

**AN ATTEMPT OF PREDICTION OF  
BIOLOGICAL ACTIVITY (Ames test)  
FUNCTION OF TOBACCOS CHEMICAL  
AND PHYSICAL CHARACTERISTICS**

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# TYPES OF TOBACCOS UNDER STUDY

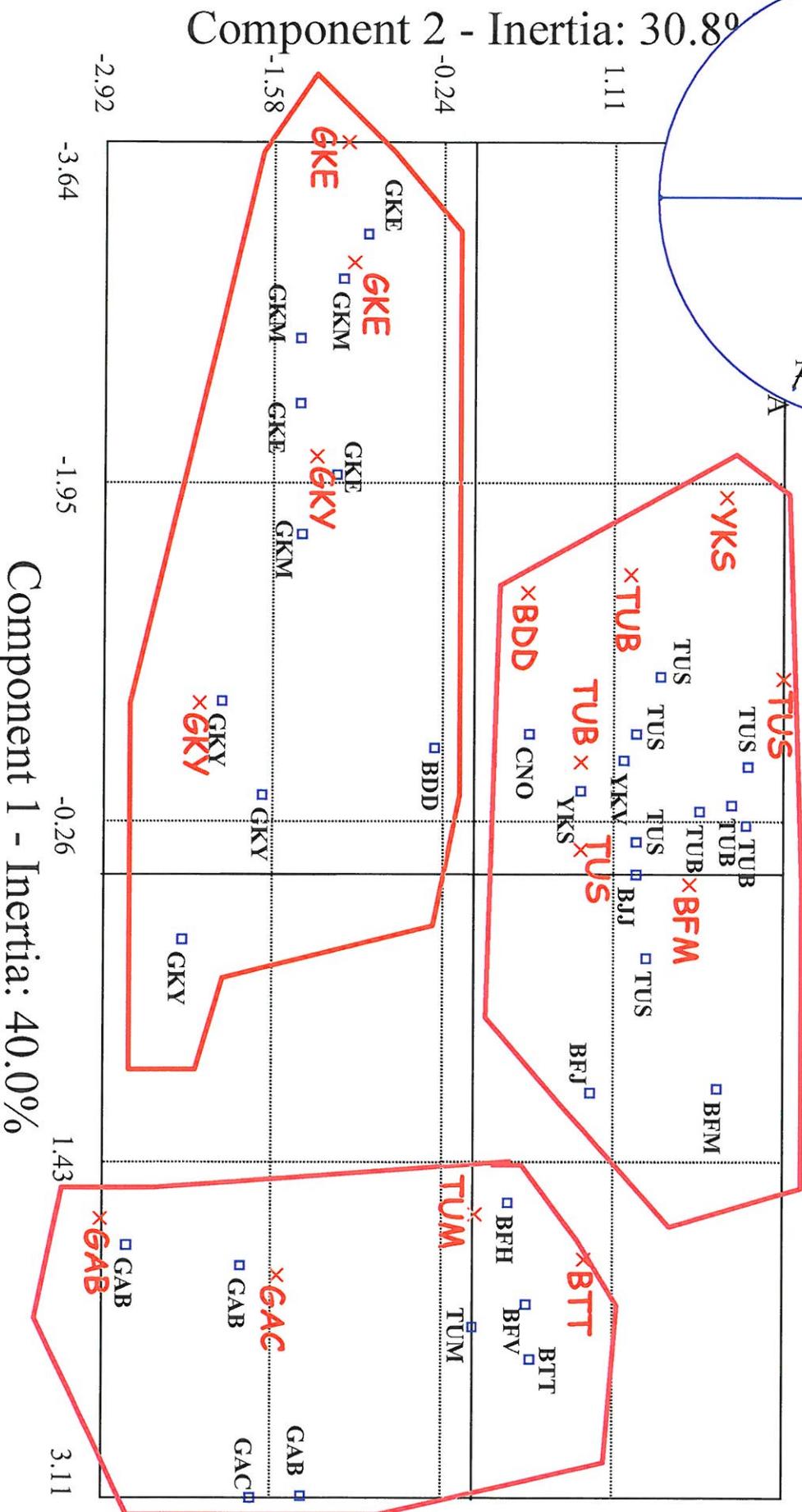
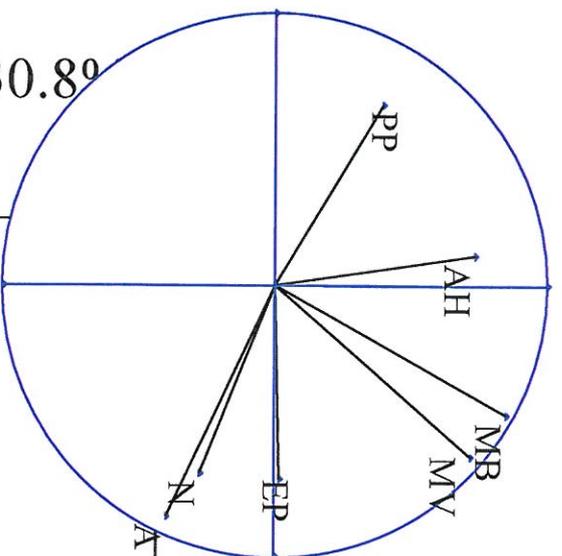
- **FLUE-CURED**
  - » 23 TOBACCO GRADES FROM 6 COUNTRIES
  - + 1 BLEND
- **BURLEY**
  - » 21 TOBACCO GRADES FROM 9 COUNTRIES
  - + 3 BLENDS
- **SUN-CURED**
  - » 15 TOBACCO GRADES FROM 4 COUNTRIES
- **DARK-AIR-CURED**
  - » 16 TOBACCO GRADES FROM 6 COUNTRIES
  - + 8 BLENDS





