which attack leaves and pods: ***Sclerotinia sclerotiorum* (white mold)**, Erysiphe diffusa (powdery mildew), *Colletotrichum lindemutianum* (anthracnose) and others.

Pytium

White mold

1.INTRODUCTION

Quality control of bean production

Quality Parameters

Chemical

- Protein
- Moisture
- Fat
- Starch

Genetical

- Resistance to plant pathologies

1.INTRODUCTION

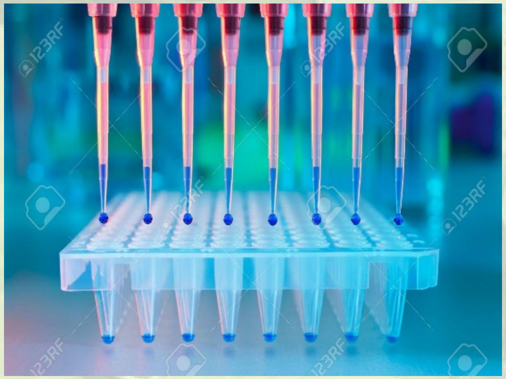
Quality control

Chemical methods

TRADITIONAL METHODOLOGIES

- **Time, Money & chemical reagents consuming**
- **Sample preparation**

Genetical



Why NIR?

- Fast
- Robust
- Nondestructive
- No sample preparation
- Many modes of measuring
- Low cost analysis

Chemical & Physical & other Information

Multi parametric analysis

"The way of analyzing chemical data, in which both elements statistical and chemical thinking are combined" ***Charles E. Miller***

Empirical modelling

Chemical data

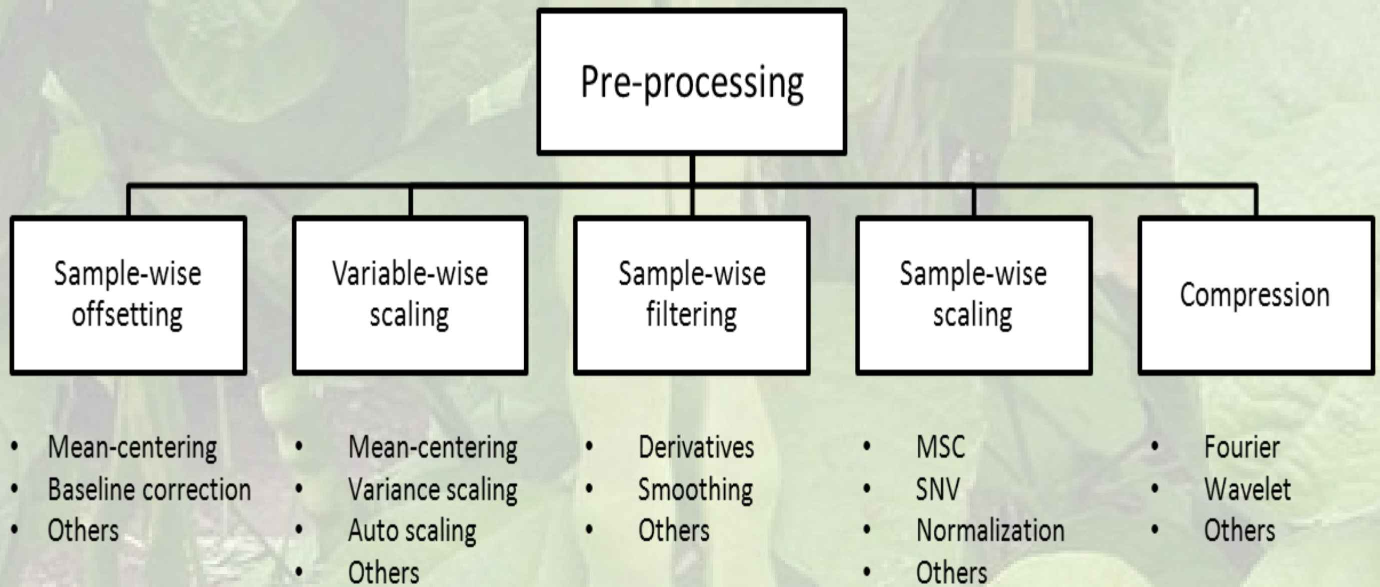
Multivariate model

"The application of multivariate, empirical modelling methods to chemical data"

C.E Miller, K.Bakeev (Ed) "Chemometrics in Process Analytical Technology (PAT)," in *Process Analytical Technology: Spectroscopic Tools and Implementation Strategies for the Chemical and Pharmaceutical Industries*, Second Edi., John Wiley & Sons, Ltd, 2010, pp. 353–438.

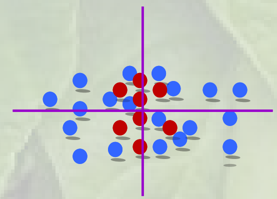
1.INTRODUCTION

Preprocessing data



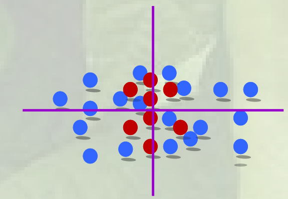
1.INTRODUCTION

Sample selection



- Kennard and Stone

Variable reduction

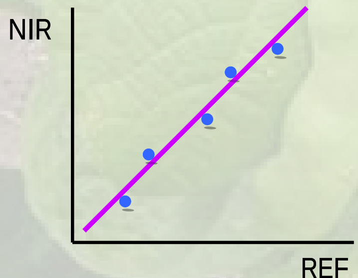


- Principal Component Analysis (PCA)

Classification

- Cluster analysis
- SIMCA
- PLS-DA

Calibration Techniques



- Partial Least Squares (PLS)
- Correlation coefficients (CC)
- Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS)

2. OBJECTIVES

OBJECTIVES

- Demonstration of strong relationships between NIR spectra and geographical characteristics and climates.

- Demonstrate NIR-Vis spectroscopy as a rapid and cost-effective method, for detecting future bean pathologies such as Pythium and white mold.

- Demonstrate that NIR modeling in bean spectra can be an alternative technique to PCR and ELISA for determining future pathologies in bean plants.

3. METHODOLOGY

3.METHODOLOGY

BEAN SEADS

Schlerotinia (White mold)

Resistance to 2 isolates of white mold (Scletorinia_V and Sclerotinia_X) that sequence analysis placed near *Erysiphe diffusa*, was evaluated on 5 plants per entry. Disease assessment was performed plant by plant 12 days after inoculation.

Pythium

Average response to four isolates was evaluated in five individual plants for each accession.

Reference Values for future pathology determination

- **Sclerotinia**

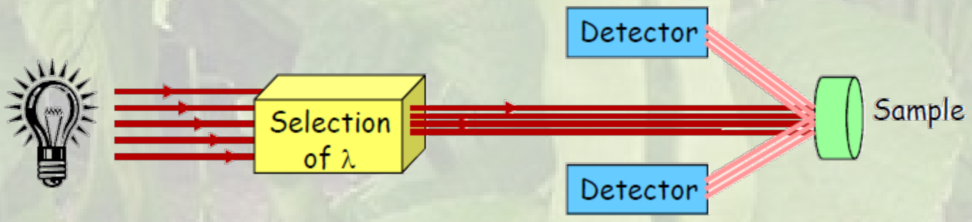
Scale = Qualitative 1, absence of symptoms - 9, death of the plant
The average response of three independent evaluations is shown

- **White mold**

P_crec: % of germination with respect to the control.
P_des: % reduction of growth of seedlings with respect to control.
The average response of four independent evaluations is shown

NEAR INFRARED APPLICATION

NIR SPECTROSCOPY



REFLECTANCE

Reference Values for future pathology determination

Bean Seeds

NIR/Vis Spectrometer

FOSS NIRSystems XDS equipped with Rapid Content Analyzer module (RCA)

(X data)

Plantation

Observation of pathologies in the grown plants

(Y data)

3.METHODOLOGY

Workflow of geographical analysis

Data set split → **Spectra pretreatment** → **Spectral range selection** → **Outlier selection** → **PCA analisys** → **Interpret**

Data structure

SAMPLES

Location	Pathologies	400-2500 nm NIR-VIS SPECTRA
1	4	4200

3.METHODOLOGY

Workflow of model development

Data set split → Spectra pretreatment → Spectral range selection → Outlier selection → Calibration → Validation

Data structure

SAMPLES	Location	Pathologies	NIR-VIS SPECTRA (400-2500 nm)
	1	4	4200

4. RESULTS

PART 1:

Establishing a relationship between the geographical location their climates and our NIR-VIS spectra

4.RESULTS

For establishing a relationship between the geographical location and our NIR-VIS spectra several algorithms and strategies have been used:

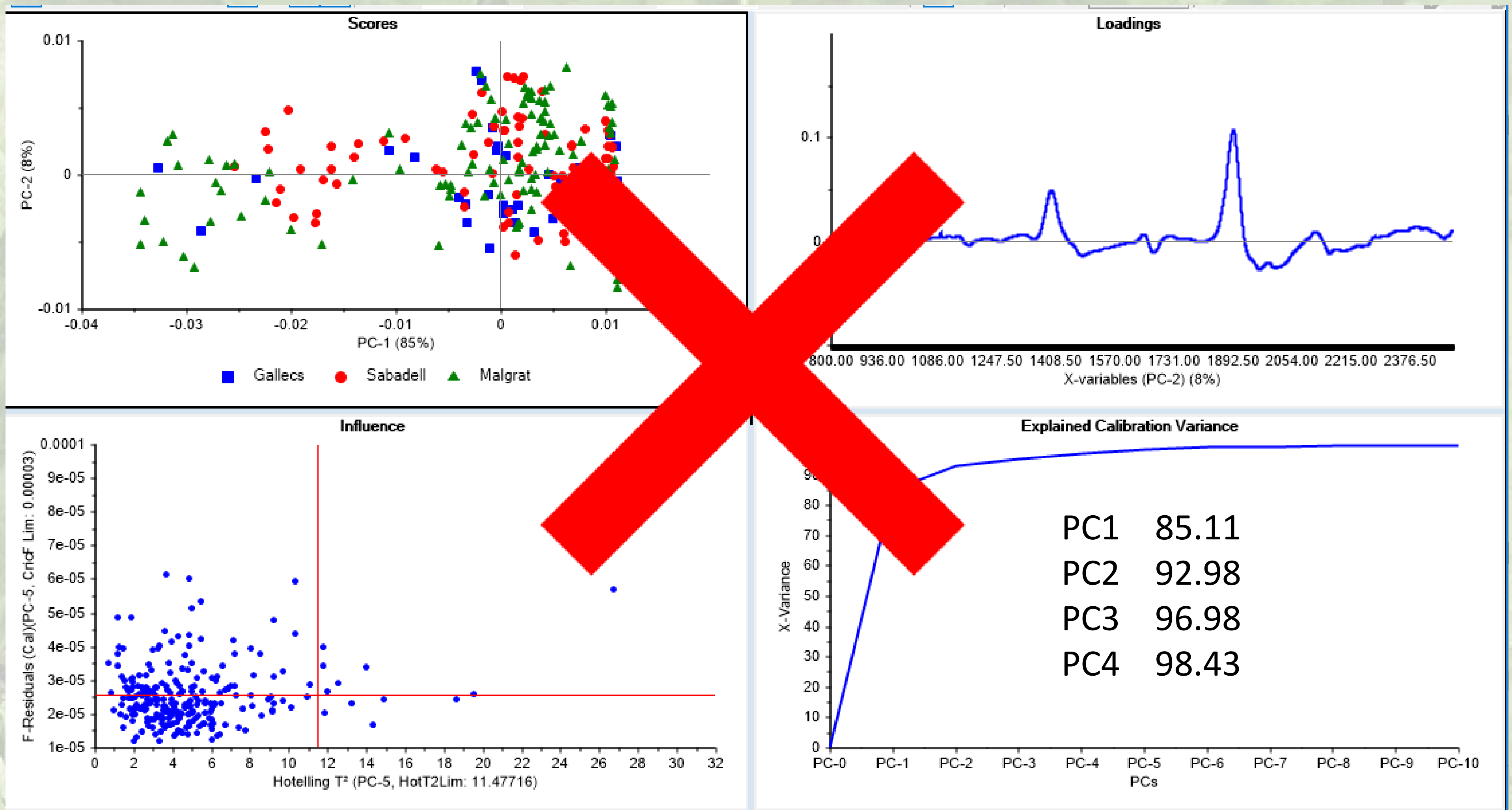
- Supervised methods
  - Cluster Analysis
    - K-medians
    - K-means
    - Hierarchical
- Non-Supervised methods
  - SIMCA
  - PLS-DA

