

Métrologie de la spectroscopie Assurance Qualité

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CALIBRATION PROCESS



INSTRUMENT DIAGNOSTICS

1. Sample preparation and spectrum acquisition

2. Calibration development

3. Routine analysis

CONTINUOUS VALIDATION



Instruments parameters :

- focus
- detector gain
- integration time
- ..

Fixed by the manufacturer (auto settings)

Operators can change:

- Type of presentation – path length ?
- Number of subsamples ?
- Number of coadds ?
- Resolution (FT-IR) ?

Instrument diagnostics

- **noise**
- **wl accuracy**
- **check cell (long term stability)**

NOISE : residues of 2 consecutive readings of the same sample
(internal or external ceramic reference)

Noise = f(optical density level) $\sim\sim$ f(sample)

- very noisy ;
- near the detector saturation – too much absorption
 - weak detector response on the borders
 - fibre optics
 - ...

RMS between spectra

$$RMS = \sqrt{\frac{\sum_{i=1}^k (a_{1i} - a_{2i})^2}{k}}$$

$$RMSC = \sqrt{\frac{\sum_{i=1}^k (a_{1i} - a_{2i} - bias)^2}{k - 1}}$$

k=number of wavelengths

ISI ISIScan

File Profiles Diagnostics Window Help

- Check Cell
- Products
- LIMS Samp

Performance Tests

- Linearize
- Gain Test
- Self Test

Main Noise Spectra Noise Summary Wavelength

Date/Time: 16/11/2012 8:34:56 Export All

Operator: RINAUser_CRAW-XDS Print All

History Export Noise Spectra

Results	Status	Bias	RMS
Wavelength Test	PASS		
Noise Test	PASS	-0.001	0.017

Number of cycles: 10 Remove water regions:

Fiber: Reference Operations Profile:

Channel: 1 CHECKCELL-XDS

Run Abort

Scan	EOC	P-P	Min.	Wavelength	Max.	Wavelength	Bias	RMS
Cycle 1	0							
Overall 1		0.451	-0.333	400	0.118	412	-0.001	0.018
seg 1		0.451	-0.333	400	0.118	412	0.001	0.040
seg 2		0.109	-0.073	1099	0.036	861	-0.004	0.019
seg 3		0.023	-0.017	1100	0.007	1346	-0.000	0.003
seg 4		0.075	-0.046	2499	0.029	2481	-0.001	0.008
Cycle 2	0							
Overall 2		0.286	-0.232	400	0.054	2488	-0.001	0.015
seg 1		0.273	-0.232	400	0.042	456	-0.008	0.034
seg 2		0.051	-0.026	1099	0.025	836	0.004	0.009
seg 3		0.027	-0.017	1100	0.010	1525	-0.000	0.003
seg 4		0.086	-0.031	2438	0.054	2488	-0.000	0.011

400-699,5
700-1099,5
1100-1699,5
1700-2499,5

Optical bandwidth

8.75 ±0.1 nm

Spectral resolution

0.5 nm

Number of data points

4200

Shenk, default, /8 80dp between 1100-2500 OK

FTIR and DISPERSIVE

1) Doubling the measurement time (same resolution!) enhances the S/N with the square root of 2.

Example: 10 seconds measurement time: S/N: 1000:1

20 seconds measurement time: S/N: 1414:1

FTIR

2) Reducing the resolution with a factor of 2 enhances the S/N with a factor of 2. (Linear)

Example: Resolution 8cm⁻¹: S/N: 1000:1

Resolution 16cm⁻¹: S/N: 2000:1

Résolution	co-adds	Time
32	16	4''
16	64	21''
8	256	2'09''
4	1024	14'33'

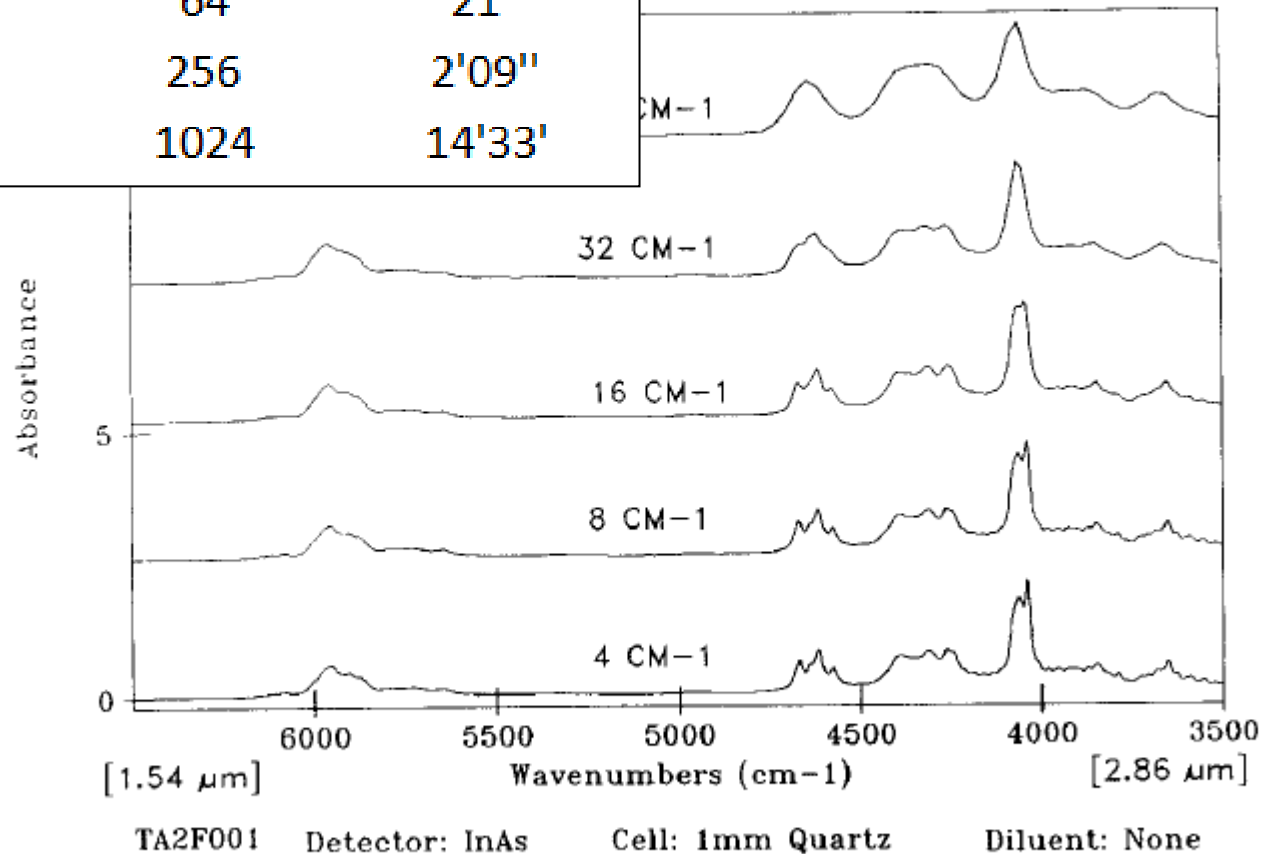
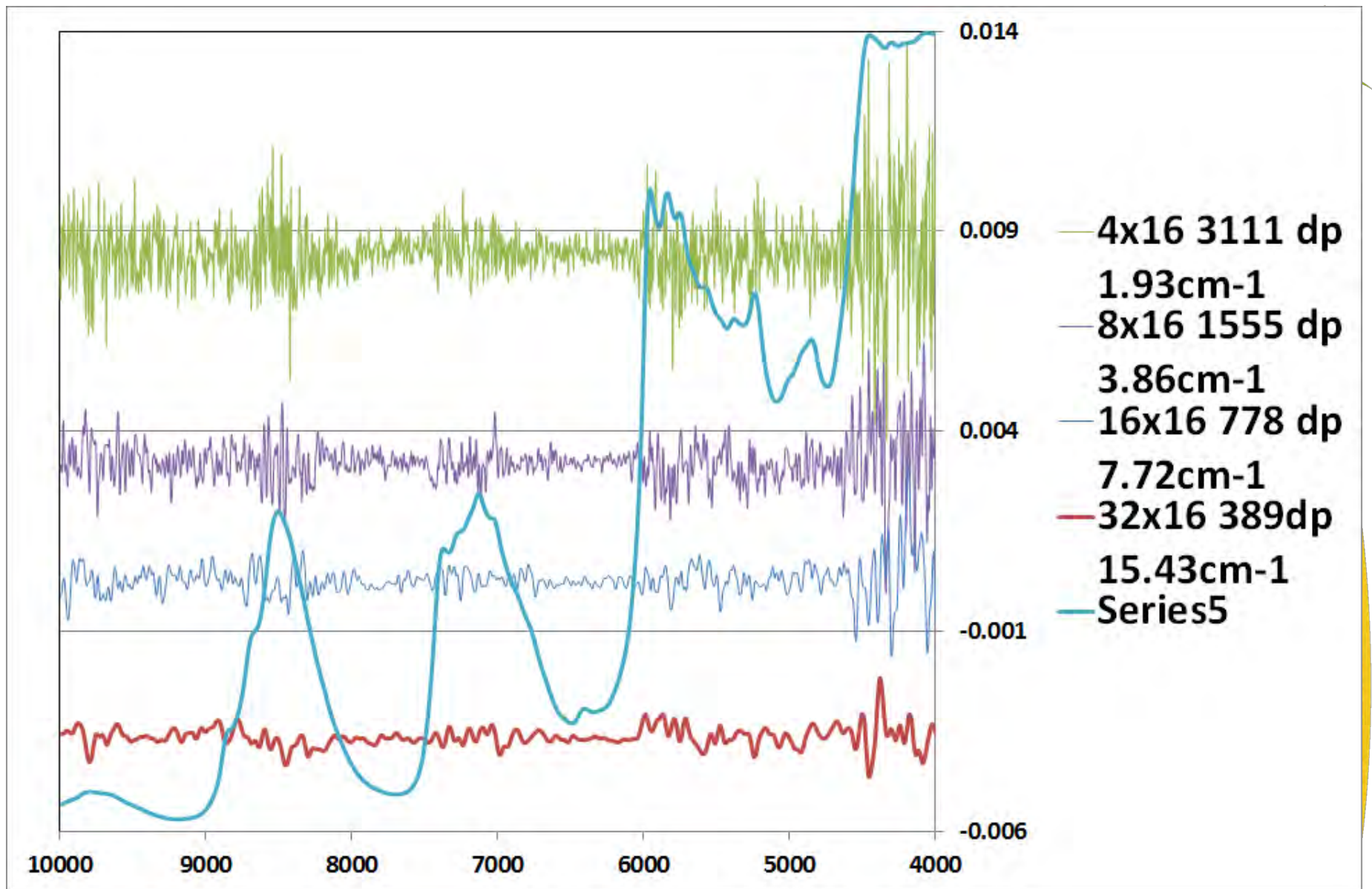


Figure 10. Spectra of toluene from 1.54 to 2.86 μm at five different spectral resolutions.



RMS between SPECTRA - 1100-2500 dispersive inst.