# Reference mapping for sun-cured 95-99

Factorial plane 1-2



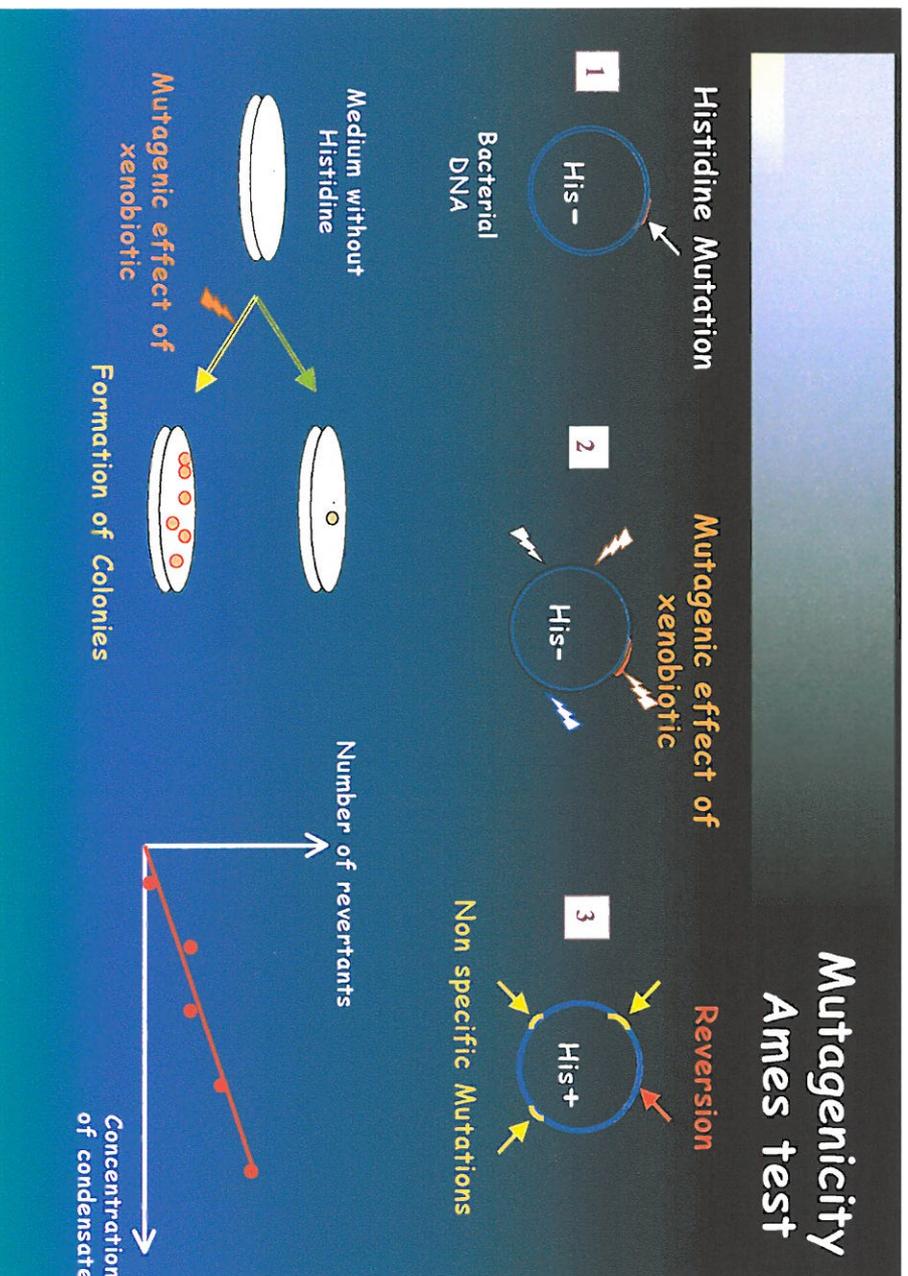
# Working study

## •Dark Air-cured

| BRASIL  | PARAGUAY | ARGENTINA | FRANCE   | INDONESIA | INDIA | CUBA | COLOM NIA | PHILIPPINES | ITALIA |
|---------|----------|-----------|----------|-----------|-------|------|-----------|-------------|--------|
| BAR1    | PAY PL1  | ARC       | FRD PL11 | INB       | IDE   | CUV  | CLC       | PI1         | TTD    |
| BAR2    | PAY PN1  |           | FRD PN11 | IOE       | IDL   | CUR  |           |             |        |
| BBA H   |          |           | FRD PL12 | INK       |       |      |           |             |        |
| BRC PN1 |          | ↘         | FRD PN12 | IOL       |       |      |           |             |        |
| BRC PL1 |          | ↘         | FRD PN13 |           |       |      |           |             |        |