4.RESULTS

As a descriptive and exploratory method of variable reduction, we have tried Principal Component Analysis in order to visualize correlations among our variables and the geographic origin

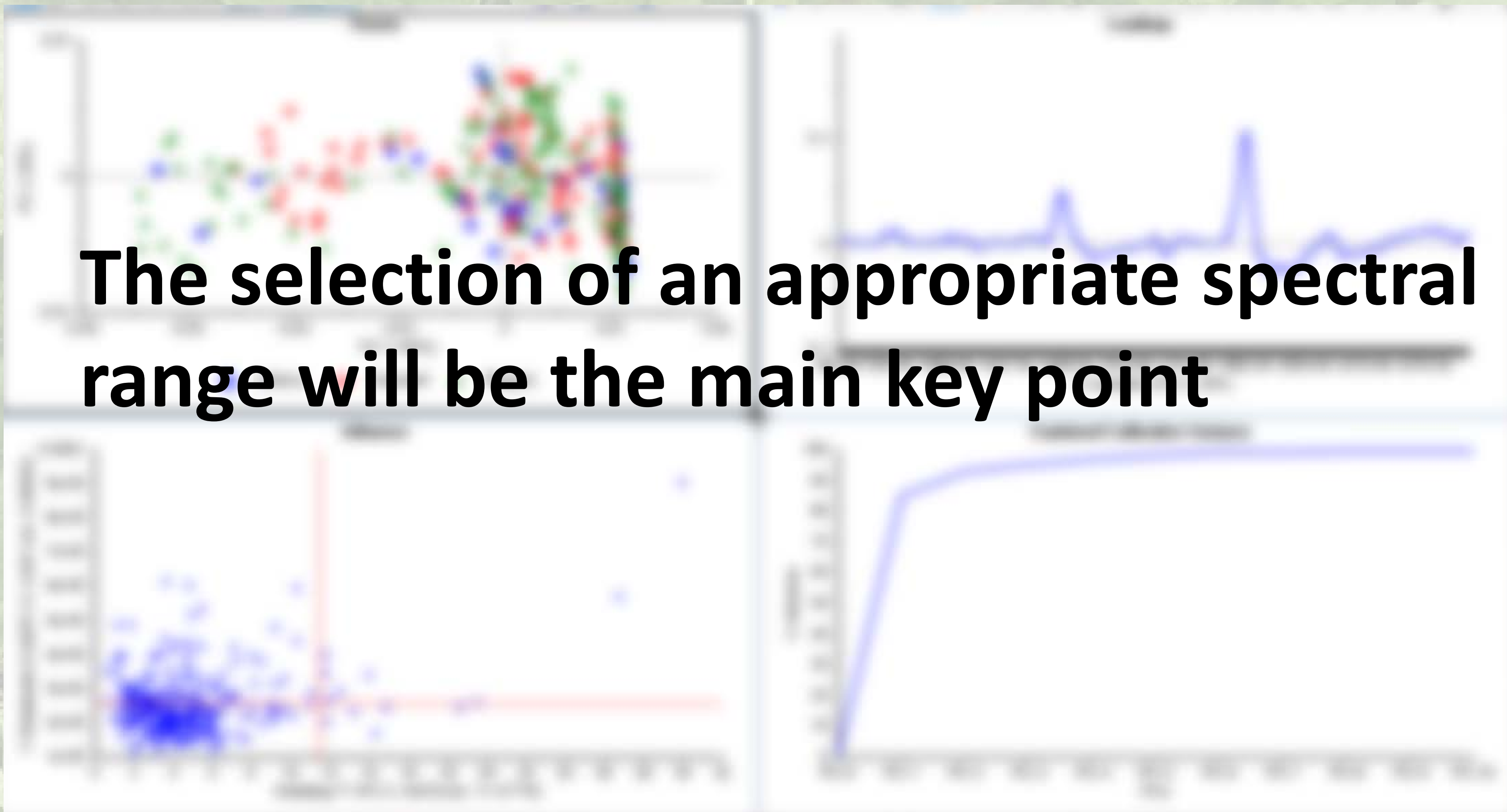
4.RESULTS

1st SG Derivative 11 smoothing points



4.RESULTS

1st SG Derivative 11 smoothing points



The selection of an appropriate spectral range will be the main key point

4.RESULTS

	A	C	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
1		Location	400	400.5	401	401.5	402	402.5	403	403.5	404	404.5	405	405.5	406	406.5
2	071_L4_B1b	4	-0.04962841	0.04962841	-0.04962841	-0.04962841	-0.04962841	8.418923	8.323947	8.213363	8.087381	7.946535	7.791586	7.623638	7.443801	7.253364
3	074_L4_B2A	4	-0.1950905	-0.1950905	-0.1950905	-0.1950905	-0.1950905	5.099743	4.958691	4.805386	4.641794	4.46982	4.291051	4.107011	3.918899	3.727648
4	074_L4_B2B	4	-0.1951563	-0.1951563	-0.1951563	-0.1951563	-0.1951563	5.087153	4.948351	4.797276	4.635773	4.465504	4.288011	4.10473	3.916954	3.725812
5	028_L4_B1A	4	-0.05060106	0.05060106	-0.05060106	-0.05060106	-0.05060106	8.531395	8.419162	8.293399	8.154834	8.00419	7.842081	7.669085	7.485689	7.292713
6	124_L4_B2A	4	-0.1835715	-0.1835715	-0.1835715	-0.1835715	-0.1835715	6.582437	6.402778	6.208258	6.001641	5.785751	5.562967	5.335105	5.103597	4.869616
7	071_L4_B1A	4	-0.04791864	0.04791864	-0.04791864	-0.04791864	-0.04791864	8.448255	8.348013	8.232958	8.103449	7.960065	7.803678	7.635228	7.455591	7.265653
8	028_L4_B1B	4	-0.05113561	0.05113561	-0.05113561	-0.05113561	-0.05113561	8.545098	8.43719	8.315353	8.180202	8.032292	7.872252	7.700856	7.518838	7.327003
9	217_L4_B1B	4	-0.0684565	-0.0684565	-0.0684565	-0.0684565	-0.0684565	8.750168	8.643576	8.521509	8.384313	8.232509	8.066875	7.8883	7.69774	7.496437
10	083_L4_B1A	4	-0.1065392	-0.1065392	-0.1065392	-0.1065392	-0.1065392	8.654555	8.519915	8.36758	8.198657	8.014532	7.816616	7.606347	7.385094	7.154316
11	083_L4_B1B	4	-0.108052	-0.108052	-0.108052	-0.108052	-0.108052	8.692506	8.554457	8.398266	8.224848	8.035321	7.831086	7.613723	7.384803	7.145971
12	217_L4_B1A	4	-0.06607383	0.06607383	-0.06607383	-0.06607383	-0.06607383	8.808926	8.705638	8.586017	8.45048	8.299625	8.134303	7.955634	7.764816	7.563065
13	133_L4_B1B	4	-0.09007233	0.09007233	-0.09007233	-0.09007233	-0.09007233	8.775386	8.650879	8.509552	8.352236	8.179892	7.993622	7.794596	7.584019	7.363189
14	214_L4_B1B	4	-0.1988832	-0.1988832	-0.1988832	-0.1988832	-0.1988832	4.913704	4.780297	4.634584	4.478513	4.31392	4.142337	3.965235	3.783785	3.599136
15	214_L4_B1C	4	-0.1962677	-0.1962677	-0.1962677	-0.1962677	-0.1962677	4.893845	4.762187	4.618301	4.46397	4.300707	4.12993	3.953169	3.77165	3.586645
16	037_L4_B2A	4	-0.0932529	-0.0932529	-0.0932529	-0.0932529	-0.0932529	8.579806	8.460199	8.323943	8.171916	8.005337	7.825466	7.633686	7.431433	7.220181
17	037_L4_B1C	4	-0.08501327	0.08501327	-0.08501327	-0.08501327	-0.08501327	9.666444	9.522546	9.360785	9.18227	8.98824	8.779823	8.558166	8.324221	8.079026
18	037_L4_B1B	4	-0.08614644	0.08614644	-0.08614644	-0.08614644	-0.08614644	9.604309	9.469338	9.315275	9.142917	8.9532	8.747312	8.52667	8.292611	8.046509
19	037_L4_B2B	4	-0.1027365	-0.1027365	-0.1027365	-0.1027365	-0.1027365	8.591467	8.465667	8.323544	8.165701	7.993091	7.80676	7.607937	7.397788	7.177599
20	133_L4_B1A	4	-0.09104189	0.09104189	-0.09104189	-0.09104189	-0.09104189	8.821633	8.692477	8.546921	8.38581	8.210115	8.020881	7.819048	7.605494	7.381249
21	048_L4_B1A	4	-0.1977875	-0.1977875	-0.1977875	-0.1977875	-0.1977875	5.25574	5.110669	4.954646	4.790055	4.618929	4.443005	4.263514	4.081177	3.89674
22	048_L4_B1B	4	-0.1943776	-0.1943776	-0.1943776	-0.1943776	-0.1943776	5.415574	5.265239	5.103743	4.933457	4.756631	4.574862	4.38941	4.201064	4.010437

The correlation coefficient between every single wavelength and the geographical location from samples