Two consecutive readings



Material	RMS (LOG*10 ⁻⁶)
Ceramic	30
Soya meal (0.4 od) (same cup)	200
Rape seed (0.8od) (Whole grains - same cup)	500
Soya meal (Sealed cup) Between 2 STDED instrum.	1000
Soya meal (refilling)	2000
Rape seed (Whole grains - refilling)	6000

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HISTOGRAM OF RMS

Set up a threshold

AVERAGE SPECTRA

After having checked the consistency of the reps.

From a set of prediction models, the number of replicates will be determined with the less repeatable parameter to be predicted.

kdst a.nir vs. xdst b.nir:

POS.	SAMPLE	R-SQUARE	RMS	BIAS	RMSC
1	01	1.0000	1219	1083	560
2	02	1.0000	673	-573	353
3	03	1.0000	208	-53	201
4	04	1.0000	353	-292	200
5	05	1.0000	1484	-1393	511
6	06	1.0000	181	45	176
7	07	1.0000	771	-729	254
8	08	1.0000	349	-120	328
9	09	1.0000	5012	3772	3303
10	10	1.0000	282	5	282
11	11	1.0000	504	-397	311
12	12	1.0000	459	428	167
13	13	1.0000	614	-342	510
14	14	1.0000	594	-513	299
15	15	1.0000	1164	-615	989
16	16	1.0000	2284	1874	1307
17	17	1.0000	317	239	210
18	18	1.0000	406	342	219
19	19	1.0000	414	192	367
20	20	1.0000	331	175	281
21	21	1.0000	1204	628	1028
22	22	1.0000	282	122	254
23	23	1.0000	2562	-2137	1414
24	24	1.0000	828	725	400
25	25	1.0000	392	-261	292
26	26	1.0000	551	-431	343
27	27	1.0000	254	139	212
28	28	1.0000	1237	1148	462
29	29	1.0000	165	88	140
30	30	1.0000	382	276	265
Overall Aves:		1.0000	1286	114	801

$$RMSEP^2 = SE_{model}^2 + SE_{nirs}^2 + SEL_{ref}^2$$



$$RMSEP^{-2} = SE_{model}^2 + \left(\frac{SE_{inst}^2}{k} + \frac{SE_{spl}^2}{m} \right) + \frac{SEL_{ref}^2}{n}$$

k : number of replicated scans or coadds

m : number of replicated samples (refillings)

n : number of replicated reference analyses

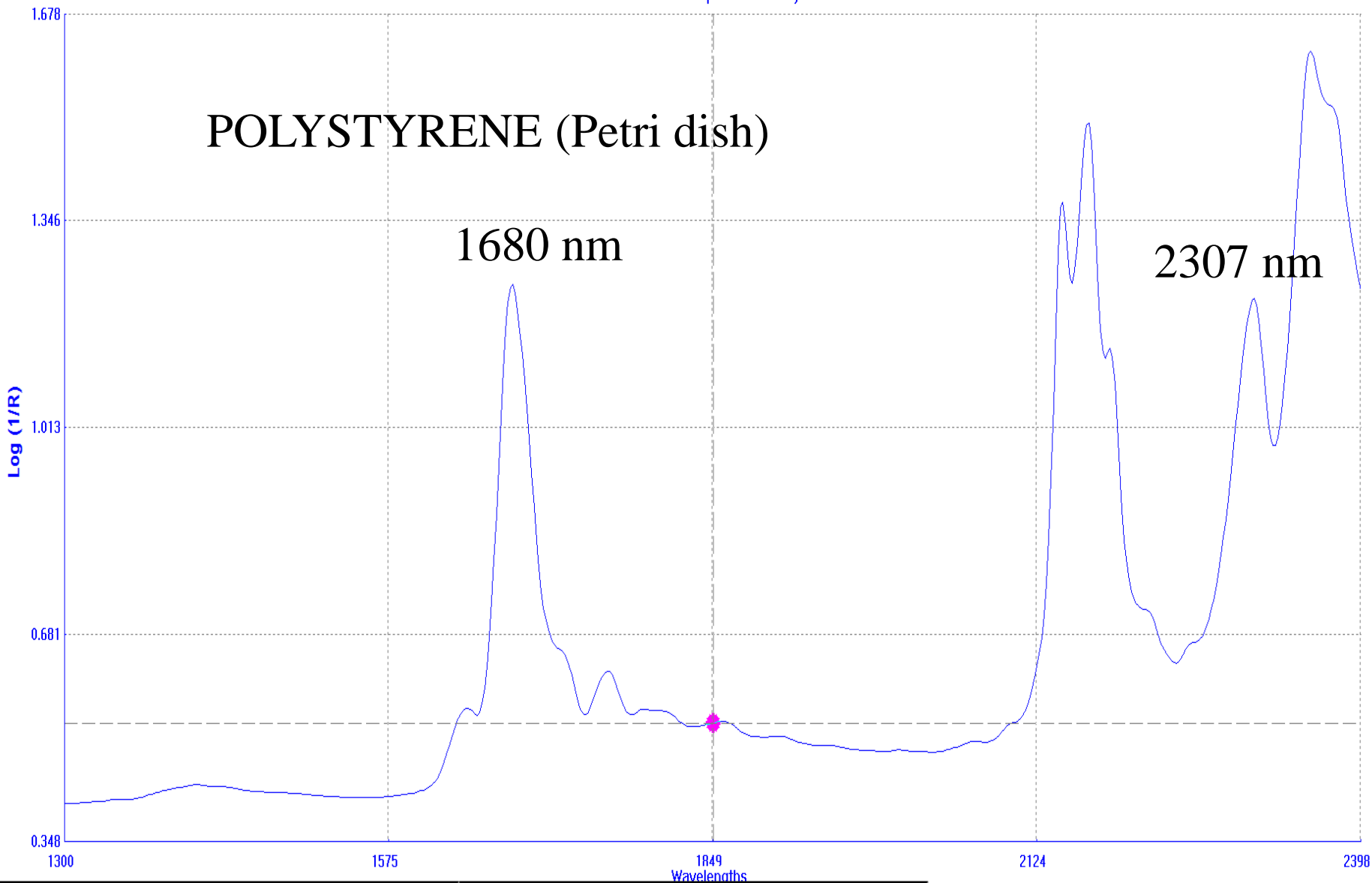
$$RMSEP_{actual}^2 = RMSEP_{observed}^2 - SEL_{ref}^2$$

Instrument diagnostics

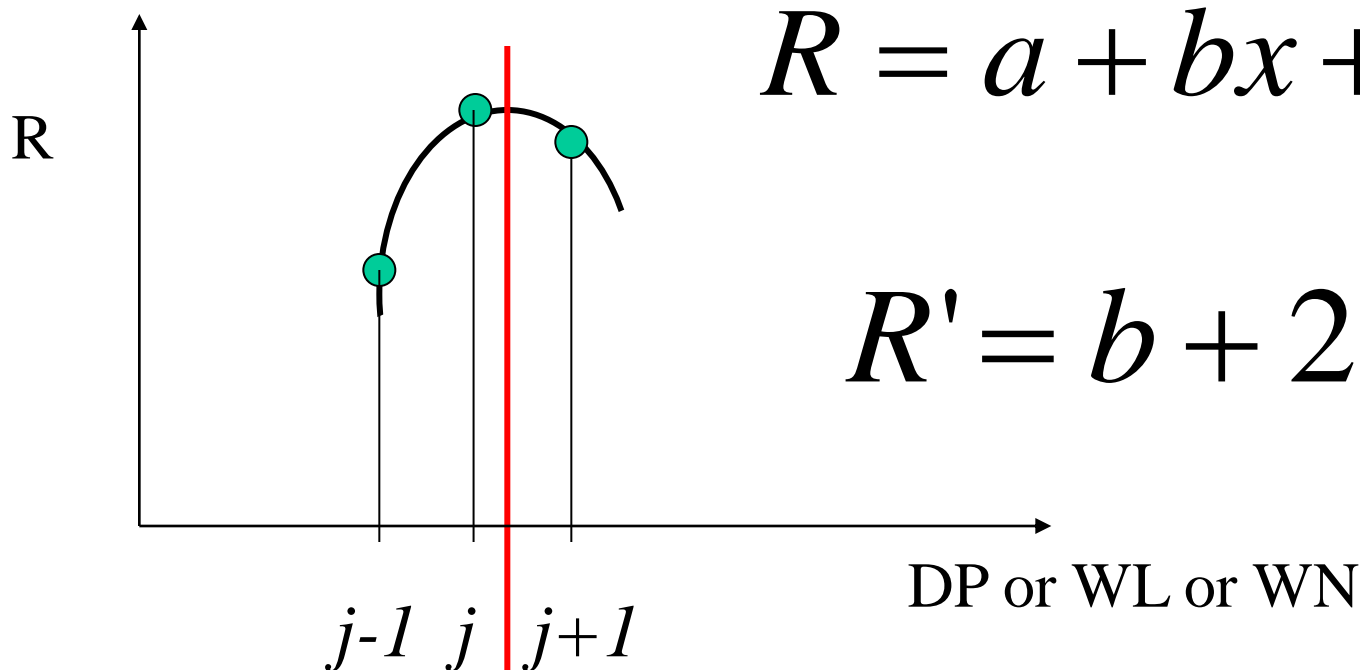
- noise
- wl accuracy
- check cell (long term stability)

Main	Noise	Spectra	Noise Summary	Wavelength			
Cycle	Peak1	Peak2	Peak3	Peak4	Peak5	Peak6	
1	526.54	800.76	1072.89	1222.50	1679.12	2307.44	
2	526.53	800.76	1072.89	1222.50	1679.12	2307.43	
3	526.53	800.76	1072.88	1222.50	1679.11	2307.43	
4	526.53	800.76	1072.88	1222.50	1679.12	2307.42	
5	526.53	800.76	1072.88	1222.50	1679.11	2307.43	
6	526.54	800.76	1072.88	1222.50	1679.11	2307.43	
7	526.53	800.76	1072.88	1222.50	1679.11	2307.43	
8	526.54	800.77	1072.88	1222.50	1679.12	2307.44	
9	526.53	800.77	1072.88	1222.49	1679.12	2307.43	
10	526.54	800.76	1072.89	1222.50	1679.12	2307.43	
Average	526.53	800.76	1072.88	1222.50	1679.12	2307.43	
Delta	0.03	0.01	0.08	0.02	0.06	-0.11	
S/D	0.003	0.003	0.003	0.003	0.003	0.005	
Minimum	526.53	800.76	1072.88	1222.49	1679.11	2307.42	
Maximum	526.54	800.77	1072.89	1222.50	1679.12	2307.44	
Max-Min	0.0101	0.0093	0.0079	0.0090	0.0077	0.0156	

POLYSTYRENE (Petri dish)



Peak search



$$R = a + bx + cx^2$$

$$R' = b + 2cx$$

$$0 = b + 2cx$$

$$\text{Min or max at } x = -\frac{b}{2c}$$

Instrument diagnostics

- noise
- wl accuracy
- check cell (long term stability)