# Mutagenicity test (Ames test) = PMUT

## VARIABLE to be PREDICTED



# •ANALYSIS = PREDICTATIVE VARIABLES

- **CHEMICAL ANALYSIS**
  - 50 CRITERIA
- **VISIBLE and Near InfraRed Spectra**
- **PHYSICAL**
  - 4 MEASUREMENTS (hardness, free burning rate, weight of tobacco, filling density)
    - Cigarettes with the same N.T.M
      - **Draw resistance ~CST**
      - width of cut = 1.0 mm
- **SMOKING**
  - 5 MEASUREMENTS ARE DONE (TAR, Nic, puff number, CO,H<sub>2</sub>O)

# Chemical measurements

**Tobacco markers**

**Burley, FC, Sun cured, Dark**

Amino Acids

ASparagiNe

ASPartic Acid

PROline

Alkaloids A

Nic, Nor, Anat,

Cotinine

Sugars

G, F, S

Cell wall compounds

Lignin, Cellulose, hemicCell

CITTric acid

MALic acid

NH<sub>3</sub>, PO<sub>4</sub>, N

P.E

Methyl Valeric ac.

Methyl Butyric ac

Polyphenols PP

Color

L,a,b,(H,c)

Aminosugars

FALA, FASN, FGLU, FPRO

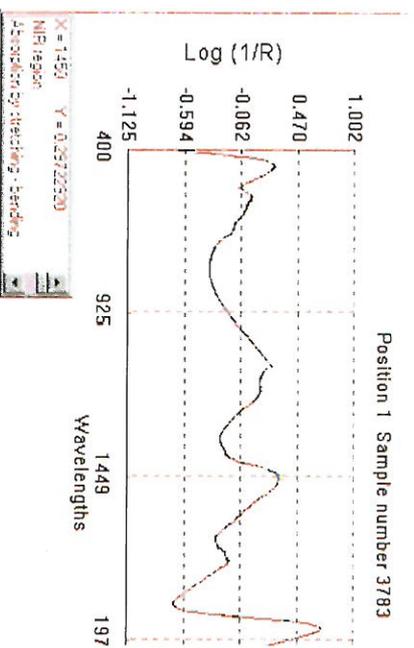
Ca, Mg, K, Ashes, Cl, NO<sub>3</sub>, Total

Alcalinity, Hydrosoluble Alcalinity.