4.RESULTS

	A	C	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
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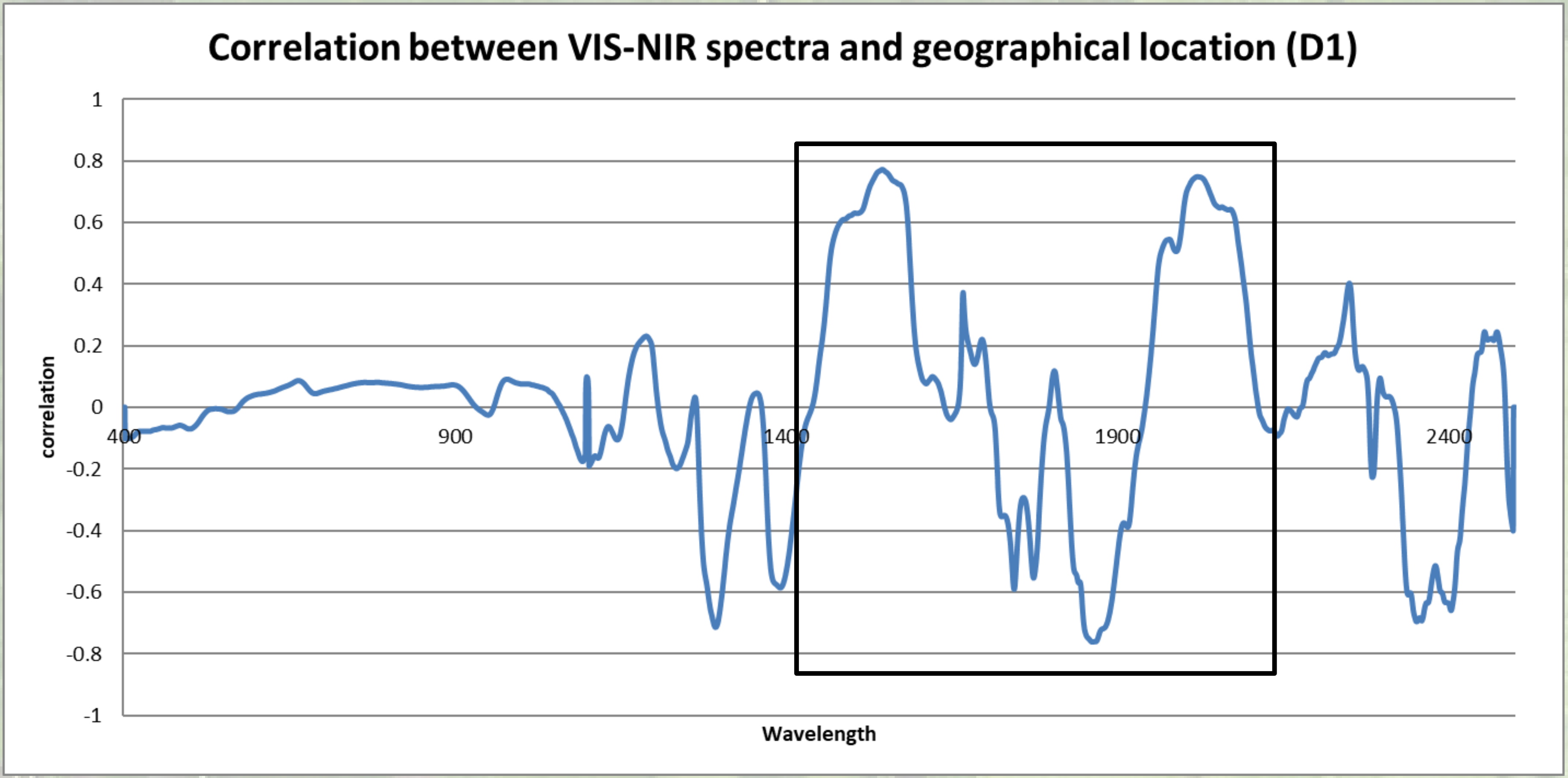
3	074_L4_B2A	4	-0.1950905	-0.1950905	-0.1950905	-0.1950905	-0.1950905	5.099743	4.958691	4.805386	4.641794	4.46982	4.291051	4.107011	3.918899	3.727648
4	074_L4_B2B	4	-0.1951563	-0.1951563	-0.1951563	-0.1951563	-0.1951563	5.087153	4.948351	4.797276	4.635773	4.465504	4.288011	4.10473	3.916954	3.725812
5	028_L4_B1A	4	-0.05060106	-0.05060106	-0.05060106	-0.05060106	-0.05060106	8.531395	8.419162	8.293399	8.154834	8.00419	7.842081	7.669085	7.485689	7.292713
6	124_L4_B2A	4	-0.1835715	-0.1835715	-0.1835715	-0.1835715	-0.1835715	6.582437	6.402778	6.208258	6.001641	5.785751	5.562967	5.335105	5.103597	4.869616
7	071_L4_B1A	4	-0.04791864	-0.04791864	-0.04791864	-0.04791864	-0.04791864	8.448255	8.348013	8.232958	8.103449	7.960065	7.803678	7.635228	7.455591	7.265653
8	028_L4_B1B	4	-0.05113561	-0.05113561	-0.05113561	-0.05113561	-0.05113561	8.545098	8.43719	8.315353	8.180202	8.032292	7.872252	7.700856	7.518838	7.327003
9	217_L4_B1B	4	-0.0684565	-0.0684565	-0.0684565	-0.0684565	-0.0684565	8.750168	8.643576	8.521509	8.384313	8.232509	8.066875	7.8883	7.69774	7.496437
10	083_L4_B1A	4	-0.1065392	-0.1065392	-0.1065392	-0.1065392	-0.1065392	8.654555	8.519915	8.36758	8.198657	8.014532	7.816616	7.606347	7.385094	7.154316
11	083_L4_B1B	4	-0.108052	-0.108052	-0.108052	-0.108052	-0.108052	8.692506	8.554457	8.398266	8.224848	8.035321	7.831086	7.613723	7.384803	7.145971
12	217_L4_B1A	4	-0.06607383	-0.06607383	-0.06607383	-0.06607383	-0.06607383	8.808926	8.705638	8.586017	8.45048	8.299625	8.134303	7.955634	7.764816	7.563065
13	133_L4_B1B	4	-0.09007233	-0.09007233	-0.09007233	-0.09007233	-0.09007233	8.775386	8.650879	8.509552	8.352236	8.179892	7.993622	7.794596	7.584019	7.363189
14	214_L4_B1B	4	-0.1988832	-0.1988832	-0.1988832	-0.1988832	-0.1988832	4.913704	4.780297	4.634584	4.478513	4.31392	4.142337	3.965235	3.783785	3.599136
15	214_L4_B1C	4	-0.1962677	-0.1962677	-0.1962677	-0.1962677	-0.1962677	4.893845	4.762187	4.618301	4.46397	4.300707	4.12993	3.953169	3.77165	3.586645
16	037_L4_B2A	4	-0.0932529	-0.0932529	-0.0932529	-0.0932529	-0.0932529	8.579806	8.460199	8.323943	8.171916	8.005337	7.825466	7.633686	7.431433	7.220181
17	037_L4_B1C	4	-0.08501327	-0.08501327	-0.08501327	-0.08501327	-0.08501327	9.666444	9.522546	9.360785	9.18227	8.98824	8.779823	8.558166	8.324221	8.079026
18	037_L4_B1B	4	-0.08614644	-0.08614644	-0.08614644	-0.08614644	-0.08614644	9.604309	9.469338	9.315275	9.142917	8.9532	8.747312	8.52667	8.292611	8.046509
19	037_L4_B2B	4	-0.1027365	-0.1027365	-0.1027365	-0.1027365	-0.1027365	8.591467	8.465667	8.323544	8.165701	7.993091	7.80676	7.607937	7.397788	7.177599
20	133_L4_B1A	4	-0.09104189	-0.09104189	-0.09104189	-0.09104189	-0.09104189	8.821633	8.692477	8.546921	8.38581	8.210115	8.020881	7.819048	7.605494	7.381249
21	048_L4_B1A	4	-0.1977875	-0.1977875	-0.1977875	-0.1977875	-0.1977875	5.25574	5.110669	4.954646	4.790055	4.618929	4.443005	4.263514	4.081177	3.89674
22	048_L4_B1B	4	-0.1943776	-0.1943776	-0.1943776	-0.1943776	-0.1943776	5.415574	5.265239	5.103743	4.933457	4.756631	4.574862	4.38941	4.201064	4.010437

The correlation coefficient between every single wavelength and the geographical location from samples