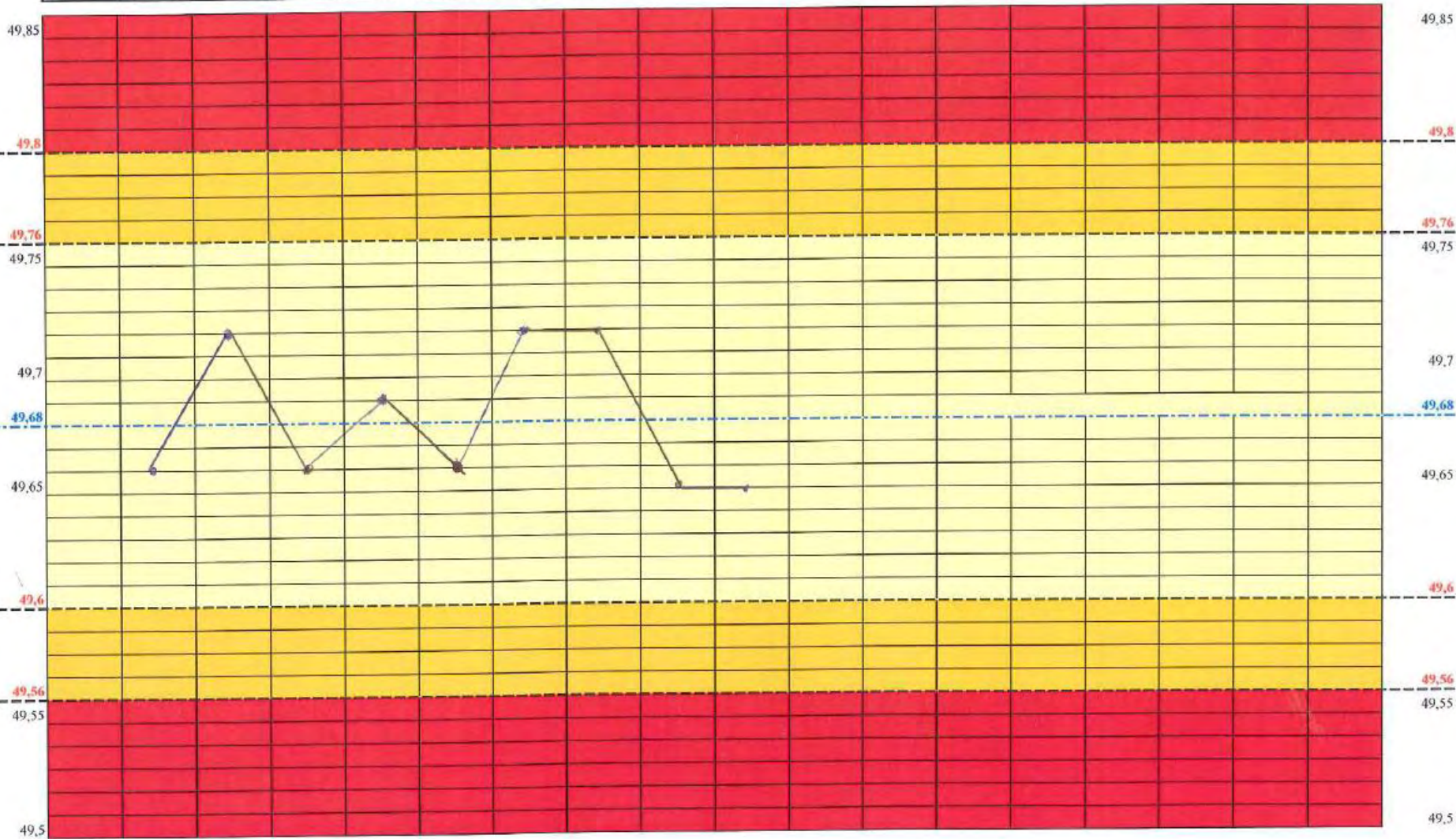
FOSS XDS D7-EQ696 CONTROL CHART

Sample : Check cell 078

Analytical parameter : Protein % MS

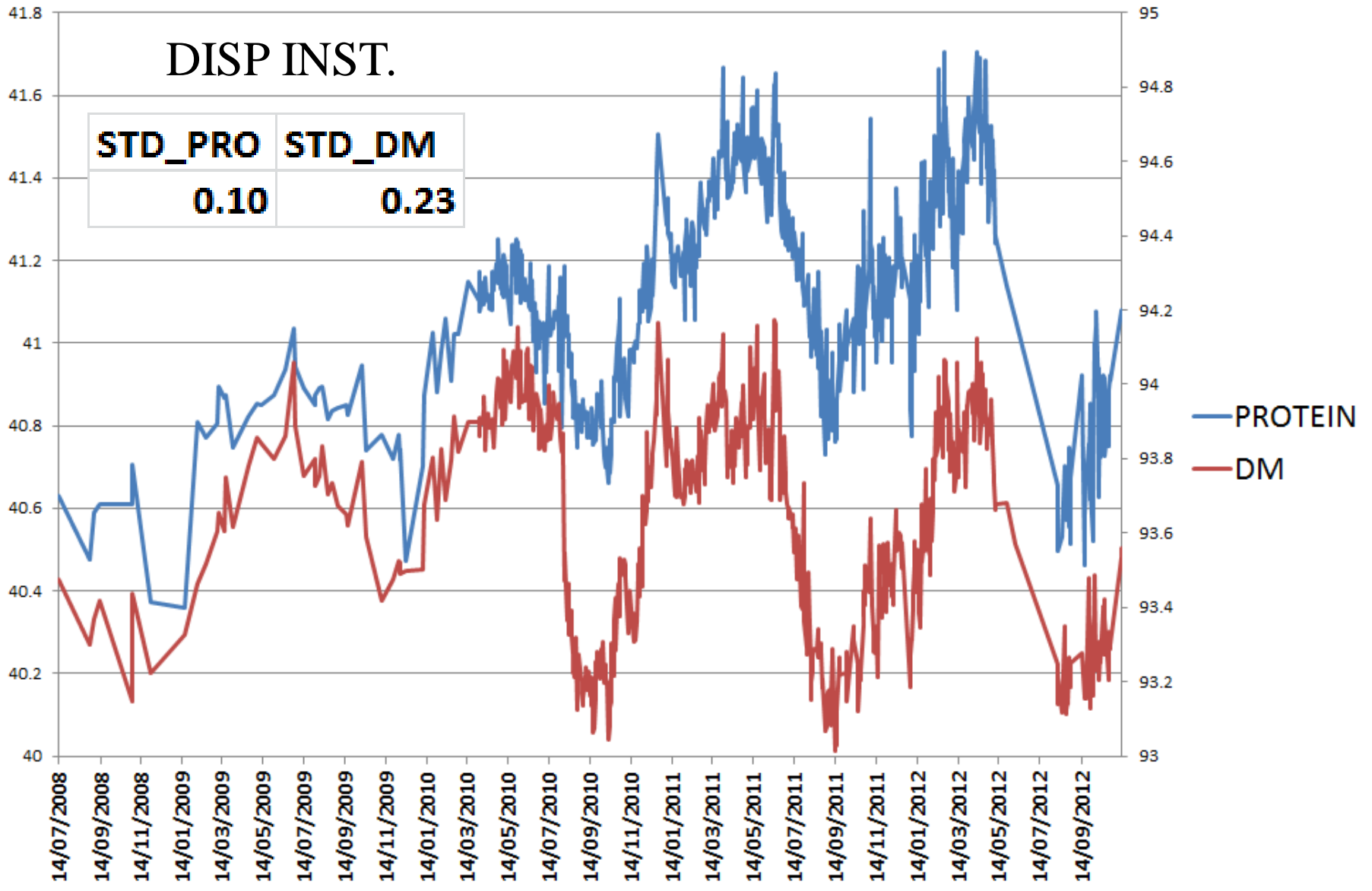
Periode

Analyst	NC	NC	AH	AH	AH	BL	MF	MF	MF						
Date	06/11/12	07/11/12	08/11/12	09/11/12	09/11/12	10/11/12	12/11	13/11	14/11/12						
Protein	49,66	49,72	49,66	49,69	49,66	49,72	49,72	49,65	49,65						
Corrective Act :															
Vin RES Labo															
Date			07/11/12	08/11/12	09/11/12	10/11/12									



DISP INST.

STD_PRO	STD_DM
0.10	0.23



If SEP = 0.50 Protein in Soyameal #

$$\mathbf{SEP^2 = SEP^2_{model} + SE^2_{nirs}}$$

$$\mathbf{0.50^2 = 0.49^2 + 0.10^2}$$

Instrument diagnostics

Validation

DATA BASE QUALITY (validate a « clean » data set)



- calibration or routine analyses

View all the raw data; observations of abnormalities
- Immediately after the scanning

In Routine Analysis

Correlations

Mahalanobis distances

H values

X residuals

...