# VISIBLE and Near InfraRed Spectra :

## Presentation of the methodology

• INTERACTION between electromagnetic waves and the level of vibration energy of molecules



• LEVEL of Absorbance

• predictive models

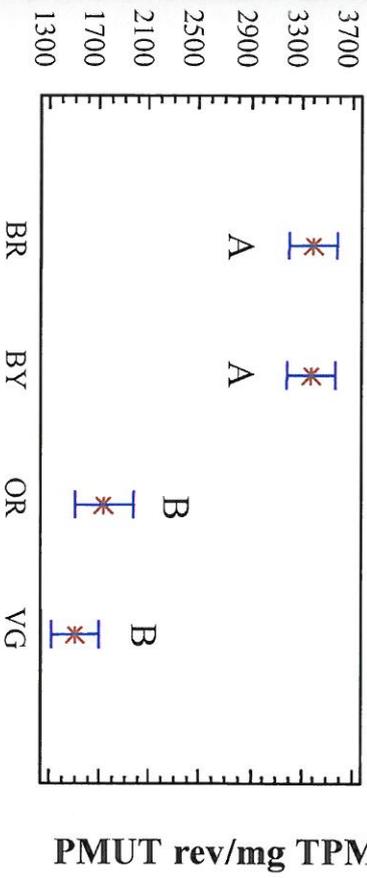
• QUANTITATIVE ANALYSIS

### • CHIMIOMETRIC APPROACH

∴ using mathematical and statistical methods to develop different models of prediction

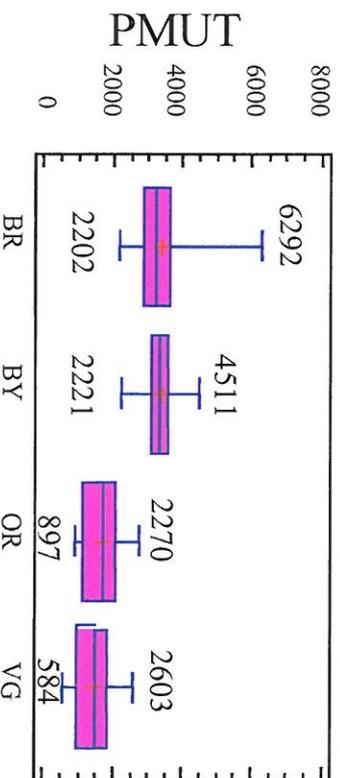
# PMUT : SPECIFIC BIOLOGICAL ACTIVITY

Means and 95,0 Percent LSD Intervals



**BR and BY belong to the same group.  
OR and VG are on an other group.**

Box-and-Whisker Plot



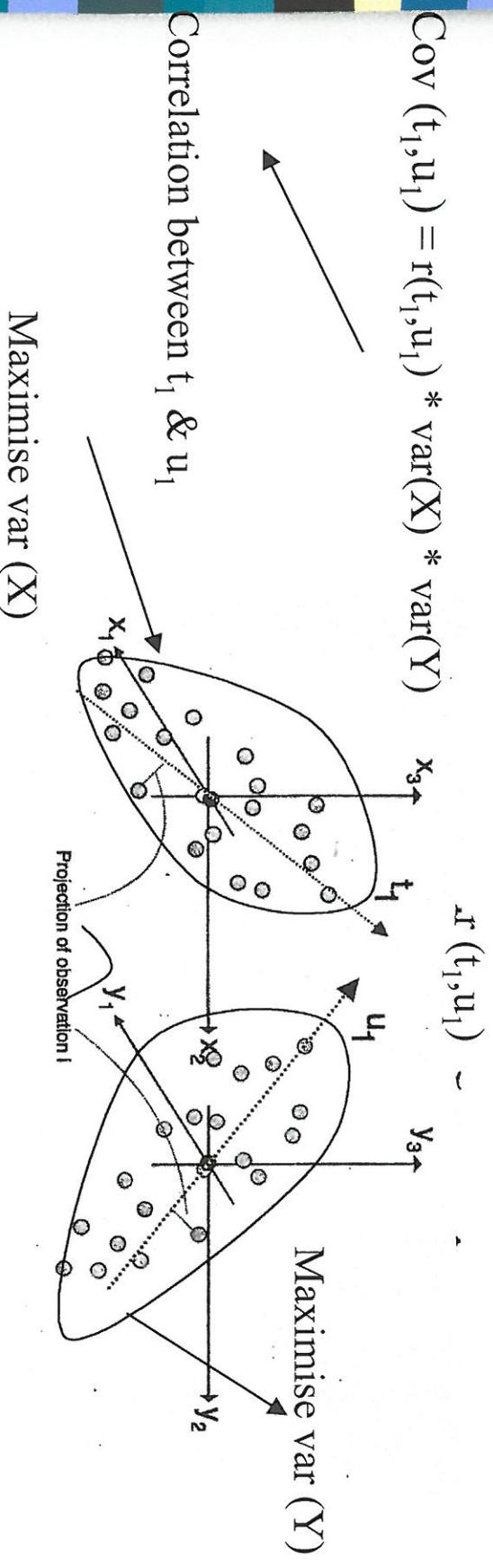
# Methods

- **Mathematical pre treatment of NIRS :**
  - Derivate and Detrending
  - Standard Normal Variante
  - Multiplicative Scatter Correction
  - Orthogonal Signal correction
  - Mix of Derivate SNV & Derivate OSC
- **Methods of obtaining prediction**
  - Linear Multiple Regression
  - Partial Least Square Regression