4.RESULTS

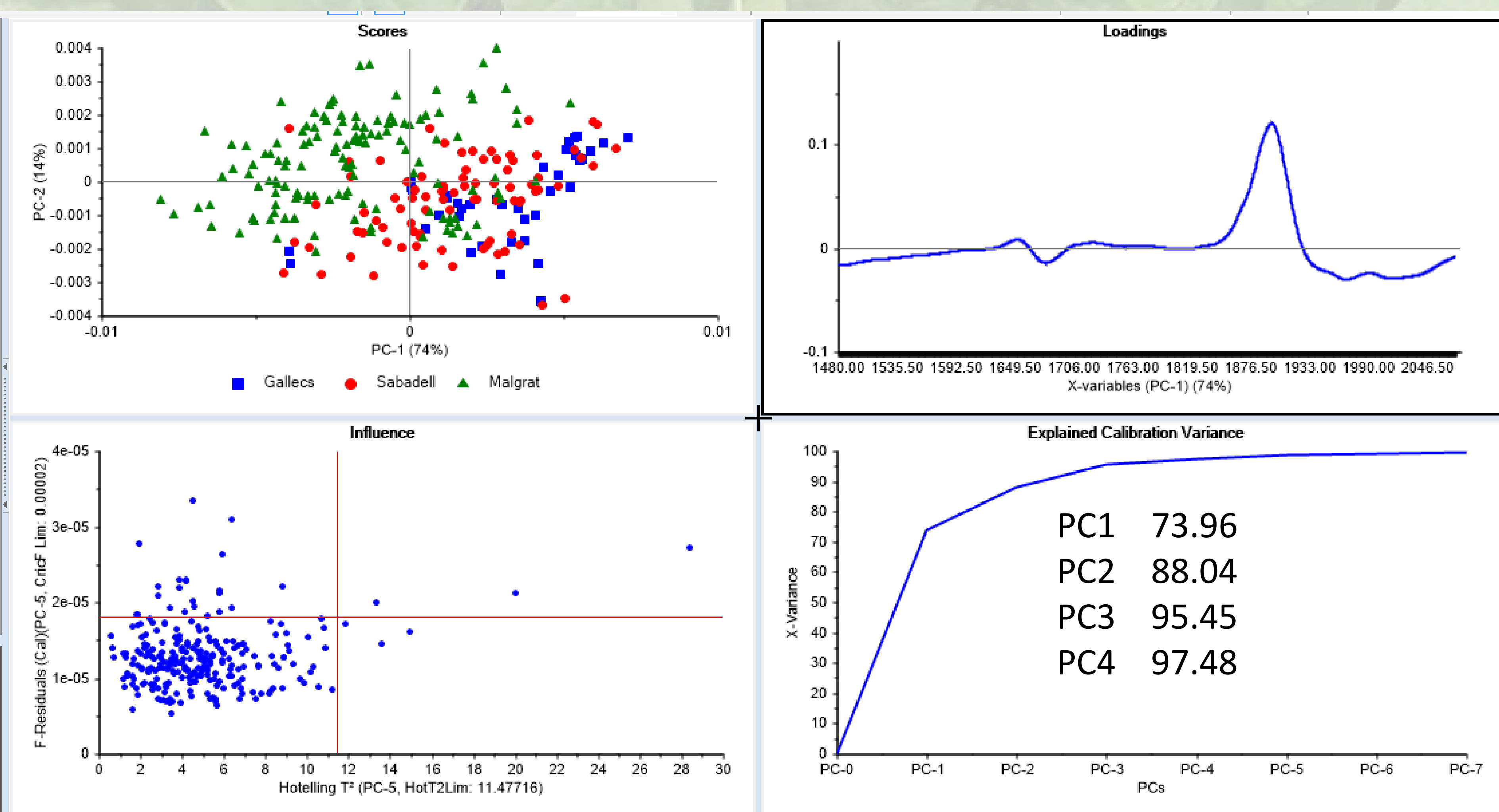


1480-2045nm

4.RESULTS

1480-2045 nm./ 1st SG Derivative/ 11 smoothing points

PCA Algorithm: Single Value Decomposition

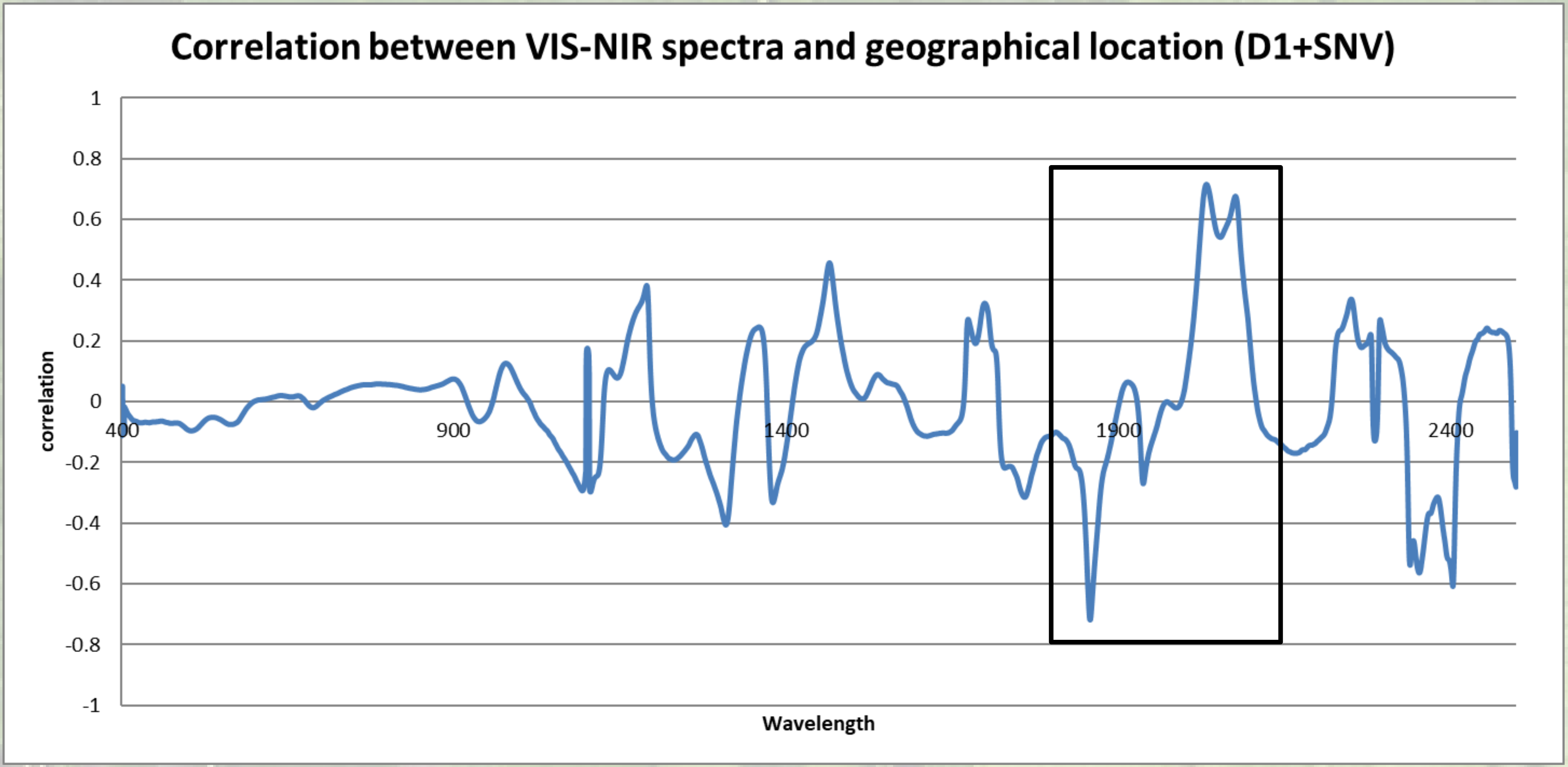


1480-2045 nm./ 1st SG Derivative/ 11 smoothing points

PCA Algorithm: Single Value Decomposition

We need to keep improving

4.RESULTS

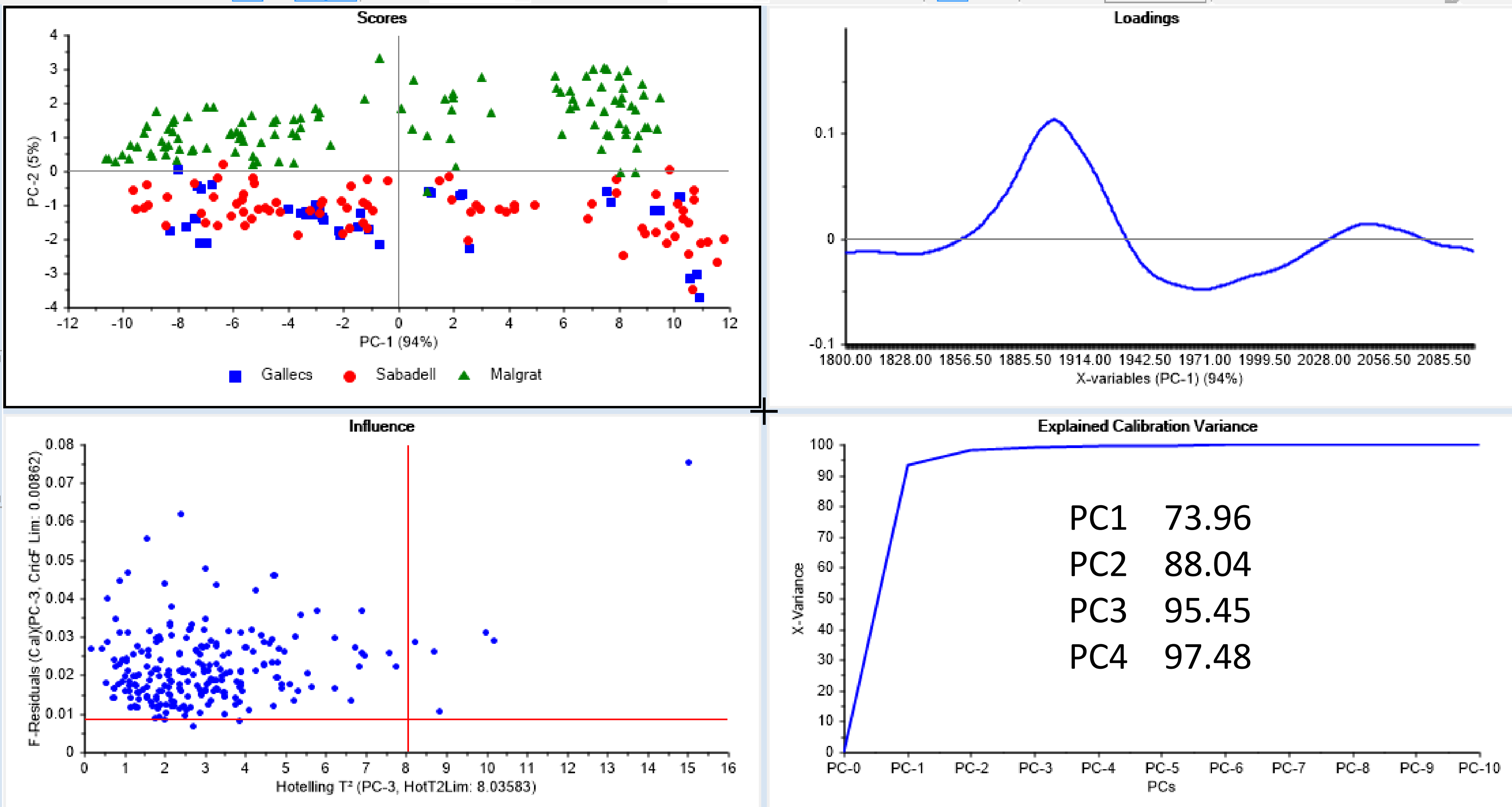


1800-2100nm

4.RESULTS

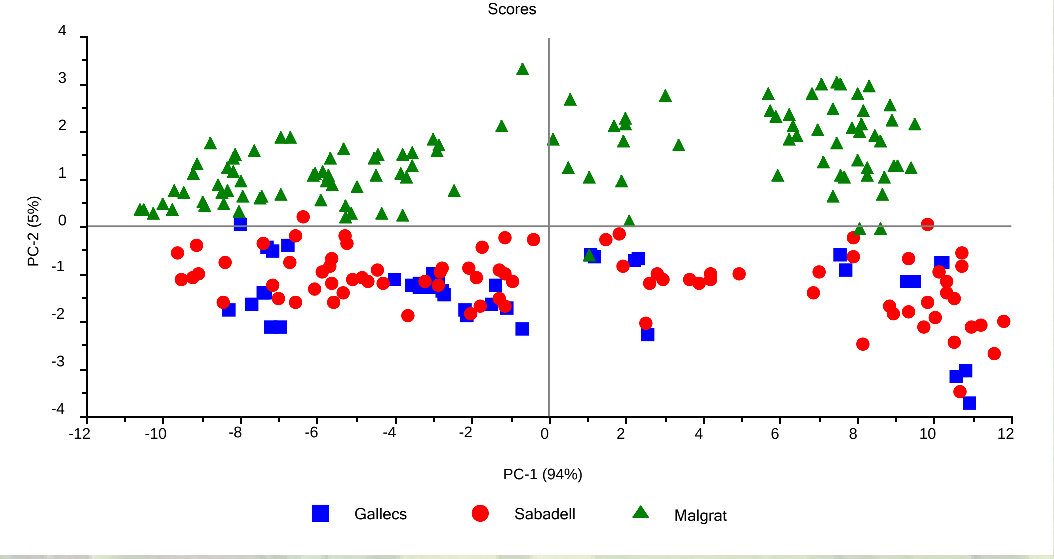
1480-2045 nm./ 1st SG Derivative+SNV/ 11 smoothing points