Pretreatment

- 1st derivative, 1,1,1

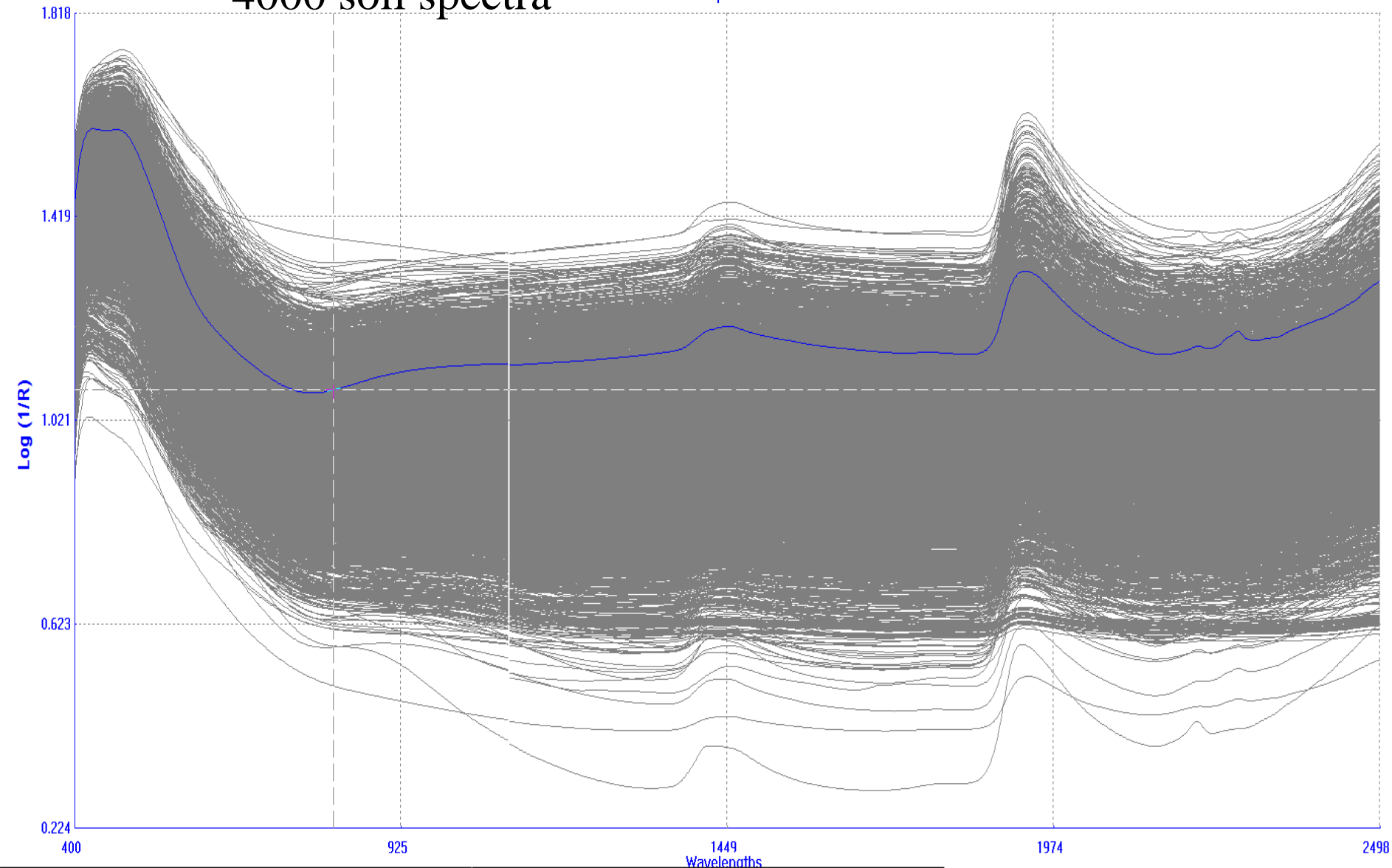
M. Westerhaus, 3rd derivative

K. Norris, 4th derivative



4000 soil spectra

Position 1 Sample number 89829

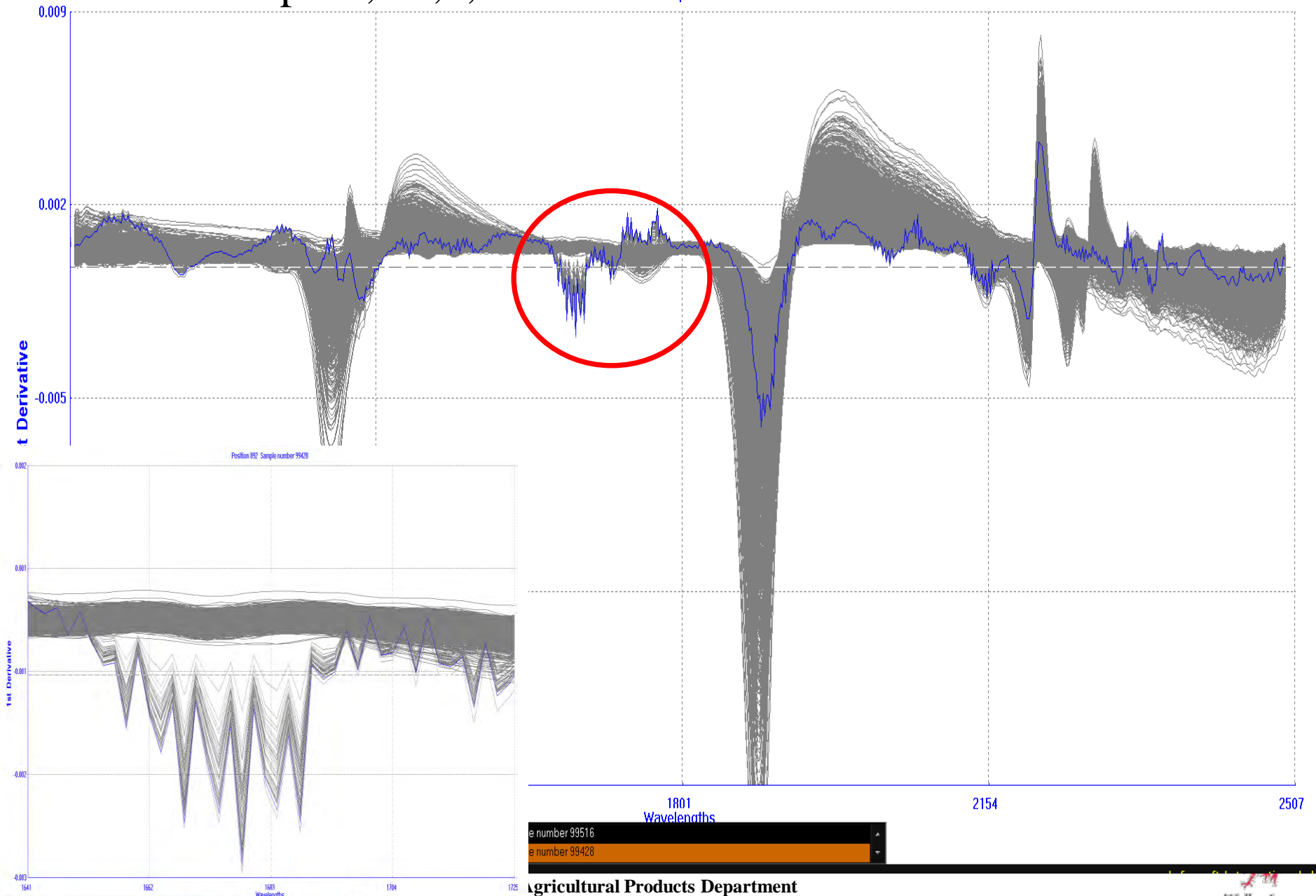


X = 816 Y = 1.07981420
Transition between VIS and NIR

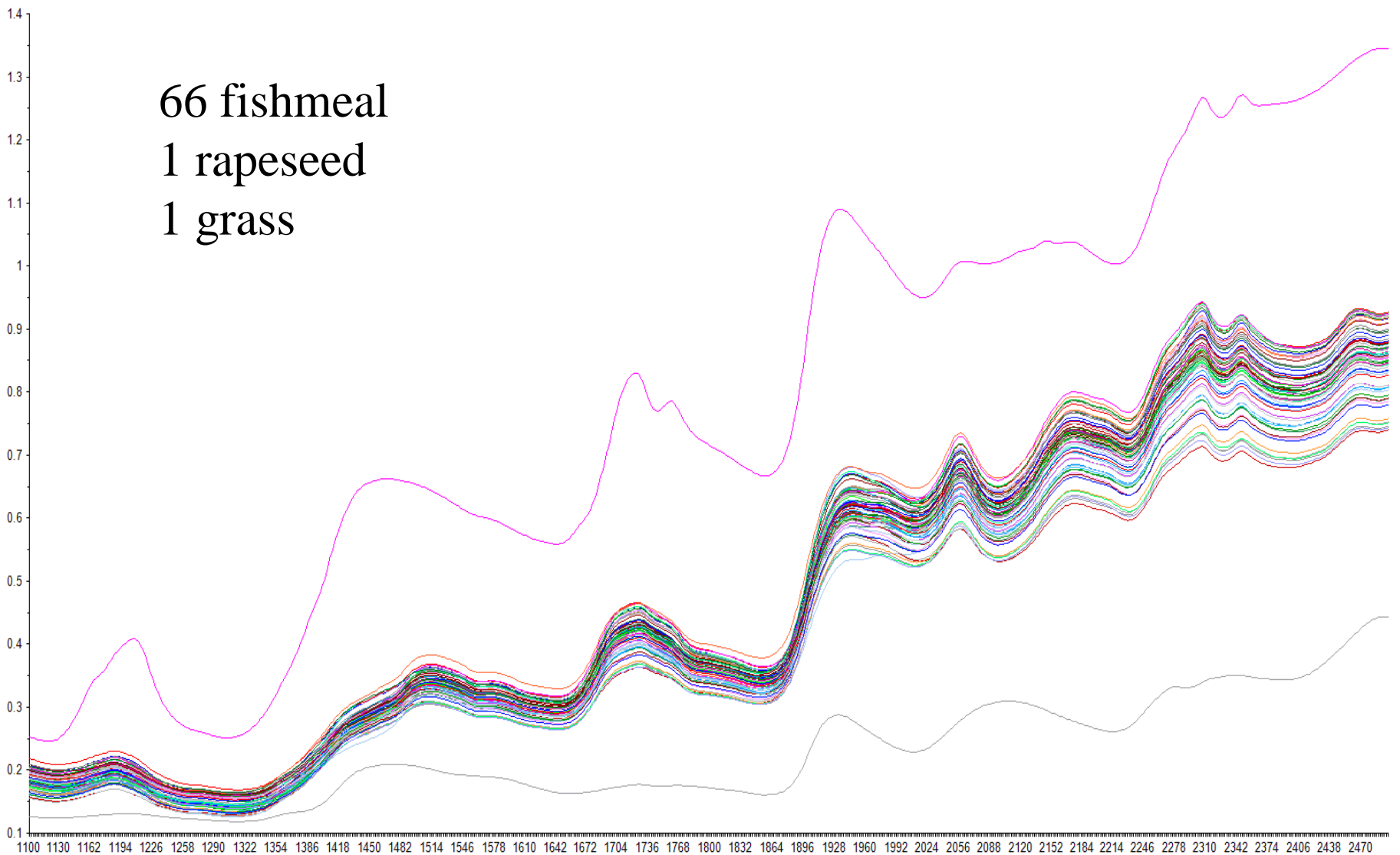
- ▲ Position 1 Sample number 89829
- ▼ Position 2 Sample number 89842