# Partial Least Squares Regression

- Purposes :
  - To link a block of explanatory variables (e.g chemical criteria) and one or many variables to explain (e.g Pmut)

$$\text{Cov}(t_1, u_1) = r(t_1, u_1) * \text{var}(X) * \text{var}(Y)$$





# Chemical block predictions results (Quality of model and variables involved)

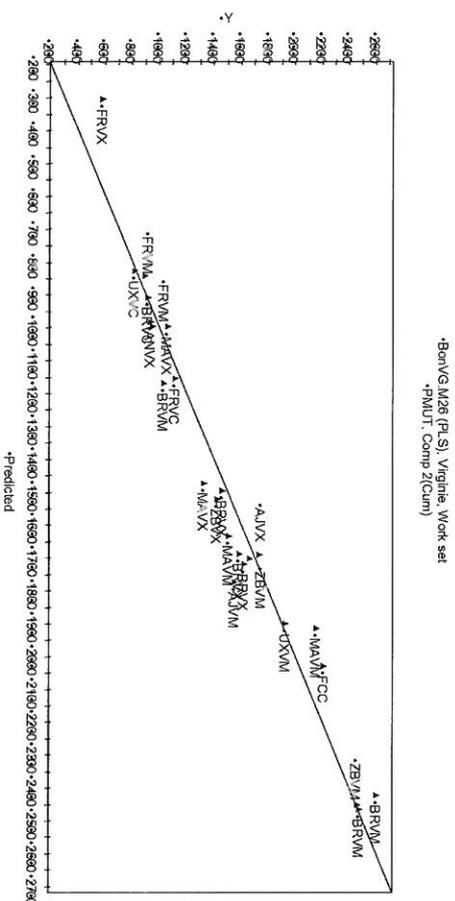
| Type / Criteria | $R^2_{adj}$ | $Q^2_{cum}$ | RMSEE | RMSEP |
|-----------------|-------------|-------------|-------|-------|
| Flue cured      | 95.3 %      | 90.4 %      | 130   | 123   |
| Burley          | 85.4 %      | 66.5 %      | 222   | 465   |
| Sun cured       | 98.5 %      | 97.5 %      | 81    |       |
| Dark air cured  | 61.8 %      | 50.2 %      | 351   |       |