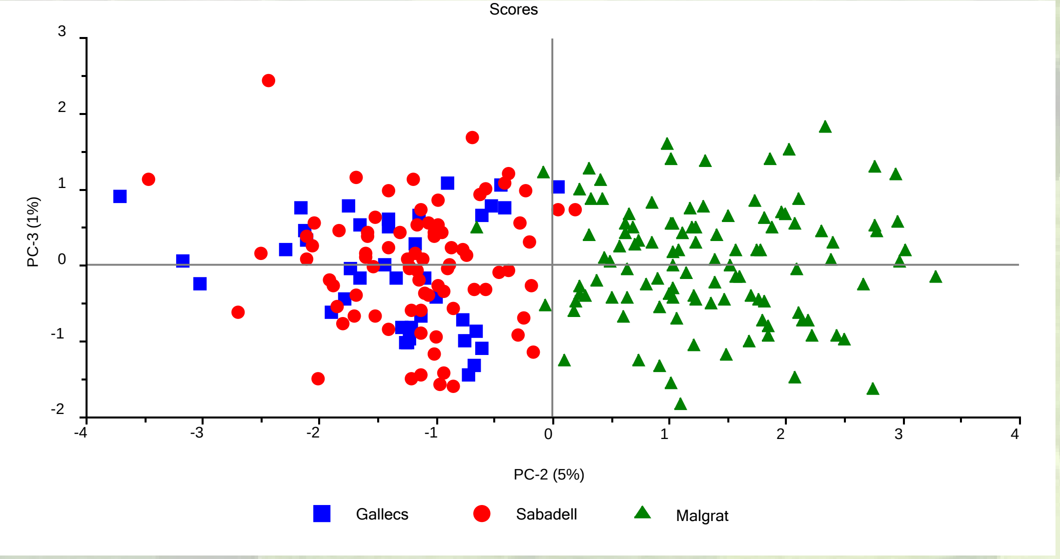
PCA Algorithm: NIPALS



4.RESULTS

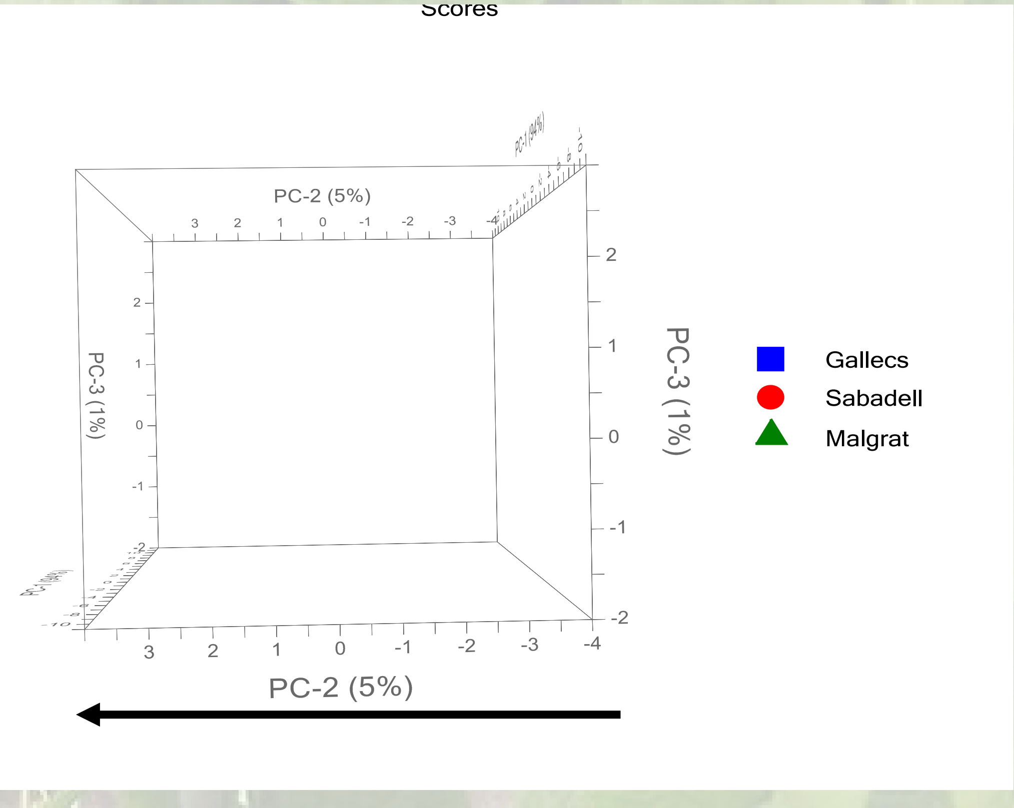
Score Plots





4.RESULTS

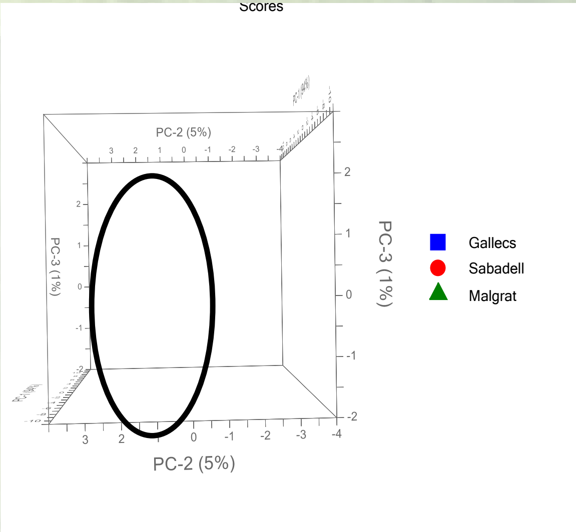
Score Plots

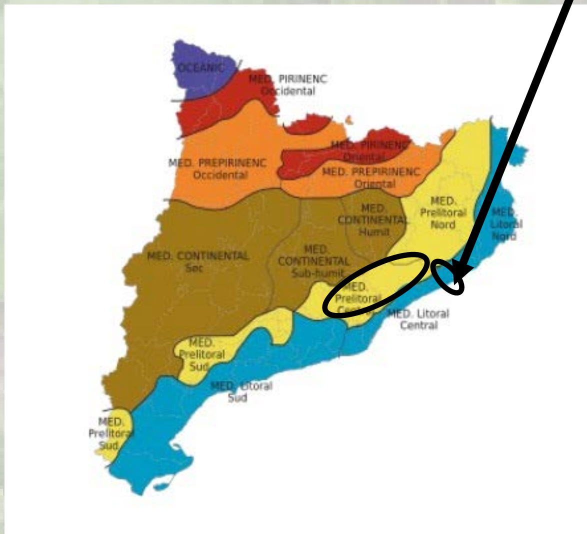


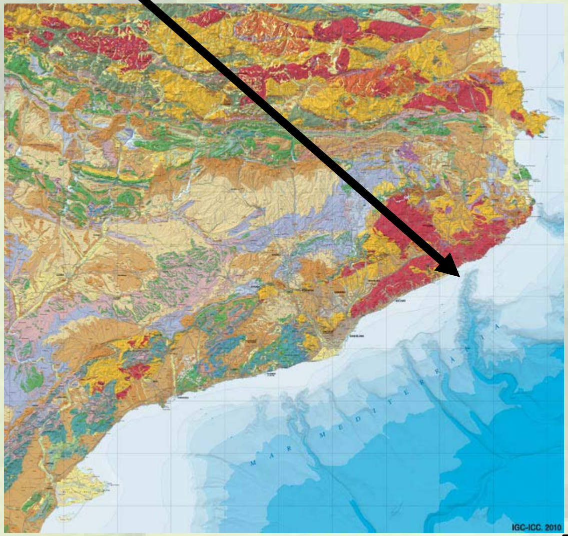
- **PC 2 explains the geographic differences between beans from Malgrat and the ones from Vallès Occidental County (Sabadell, Gallecs).**
- **PCA is not able to distinguish differences between samples from Sabadell and from Gallecs.**