Soil samples ; d1,1,1

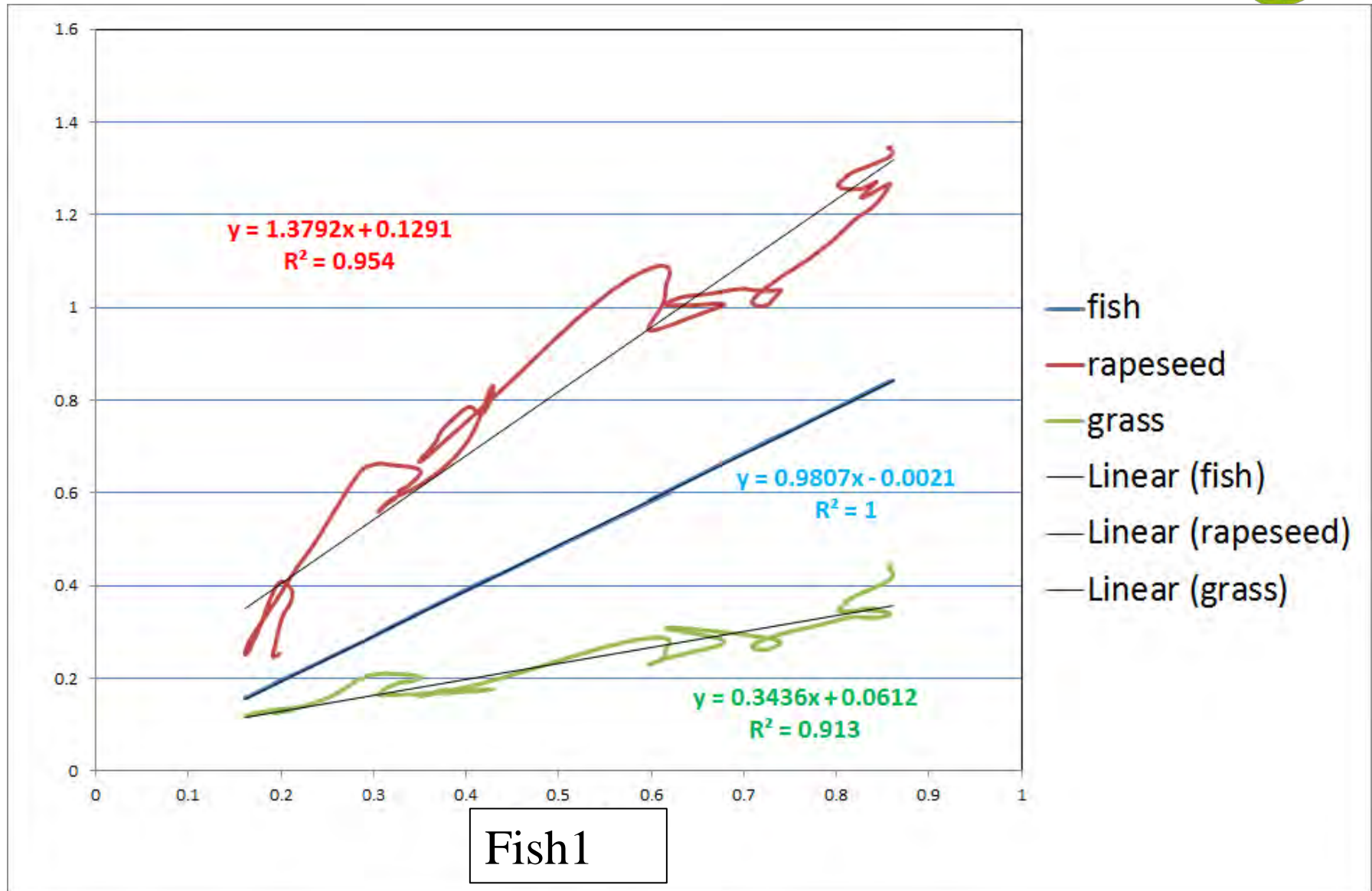
Position 892 Sample number 99428



66 fishmeal
1 rapeseed
1 grass



CORRELATION



Array Editor - rho

Stack: Base

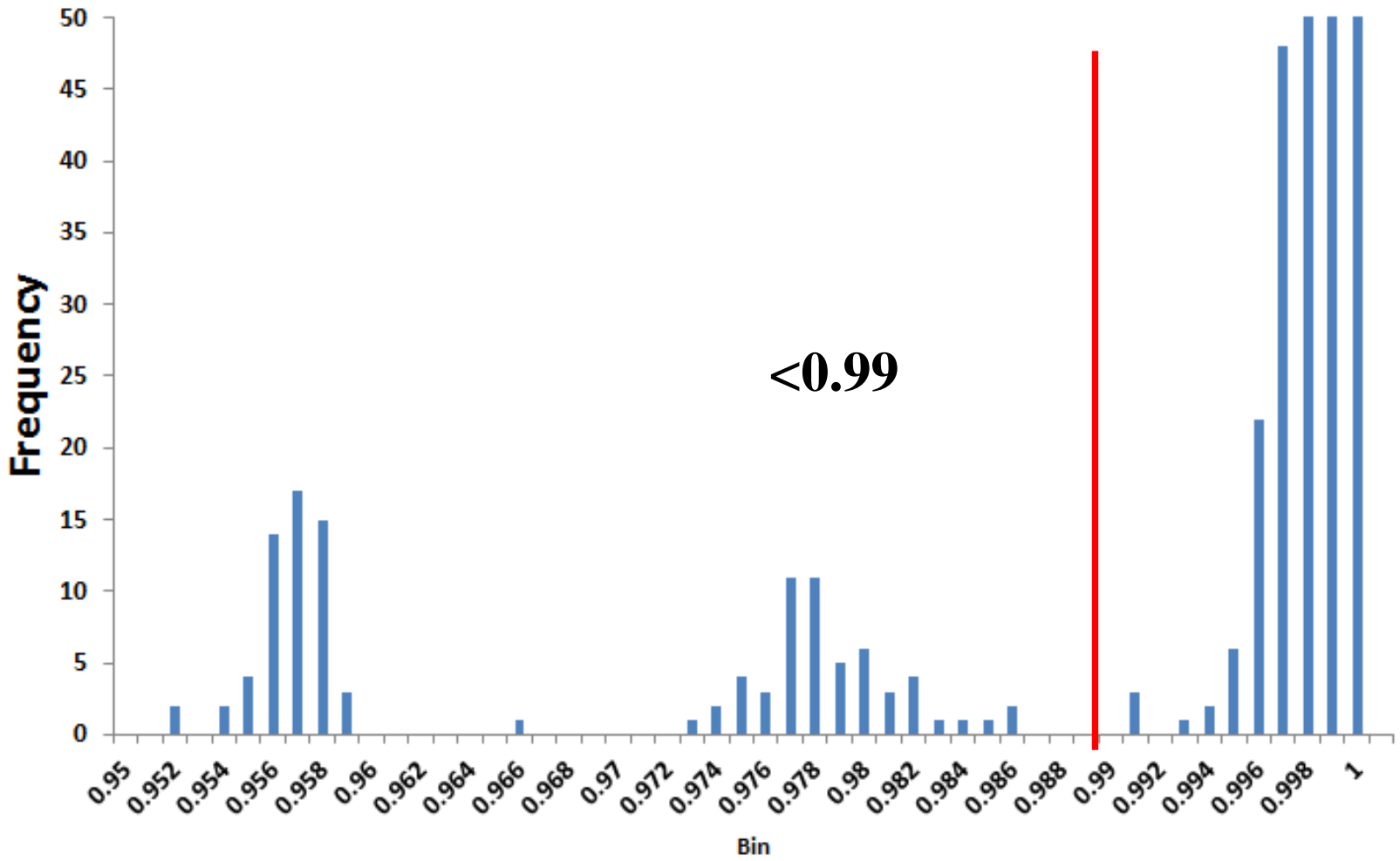
	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68
49	0.9998	0.9997	0.9990	0.9989	0.9999	0.9998	0.9997	0.9999	0.9998	0.9993	0.9997	0.9996	0.9994	0.9790	0.9573
50	0.9998	0.9990	0.9992	0.9981	0.9993	0.9998	0.9995	0.9997	0.9997	0.9993	0.9997	0.9994	0.9993	0.9759	0.9578
51	0.9994	0.9999	0.9985	0.9996	0.9999	0.9995	0.9997	0.9998	0.9995	0.9989	0.9993	0.9992	0.9990	0.9827	0.9563
52	0.9996	0.9996	0.9986	0.9994	0.9998	0.9997	1.0000	0.9998	0.9996	0.9989	0.9995	0.9992	0.9989	0.9807	0.9575
53	0.9995	0.9988	0.9986	0.9986	0.9992	0.9996	0.9997	0.9995	0.9995	0.9988	0.9994	0.9989	0.9987	0.9775	0.9589
54	1	0.9995	0.9997	0.9981	0.9997	1.0000	0.9994	0.9999	1.0000	0.9998	1.0000	0.9999	0.9998	0.9770	0.9565
55	0.9995	1	0.9989	0.9991	0.9999	0.9996	0.9994	0.9998	0.9996	0.9992	0.9994	0.9995	0.9994	0.9814	0.9552
56	0.9997	0.9989	1	0.9966	0.9989	0.9996	0.9983	0.9993	0.9997	1.0000	0.9997	0.9998	0.9999	0.9750	0.9553
57	0.9981	0.9991	0.9966	1	0.9992	0.9984	0.9995	0.9989	0.9983	0.9971	0.9980	0.9976	0.9972	0.9856	0.9568
58	0.9997	0.9999	0.9989	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999
59	1.0000	0.9996	0.9996	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999
60	0.9994	0.9994	0.9983	0.9999	0.9998	0.9997	0.9996	0.9996	0.9996	0.9797	0.9570				
61	0.9999	0.9998	0.9993	0.9999	0.9998	0.9999	0.9998	0.9998	0.9998	0.9780	0.9567				
62	1.0000	0.9996	0.9997	0.9999	0.9999	0.9999	0.9998	0.9998	0.9998	0.9780	0.9567				
63	0.9998	0.9992	1.0000	0.9999	0.9999	0.9999	0.9998	0.9998	0.9998	0.9780	0.9567				
64	1.0000	0.9994	0.9997	0.9999	0.9999	0.9999	1.0000	0.9999	0.9999	0.9758	0.9556				
65	0.9999	0.9995	0.9998	0.9999	0.9999	0.9999	0.9999	1.0000	0.9999	0.9758	0.9556				
66	0.9998	0.9994	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9772	0.9571				
67	0.9770	0.9814	0.9750	0.9999	0.9999	0.9999	0.9998	0.9998	0.9998	0.9772	0.9571				
68	0.9565	0.9552	0.9553	0.9999	0.9999	0.9999	0.9999	0.9999	0.9999	0.9767	0.9555				
69				0.9999	0.9999	0.9999	1	1.0000	0.9999	0.9767	0.9555				


rapeseed
grass

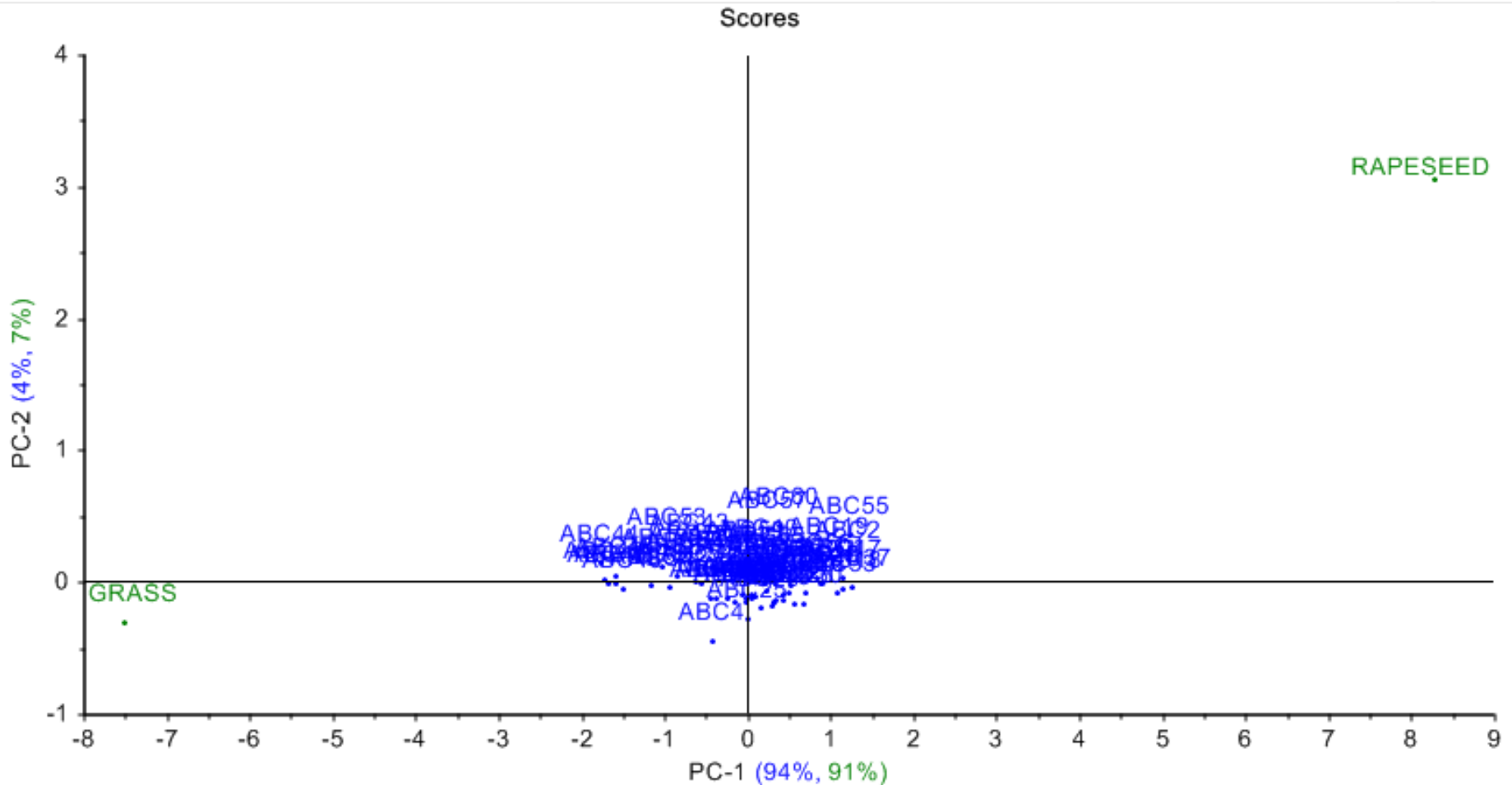
0.9998	1.0000	1	0.9758	0.9551
0.9772	0.9767	0.9758	1	0.9517
0.9571	0.9555	0.9551	0.9517	1