$R^2_{Y_{adj}}$  : Quality of reconstitution

$Q^2_{cum}$  : Quality of prediction by cross validation

RMSEE : Root Mean Square error of Estimation

RMSEP : Root Mean Square error of Prediction



• RMSEE=129  
• since P=0.07, Umbralce Ab=2002.09.23 11.52

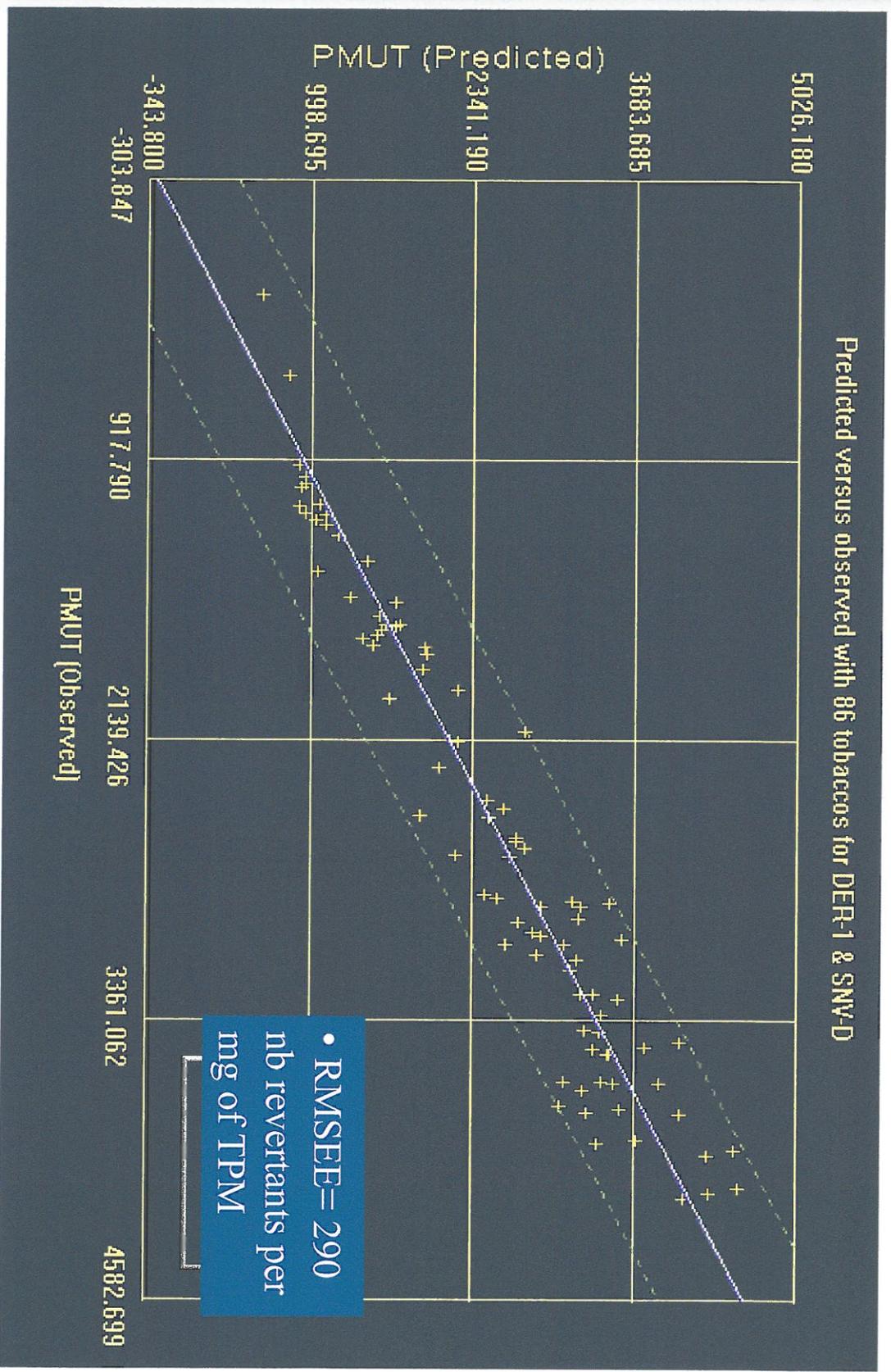
| Variables    | F.C. | S.C. | Bey | D.A.C |
|--------------|------|------|-----|-------|
| N.932        |      |      |     |       |
| A            |      |      |     |       |
| C.932        |      |      |     |       |
| Normicotine  |      |      |     |       |
| Nicotine     |      |      |     |       |
| Anatabine    |      |      |     |       |
| Hardness     |      |      |     |       |
| PP           |      |      |     |       |
| NO3          |      |      |     |       |
| CITFL        |      |      |     |       |
| PRO          |      |      |     |       |
| K            |      |      |     |       |
| P.E          |      |      |     |       |
| Color(L,a,b) |      |      |     |       |
| TAR          |      |      |     |       |