4.RESULTS

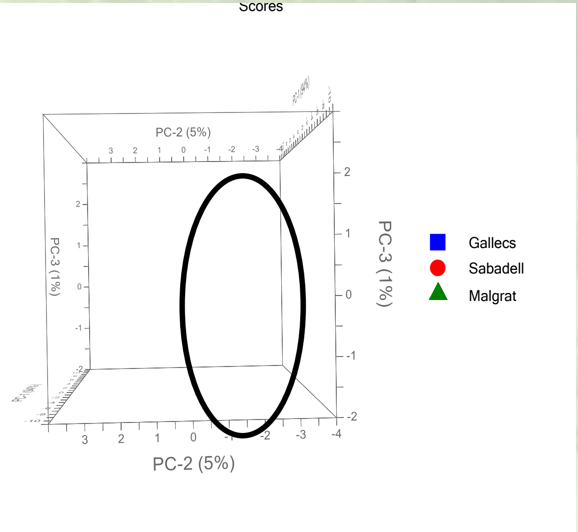
Malgrat

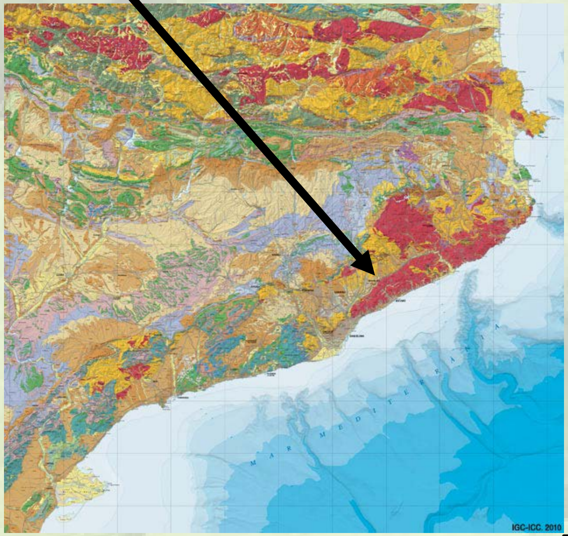




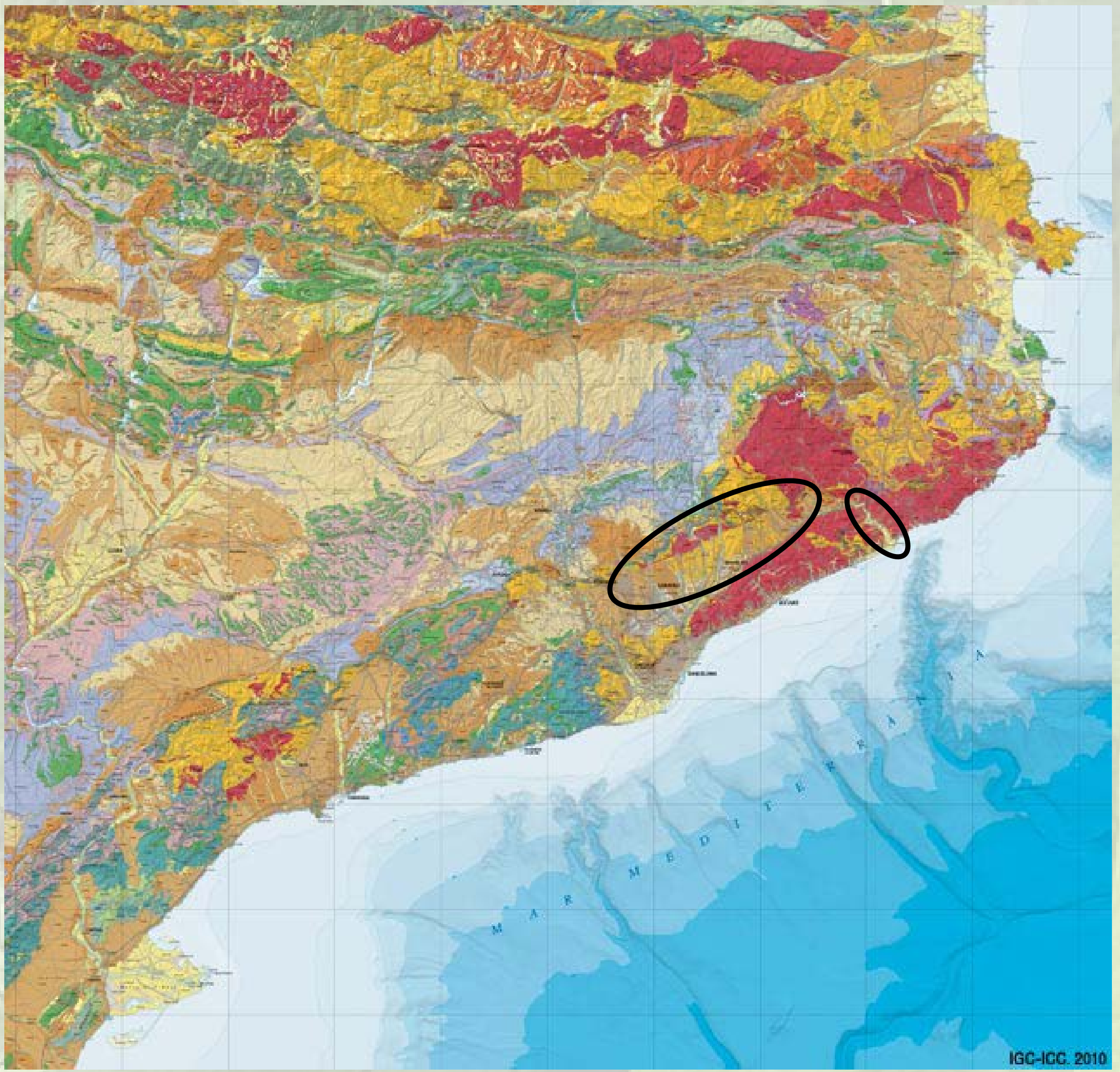


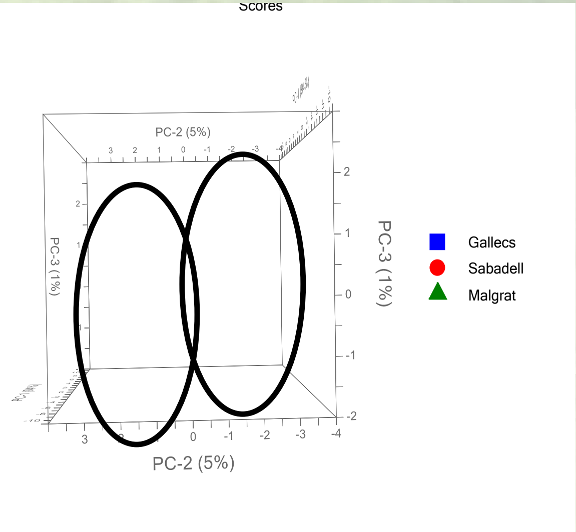
Sabadell and Gallecs





4.RESULTS



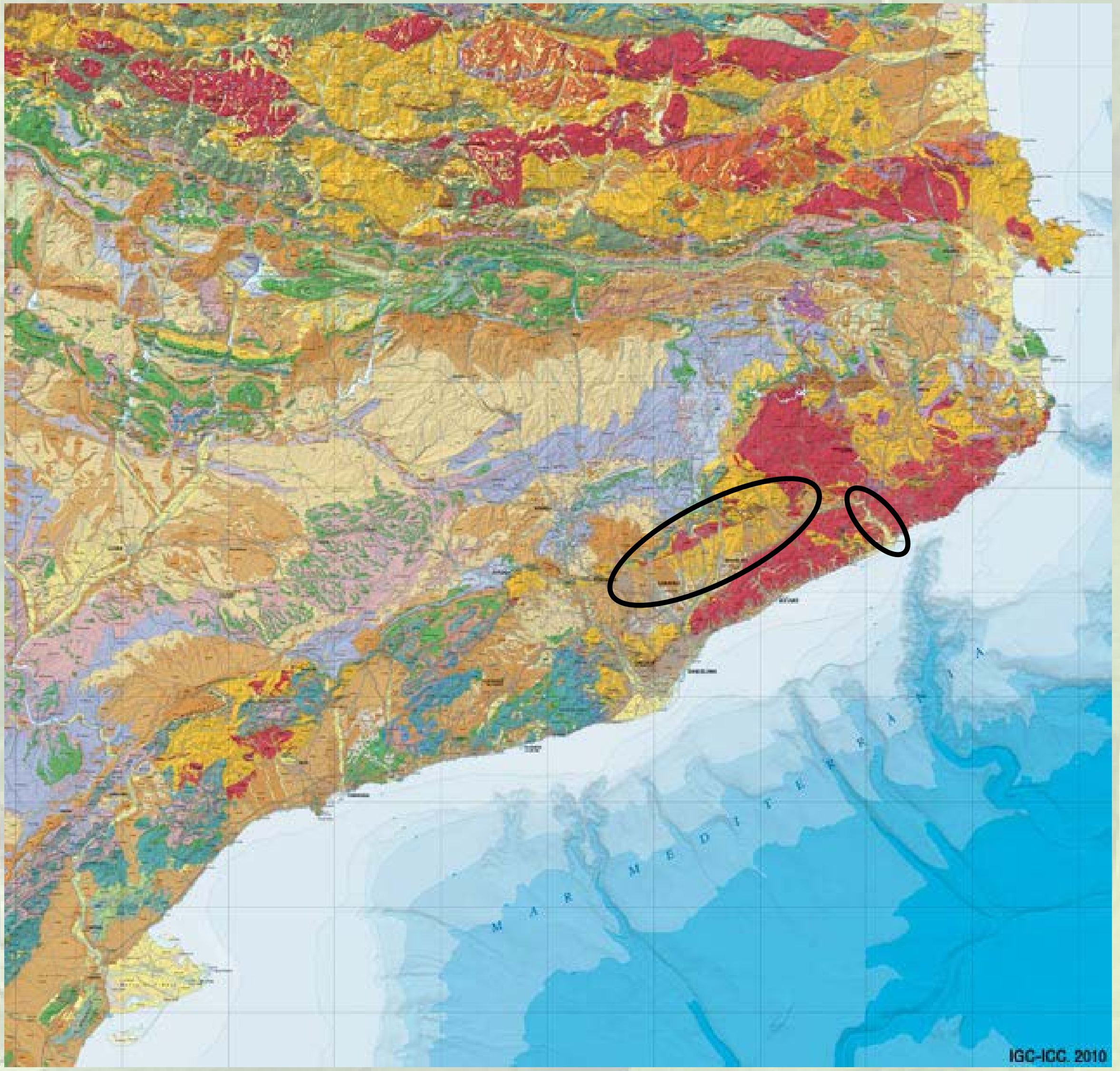


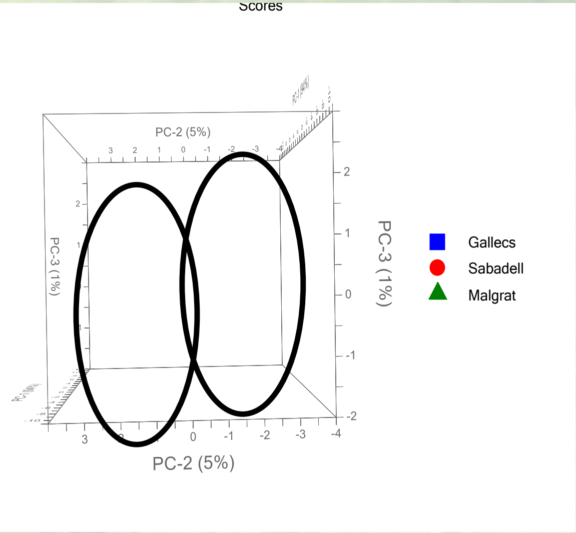
The same type of soil (Dh-Q/Si)

- **Sandstone**
- **Shale**
- **Conglomerate**

Soils with high Calcium content

4.RESULTS



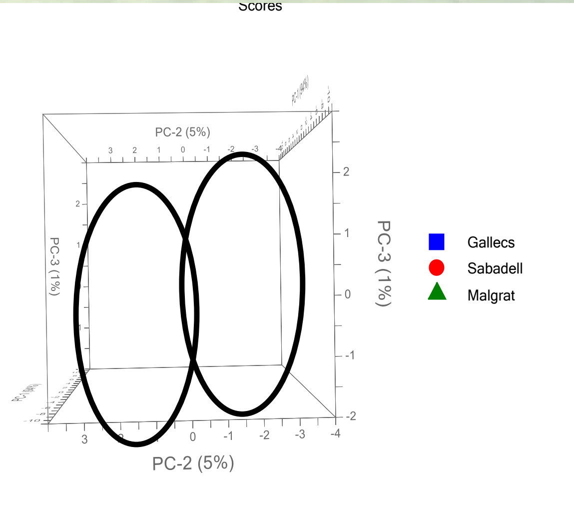


The differences observed in the PCA analysis from the bean spectra are not because of the soil.

4.RESULTS

Different Mediterranean climates

- **Malgrat:** Central Litoral Mediterranean climate
- **Sabadell and Gallecs:** Central Prelitoral Mediterranean climate

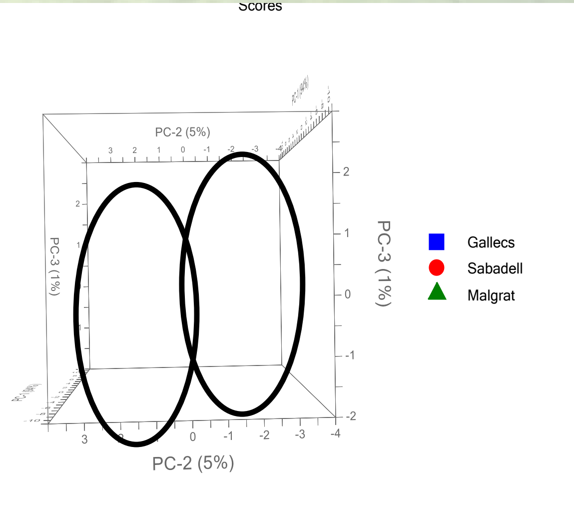


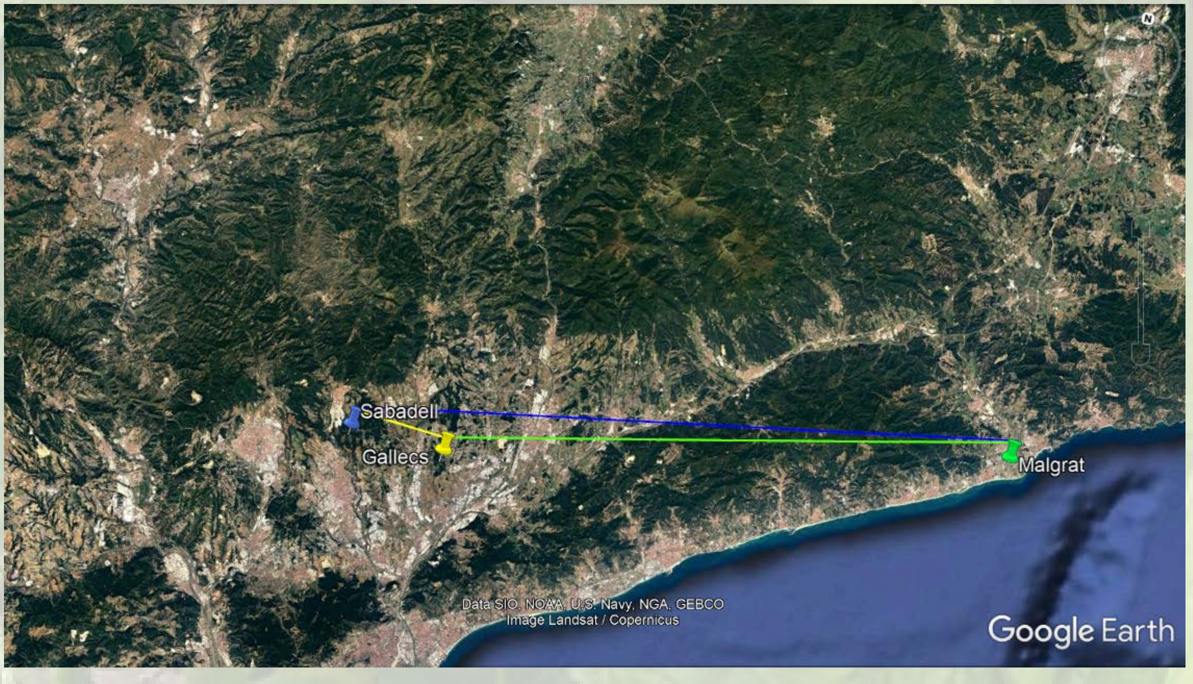
- Similar annual precipitation to Vallès county but with more possibility of hard storms because of the orography.
- Warmer temperatures in winter and softer summers than in Vallès