Histogram of R between each pair

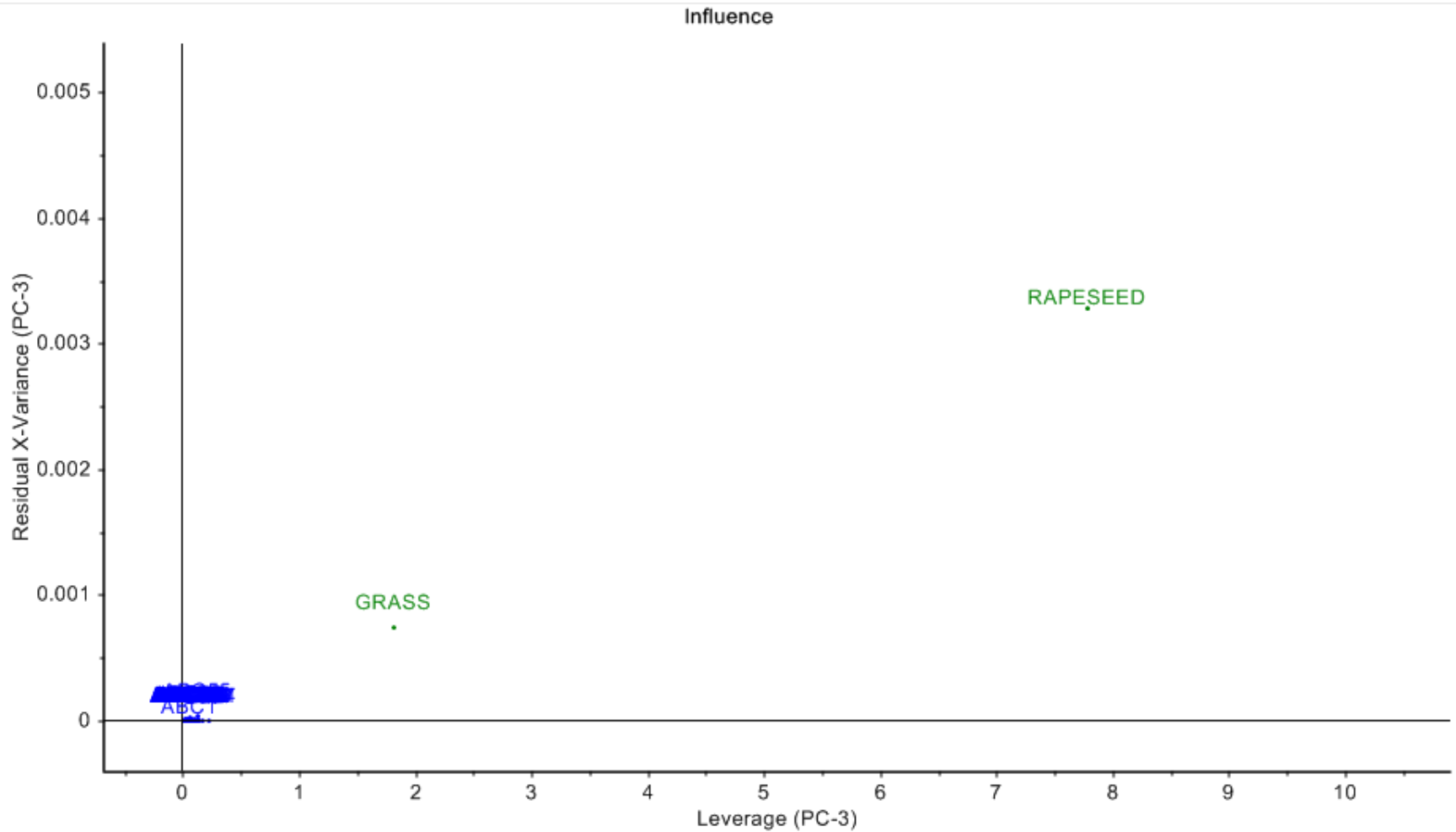


H statistic, Leverage (Hotelling T²), Mahalanobis distance, GH, 



CALCULATE A PCA and PROJECT THE UNKNOWNNS

X residuals and leverage



MONITORING

1- Verify that all the samples involved are PREDICTABLE
= verify that the routine samples are in the calibration ranges (X and Y ranges)

2- Select 10-20 samples, perform reference methods and calculate de prediction statistics