# Comparison of NIRS models

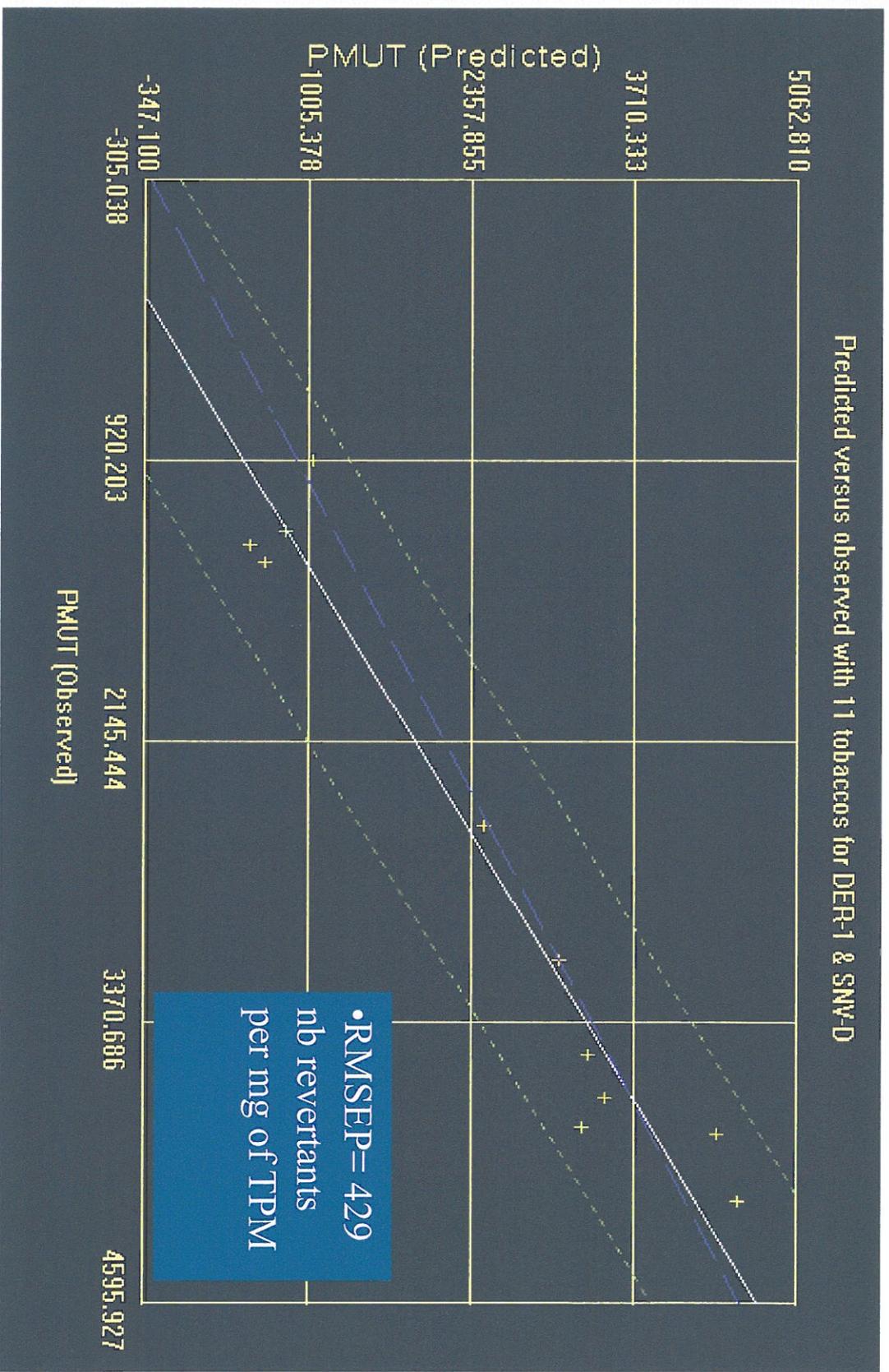
NIRS block : all types of tobaccos treated together.

|                        | ALL TYPES OF TOBACCOS |                    |            |            |
|------------------------|-----------------------|--------------------|------------|------------|
| data treat. & Criteria | R <sup>2</sup> ajust  | Q <sup>2</sup> cum | RMSEE      | RMSEP      |
| OSC                    | 88.00%                | 88.20%             | 348        | 1282       |
| <b>OSCIR</b>           | <b>88.30%</b>         | <b>87.80%</b>      | <b>356</b> | <b>249</b> |
| DerOSCIR               | 93.20%                | 92.70%             | 272        | 581        |
| MSC                    | 82.80%                | 76.90%             | 440        | 439        |
| MSCIR                  | 81.60%                | 79.60%             | 449        | 527        |
| SNV                    | 79.50%                | 75.80%             | 477        | 676        |
| SNVIR                  | 81.70%                | 79.80%             | 448        | 528        |
| DerSNVdetrndIR         | 92.70%                | 82.40%             | 290        | <b>429</b> |