4.RESULTS

Different Mediterranean climates

- **Malgrat:** Central Litoral Mediterranean climate
- **Sabadell and Gallecs:** Central Prelitoral Mediterranean climate





Sabadell-Malgrat: 72,3 km
Gallecs-Malgrat: 47,8 km
Sabadell-Gallecs: 7,76 km

PART 2:

Detection of future bean pathologies such as Pythium and white mold by using NIR-Vis spectroscopy and Partial Least Squares Regression (PLSR)

4.RESULTS

Division of datasets

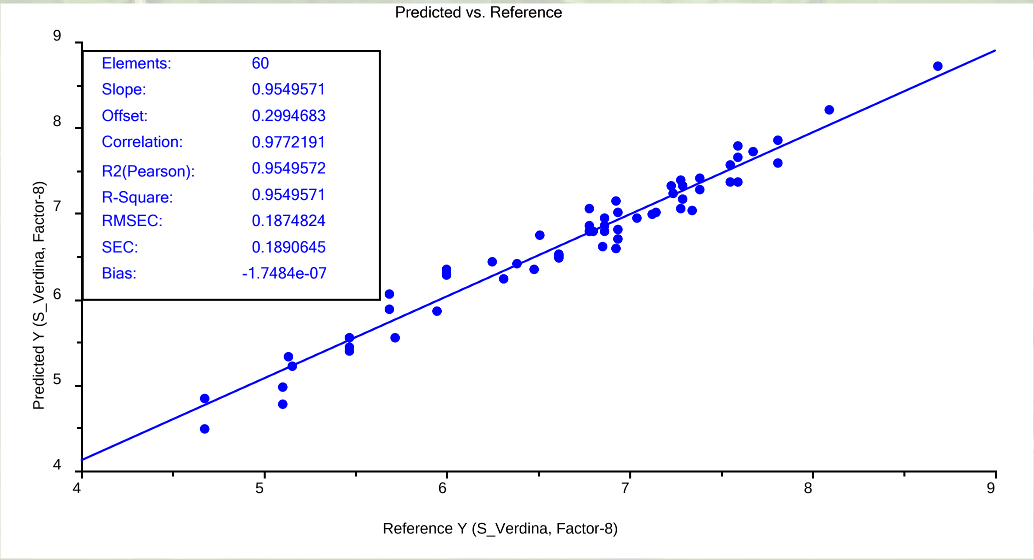
PATHOLOGIES

Sclerotinia_V	CALIBRATION 60 samples VALIDATION 214 samples
Sclerotinia_X	CALIBRATION 60 y VALIDATION 200 samples
Pythium_crec	CALIBRATION 64 samples VALIDATION 109 samples
Pythium_des	CALIBRATION 57 samples VALIDATION 60 samples

4.RESULTS

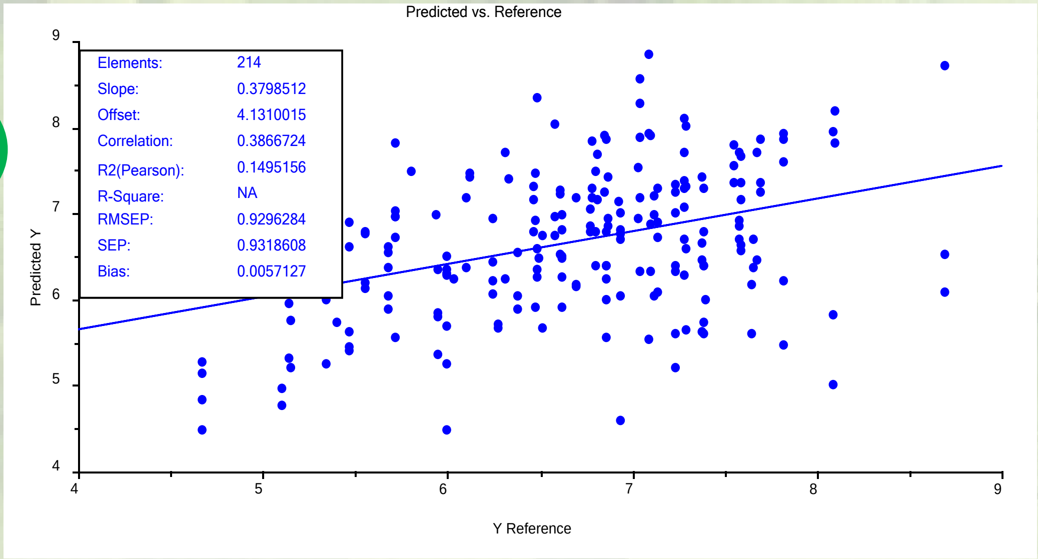
Sclerotinia_V
8 PLS components
Range :1900-2500nm
Pretreatment: SG 2D 11points 2order
Calibration range: 4.67-8.7
RMSEC= 0.19
Prediction range: 4.67-8.7
RMSEP= 0.87

Calibration



Average of residual	0.01
Standard deviation of residual	0.93
t-calculated	0.93
t(214,0,05)	1.97

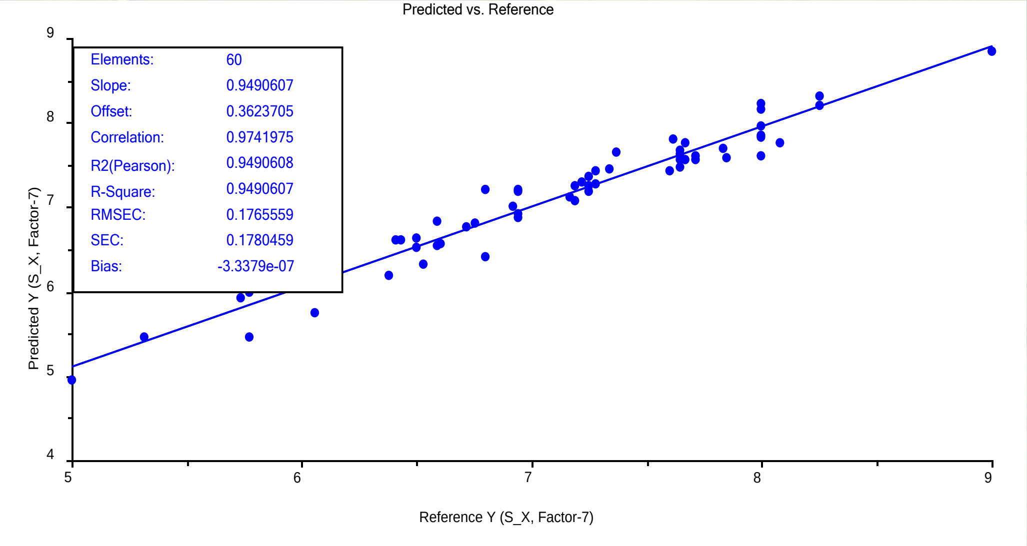
Prediction



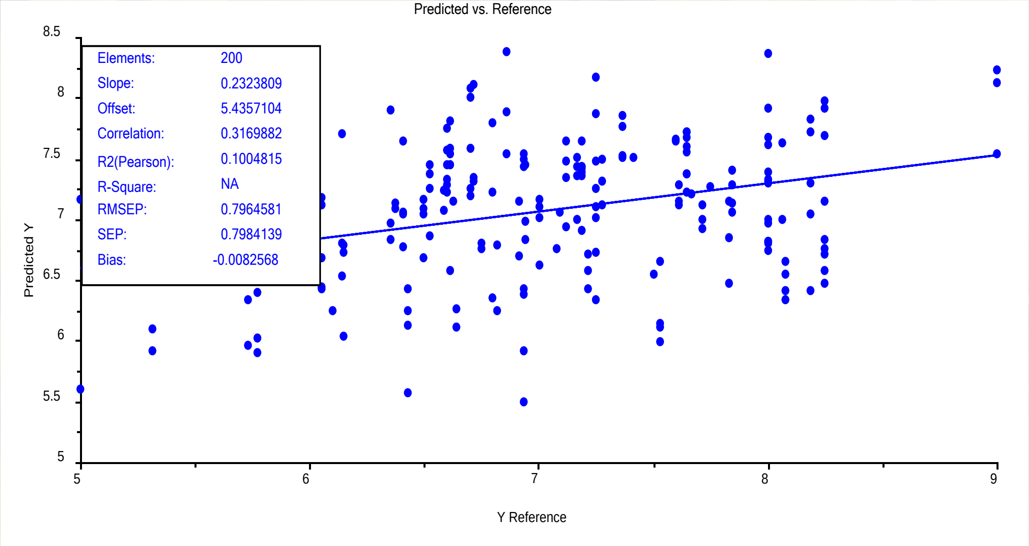
4.RESULTS

Sclerotinia_X
7 PLS components
Range :2000-2500nm
Pretreatment: SG 2D 11points 2order
Calibration range: 5-9
RMSEC= 0.19
Prediction range: 5-9
RMSEP= 0.79

Calibration



Prediction

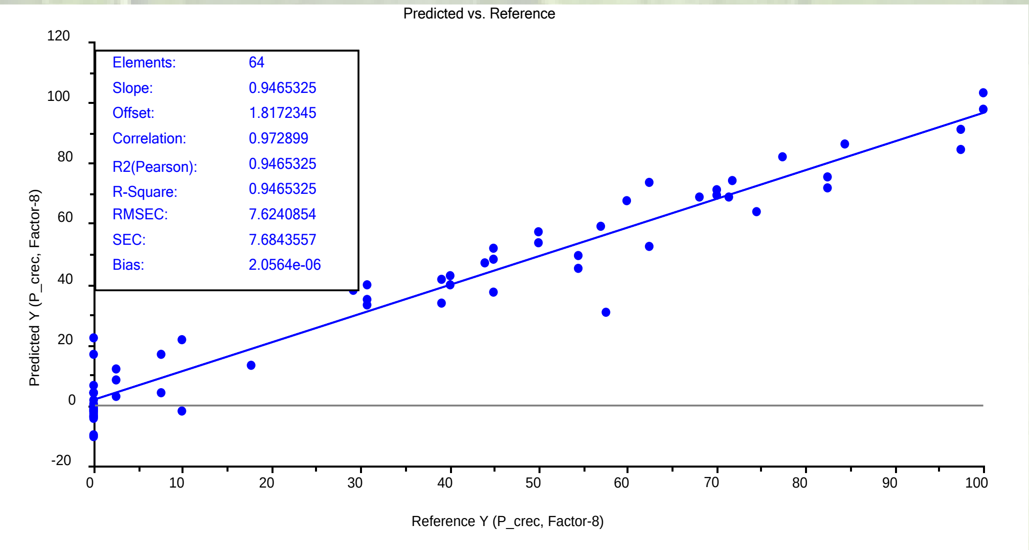


Average of residual	-0.01
Standard deviation of residual	0.80
t-calculated	0.88
t(214,0,05)	1.97