MAINTENANCE

- Recalibration by additional new samples when the MONITORING shows deficiency



COEFFICIENT OF DETERMINATION

$$R^2 = \frac{SDy^2 - SEC^2}{SDy^2}$$

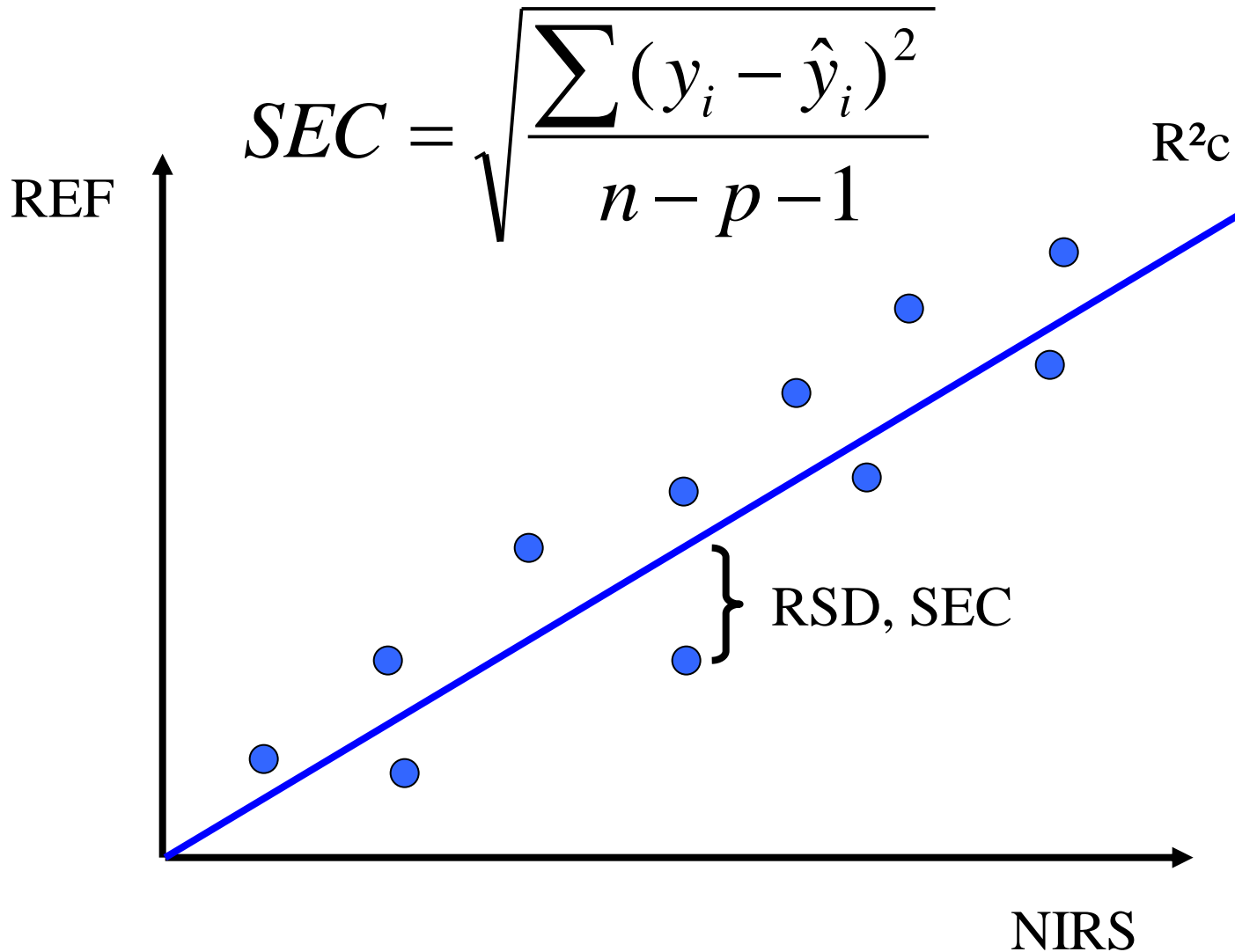
STANDARD ERROR OF CALIBRATION

$$SEC = \sqrt{\frac{\sum (y_i - \hat{y}_i)^2}{n - p - 1}}$$

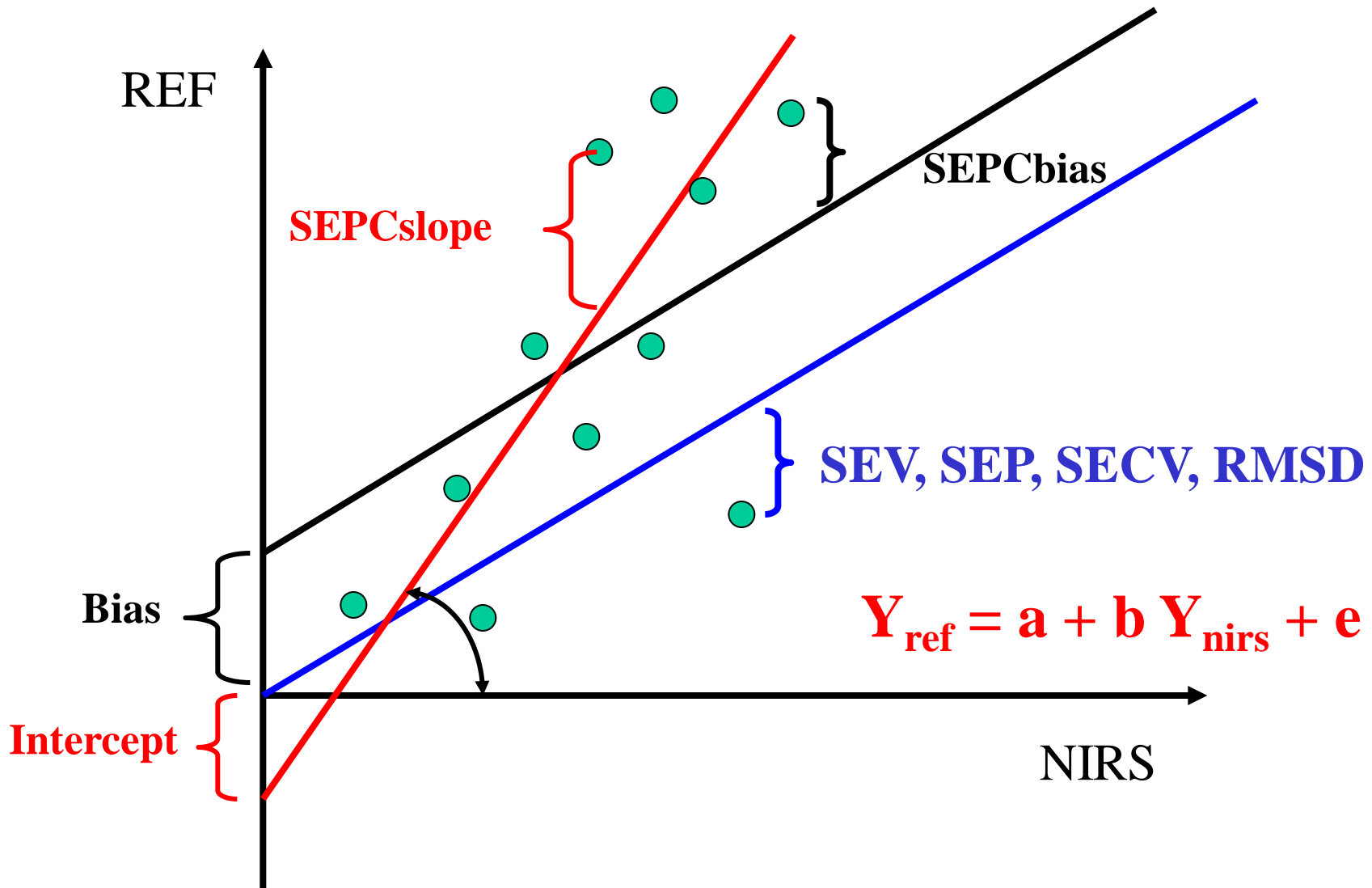
STANDARD ERROR OF PREDICTION

$$SEV = SECV = RMSEP = \sqrt{\frac{\sum (y_i - \hat{y}_i)^2}{n}}$$

Calibration statistics



Validation statistics



Calibration results	
Parameters	FAT
Units	%
N	65
Outliers	0
Min	6.39
Mean	10.9
Max	15.08
SD	1.59
R2C	0.96
R2CV	0.94
SEL-Reproductibility	0.25
SEC	0.33
SECV	0.38
NIR_repeatabilty	0.19
RPDC	4.82
RPDCV	4.18
Number of terms	4
Segments of CV	4
WL-Range/step	1100-2498/2
Pretreatment (s)	SNVD-144

Validation results	
Parameters	FAT
Units	%
N	20
Outliers	1
Min	6
Mean	10
Max	4
SD	1.41
R2P	0.95
SEL-Reproductibility	0.25
RMSEP	0.45
SEP	0.41
RSD	0.35
NIR_repeatabilty	0.19
RPDP	3.95
BIAS	-0.11
INTERCEPT	0.11
SLOPE	0.89
AveGH	5.6
AveNH	2.5

From a « CLEAN » spectral data base

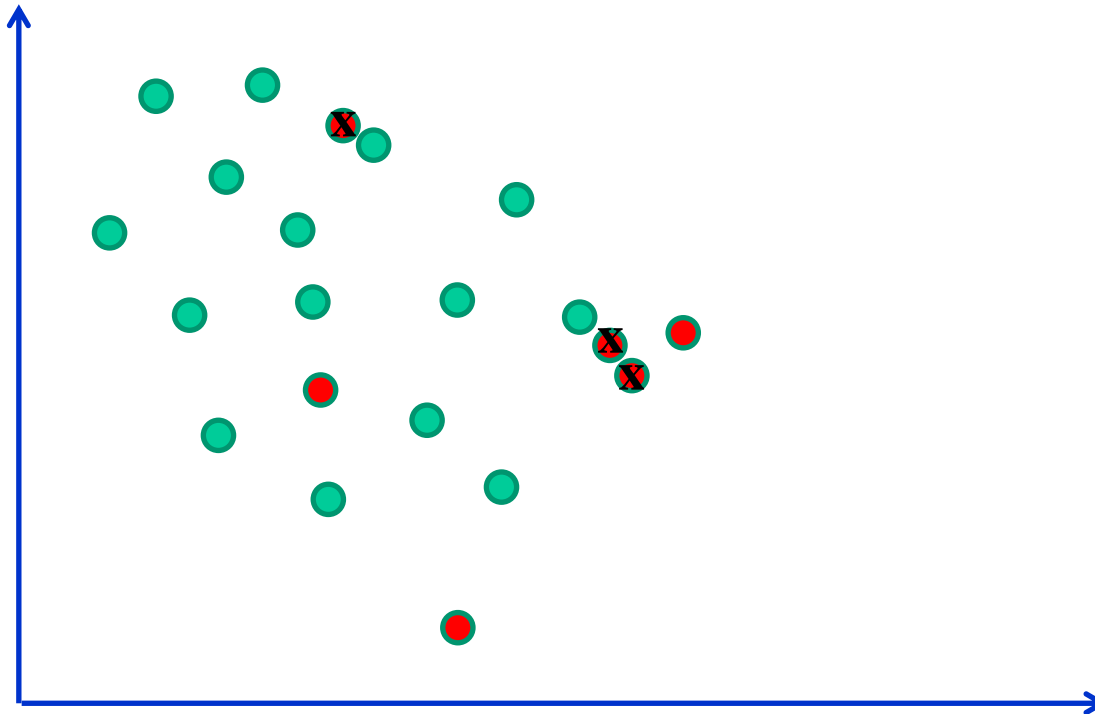
Before selecting monitoring samples, be sure outliers are removed.

Expanding a data set with too extreme points will lead to less performance

Select samples which carry information not yet represented in the data set.

DUPLEX, Kennard & Stones, NH (expand calibration)
PICKS, ...

EXPANDABLE CONCEPT : Look at the NH of the new spectra with all the previous ones and between the new points themselves



Experiment : 66 fishmeal samples (demo.cal) and 114 #

EQA1 :

Constituent	N	SEC	RSQ	SECV	1-VR
PROTEIN	60	0.7744	0.9437	1.0449	0.8957

Routine samples 114 #

Selected 20 by Expand.exe (NH, WinISI) + wet chemistry

MONITOR on the 20 # → RMSEP = 2.24 ☹️

EQA2 :

Constituent	N	SEC	RSQ	SECV	1-VR
PROTEIN	77	0.6295	0.9697	1.0823	0.9094

Routine samples 94 #

Selected 20 by Expand.exe + wet chemistry

MONITOR

RMSEP = 0.80 ☺️

ISO 12099:2010

Animal feeding stuffs, cereals and milled cereal products -- Guidelines for the application of near infrared spectrometry

SLOPE & BIAS correction of the predicted values

x = vector of N predicted values

y = vector of N reference values

$$y = a + bx + e$$

$$b = \frac{\sum (x - \bar{x})(y - \bar{y})}{\sum (x - \bar{x})^2} = \frac{\text{cov}(x, y)}{\text{var}(x)}$$

$$a = \bar{y} - b\bar{x}$$

SLOPE & BIAS correction of the predicted values

$$\text{Bias} \neq 0.0 ? \quad \text{Bias} = \bar{y} - \bar{x}$$

$$SEP = \sqrt{\frac{\sum (y - x + \text{Bias})^2}{n - 1}}$$

$$\text{BiasConfidentLimit} = \pm(t_{(1-\alpha/2)} \cdot SEP) / \sqrt{n}$$

If SEP=1, N=20 and $\alpha=5\%$,

$$BCL = \pm(2.09 * 1) / \sqrt{20} = \pm 0.48$$

Slope \neq 1?

$$\text{SlopeConfidentLimit} = b \pm t_{(1-\alpha/2)} \cdot \sqrt{RSD^2 / SSD_x}$$

$$RSD = \sqrt{\frac{\sum_{i=1}^n (y - (a + b \cdot x))^2}{n - 2}} \quad SSD_x = Sdx^2 \cdot (n - 1)$$

If $RSD = 1$, $Sdx = 2$, $N = 20$ and $\alpha = 5\%$

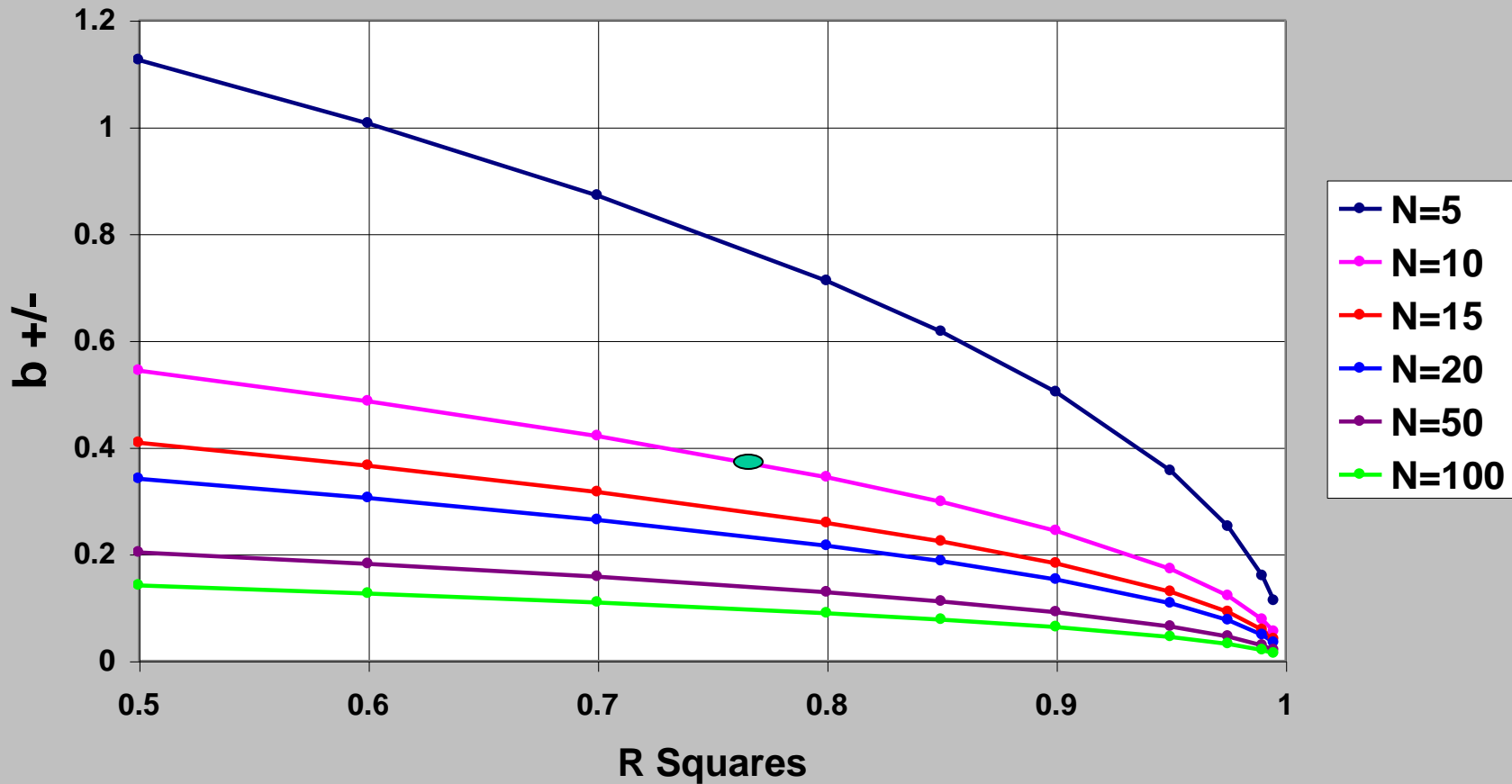
$$\text{SlopeConfidentLimit} = b \pm 2.09 * \sqrt{1 / (2^2 * 19)}$$