# • PREDICTION OF PMUT with Nirs and DER1 & SNVD

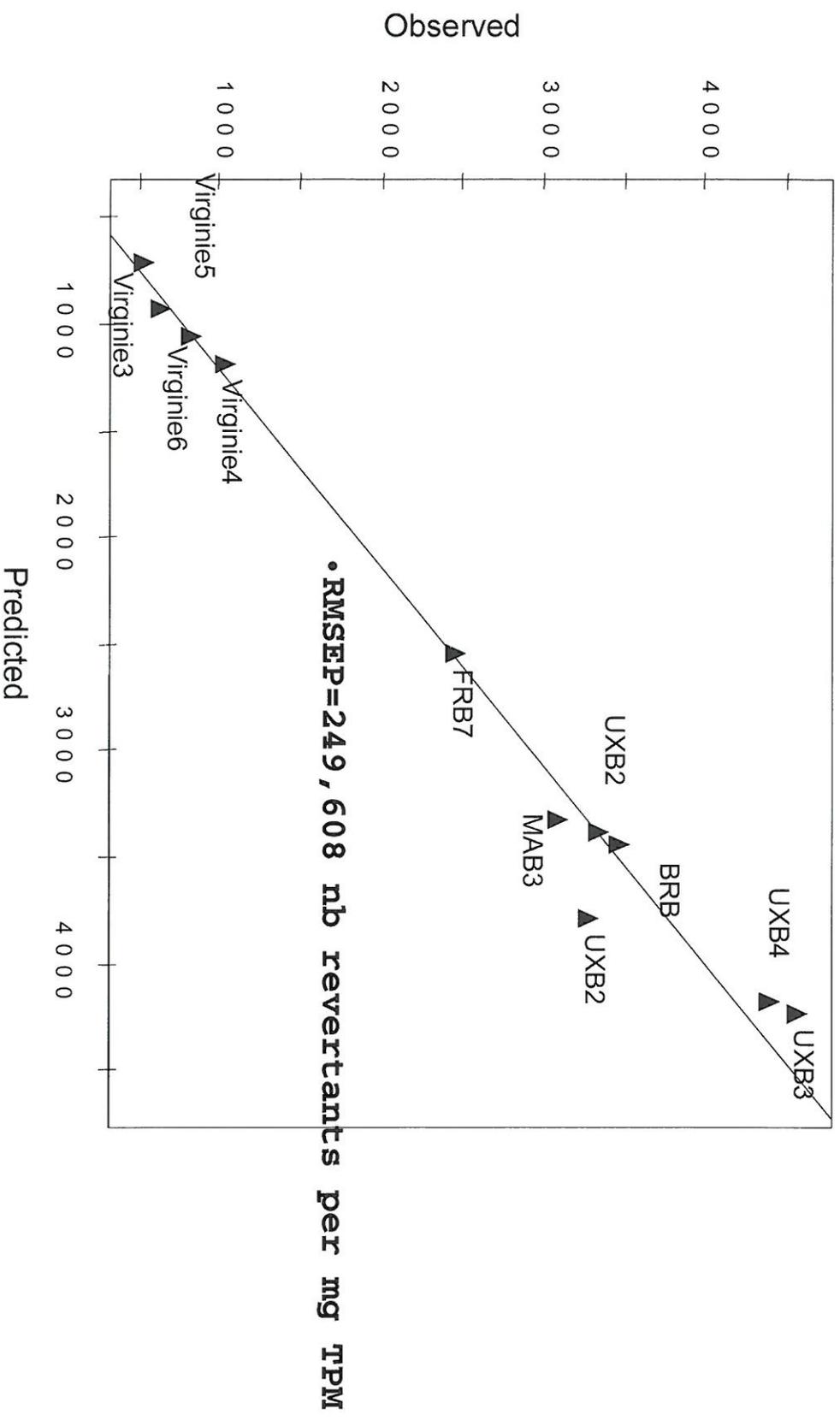


# • PREDICTION OF PMUT with Nirs and DER1&SNVD





# Forecasting of new samples realised with O.S.C. in the near infrared part.



• Simca-P 8.0 by Umetrics AB 2001-09-11 15:32

# CONCLUSION

## MAIN RESULTS

- **CHEMICAL BLOCK**
  - Accurate models are obtained.
  - Existence of relationship between some criteria and PMUT is confirmed.
- **NIRS BLOCK**
  - An unique PMUT response-function is obtained for all type of tobacco.
  - Orthogonal Signal Correction in our data give better result than others transformations.

## INTEREST :

- **ECONOMICAL INTEREST**



# CONCLUSION

## PROSPECTS

**WE INTEND TO CHECK ADDITIONAL  
OBSERVATIONS TO VALIDATE THESE  
MODELS  
AND  
TO TEST OTHER STATISTICAL METHODS  
such as MULTIBLOCK PLS to take into account  
the information from each block (chemical,  
NIRS,...)**