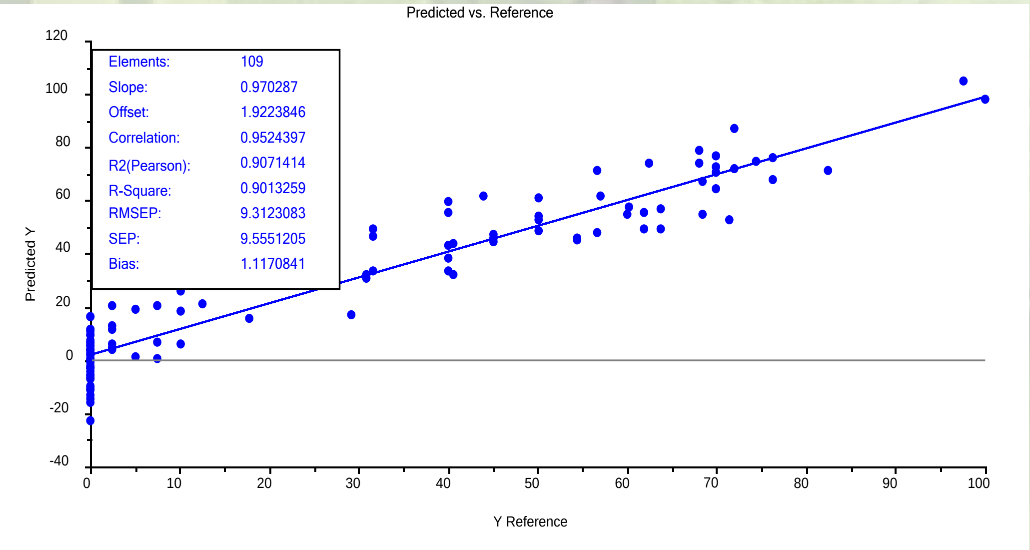
4.RESULTS

Pythium Crec %
8 PLS components
Range: 900-2500nm
Pretreatment: SG 2D 11points 2order
Calibration range: 0-100%
RMSEC= 7.62
Prediction range: 0-100%
RMSEP= 9.31

Calibration



Prediction



Average of residual	1.12
Standard deviation of residual	9.29
t-calculated	0.21
t(214,0,05)	1.98

4.RESULTS

Pythium Des %

7 PLS components

Range: 1900-2500nm

Pretreatment: SG 2D 11points 2order

Calibration range: 48.3-86.7%

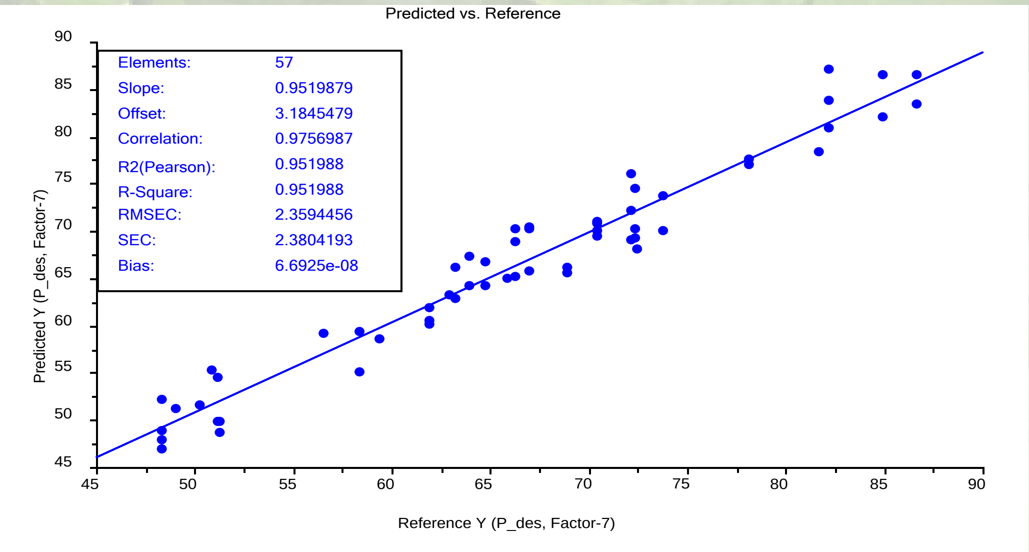
RMSEC= 7.62

Prediction range: 48.3-82.2%

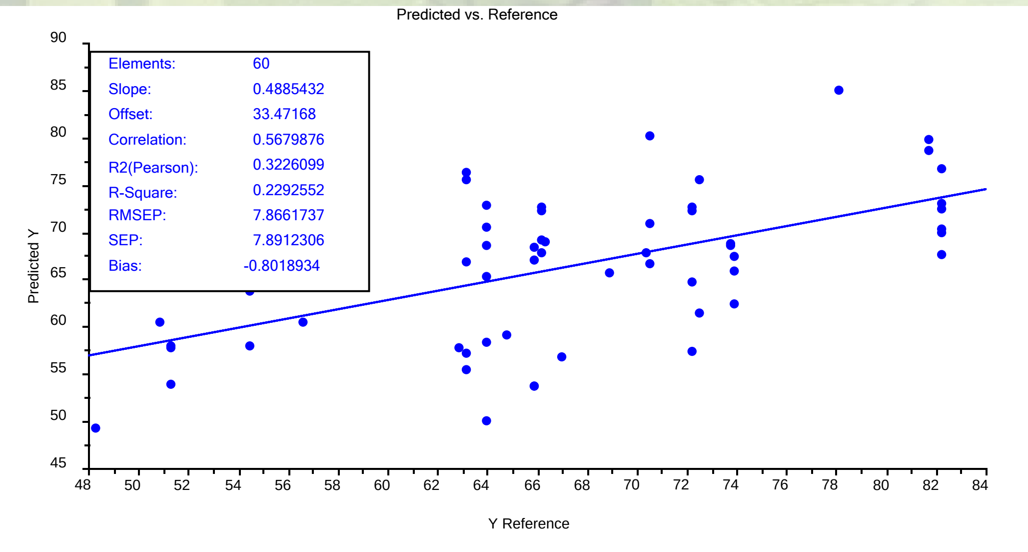
RMSEP= 7.87

Average of residual	-0.80
Standard deviation of residual	7.89
t-calculated	0.43
t(214,0,05)	2.00

Calibration



Prediction



4.RESULTS

Summary

CALIBRATION

Pathology	Pretreatments	Spectral Range	Samples No.	Slop	Correlation	RMSEC	Factor	Explained Y
Sclerotinia_V	SG 2D 11points	1900-2500nm	60	0.955	0.977	0.187	8	95.47
Sclerotinia_X	SG 2D 11points	2000-2500nm	60	0.949	0.974	0.177	7	94.90
Pythium_crec	SG 2D 11points	900-2500nm	64	0.947	0.973	7.624	8	94.65
Pythium_des	SG 2D 11points	1900-2500nm	57	0.952	0.976	2.359	7	95.19

VALIDATION

Pathology	Samples No.	Slop	Correlation	RMSEP
Sclerotinia_V	214	0.3785	0.3866	0.9296
Sclerotinia_X	200	0.232	0.3169	0.7964
Pythium_crec	109	0.9702	0.9524	9.3123
Pythium_des	60	0.4885	0.5679	7.8661

5. CONCLUSIONS

5.CONCLUSIONS

- **Relationships between NIR spectra and climates have been demonstrated.**
- **The wavelength range selection is the most important step for obtaining good results for this purpose.**
- **Because of the 3 different places have the same type of soil we haven’t been able to demonstrate a relationship between types of soil and NIR spectra.**
- **The results of validation for this 4 pathology parameters show us low residual and error values and good predictive performances.**
- **NIR modeling data from bean spectra can be an alternative technique to PCR and ELISA for determining future pathologies in bean plants.**

Acknowlegements

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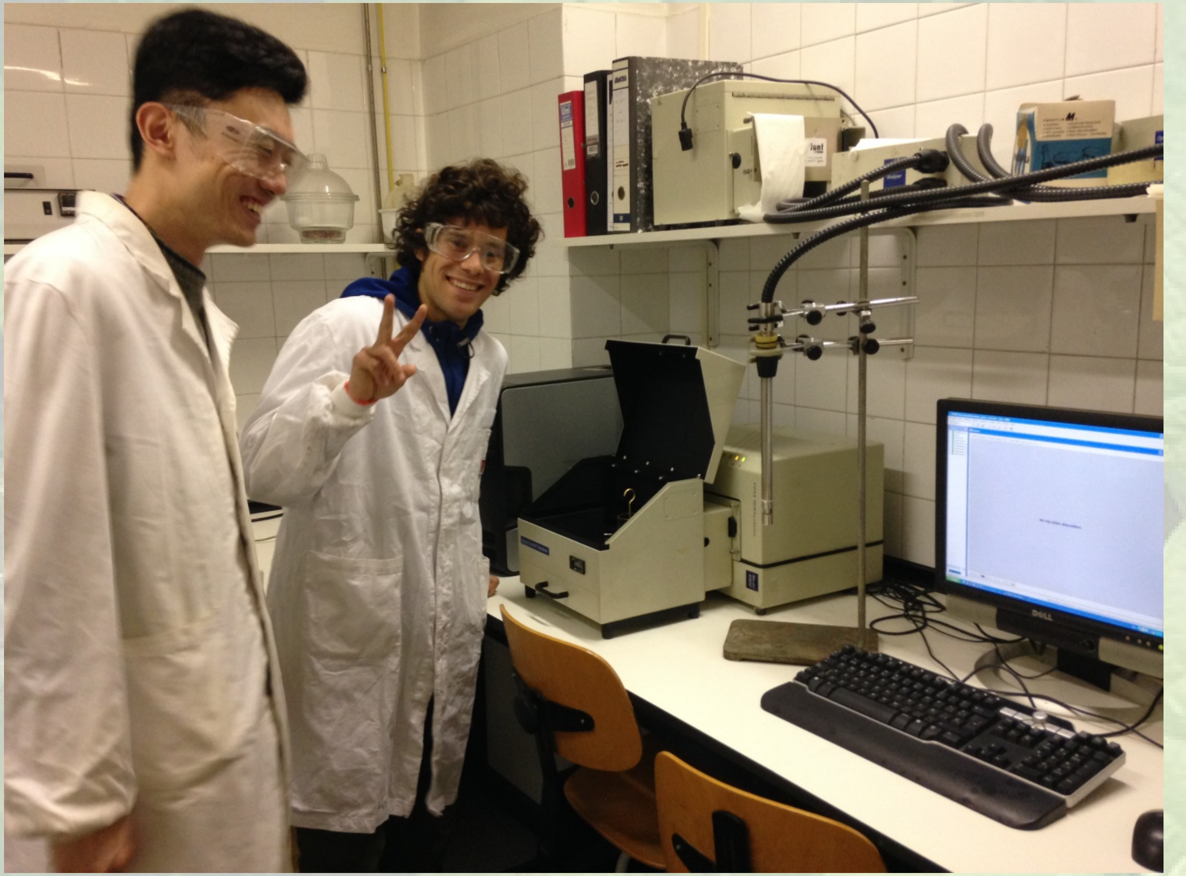
UAB
Universitat Autònoma de Barcelona

euss enginyeria

Fundació Miquel Agustí




Thanks!!!
Any question???

Applied Chemometrics Research Group
Universitat Autònoma de Barcelona

Prediction of bean plants pathologies, and geographical origin by using NIR-Vis spectroscopy and chemometrics

J. Cruz, M. Alcalà , F. Casañas, A. Rivera, J.Sabaté, J. Simó, M. Plans

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UAB Universitat Autònoma de Barcelona

The Council For CNIRS Near-Infrared Spectroscopy

Chambersburg, August 1st 2018