Slope Confident Limits : b-0.24 and b+0.24

SLOPE & BIAS correction

$\alpha=5\%$

Slope Confident Limits



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SEP # SECV ?

$$SEP = \sqrt{\frac{\sum_{i=1}^n (e_i - \bar{e})^2}{n-1}}$$

The unexplained error confidence limit (UECL) is calculated from an F -test (ratio of 2 variances)

$$UECL = SEC \cdot \sqrt{F(\alpha; \nu, M)}$$

α : the probability of making a type I error

$\nu = n-1$: numerator DF associated with SEP

$M = n_c - p - 1$: denominator DF associated with SEC

EXAMPLE With $n = 20$, $\alpha = 0,05$, $M = 100$, and $sSEP = 1$,
 $TUE = 1,30$ (10)

This means that, with 20 samples, a SEP can be accepted that is up to 30 % larger than the SEC.

$$\sqrt{F(a; v, M)}$$

Degrees of freedom (SEP) ^a	$\sqrt{[F(\alpha; v, M)]}$				
	Degrees of freedom (SEC) ^b				
	50	100	200	500	1000
5	1,55	1,52	1,50	1,49	1,49
6	1,51	1,48	1,46	1,45	1,45
7	1,48	1,45	1,43	1,42	1,42
8	1,46	1,43	1,41	1,40	1,40
9	1,44	1,41	1,39	1,38	1,37
10	1,42	1,39	1,37	1,36	1,36
11	1,41	1,37	1,36	1,34	1,34
12	1,40	1,36	1,34	1,33	1,33
13	1,39	1,35	1,33	1,32	1,32
14	1,38	1,34	1,32	1,31	1,30
15	1,37	1,33	1,31	1,30	1,29
16	1,36	1,32	1,30	1,29	1,29
17	1,35	1,31	1,29	1,28	1,28
18	1,30	1,31	1,29	1,27	1,27
19	1,34	1,30	1,28	1,27	1,26
29	1,30	1,26	1,23	1,22	1,22
49	1,27	1,22	1,19	1,17	1,17
99	1,24	1,18	1,15	1,13	1,12
199	1,22	1,16	1,12	1,10	1,09
499	1,21	1,14	1,11	1,08	1,07
999	1,20	1,14	1,10	1,07	1,05

Va



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test to monitor eqa 14/11/11

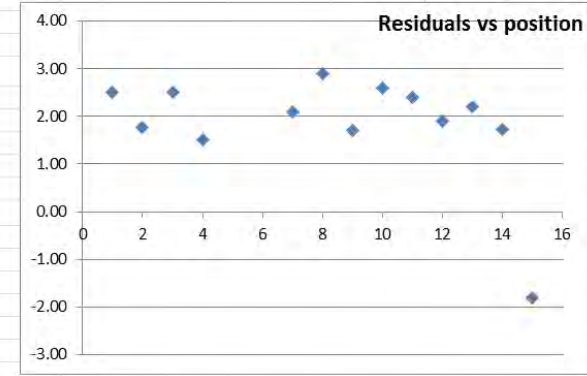
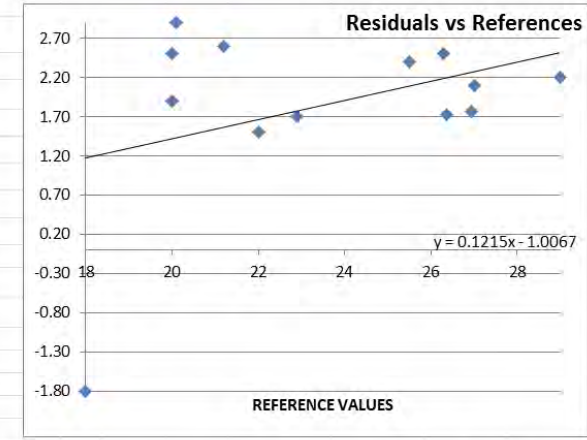
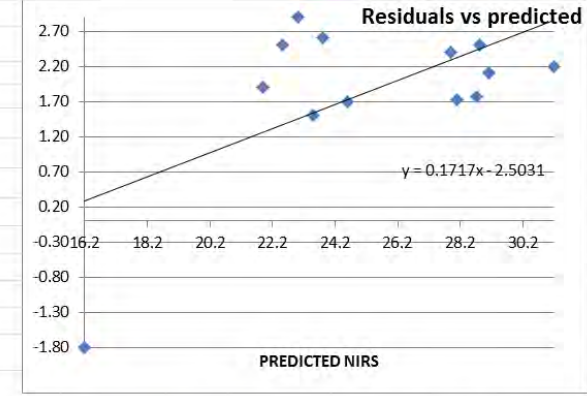
Ref Values = f (Pred Values)

	Ref Values	Pred Values
N=	13	
Average=	23.48	25.33
Min=	18.00	16.20
Max=	29.00	31.20
SD=	3.518	4.09
RMSEP=	2.163	
BIAS=	1.846	
SEPC=	1.172	
RSDyx=	0.980	
Slope=	0.828	
Intercept=	2.503	
RSQ=	0.929	
RPD=	3.751	
Least rectangle slope=	0.859	
Least rectangle intercept=	1.715	
RMSEPrec=	0.909	

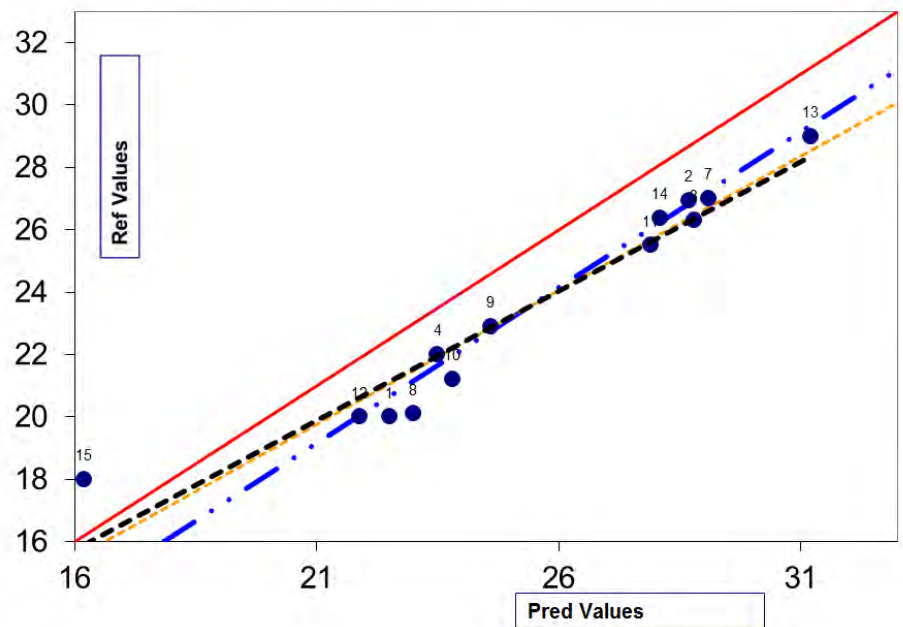
CALIBRATION INFORMATION

N=	100	
SECV=	0.15	
Number of Terms =	10	
Alpha=	0.05	
Tvalue=	2.16	
Fvalue=	1.86	
Tobs_bias=	2.957	S
F_sep=	0.279	S
Tobs_slope=	2.485	S
MAE=	0.354	
Quartile75=	0.654	

Probability
0.0120
3.028E-02



test to monitor eqa 14/11/11



- 45°
- 45°-Bias
- - - Least Rec
- - - Linear ()

USE FOR MONITOR or CALIBRATION TRANSFER



ISO 12099:2010

Animal feeding stuffs, cereals and milled cereal products -- Guidelines for the application of near infrared spectrometry

- **Validation sample selection**
- **Bias # 0 ?**
- **Slope # 1?**
- **SEP # SECV ?**



DETERMINATION OF MOISTURE,
 PROTEIN, FAT, CRUDE FIBRE, STARCH,
 AND ASH IN FEED
 BY NEAR INFRARED SPECTROSCOPY
 (PA-IR-NIRFEED -rev02)

Anne Mouteau, Pierre Dardenne and

Vincent Baeten

With the collaboration of

Emma Mukandoli – Marianne Flahaux

Walloon Agricultural Research Centre

Quality Department

November 2010

VALIDATION REPORT Ver 03

Walloon Agricultural Research Centre

Centre wallon de Recherches agronomiques



DETERMINATION OF MOISTURE, PROTEIN, FAT, CRUDE FIBRE, STARCH, AND ASH IN FEED BY NEAR INFRARED SPECTROSCOPY (PA-IR-NIRFEED -rev02)



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 - INSTRUMENT DIAGNOSTICS
 - CHECK CELL CONTROL CHART



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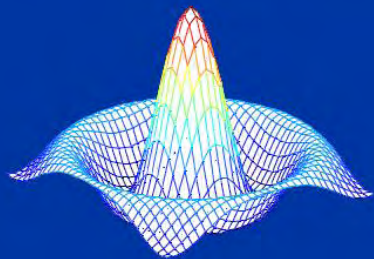
Quentin Arnould

Centre wallon de Recherches agronomiques



Vibrational spectroscopy and Chemometrics

*Training session
18-22 February 2013*



Vibrational Spectroscopy

NIR/MIR/RAMAN

Theory and applications, exper

NIR microscopy/Hyperspectral
MEMs/instrument standardiza

Chemometrics applied to vibrational data

Exploratory analysis:

Data visualisation

Principal component analysis

Outlier detection

Uncertainty estimation

Quantification and classification

Multivariate calibration:

Partial least squares PLS

Multiple linear regression MLR

Support vector machines SVM

<http://www.icnirs.org/>

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27 Nov 2012

Location : Morocco



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- NIR-2013**
Information supplied by : Véronique BELLON-MAUREL
8 OCT 2012
- Launch of the First International virtual training on NIRS technology organized by the University of Córdoba**
Information supplied by : Pierre Dardenne
23 MAY 2012

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Next ICNIRS conference...



ICNIRS 2013 will be held in Villeneuve d'Ascq (Lille) France

Wallonie



Chimiométrie 2012

5 - 06 Déc 2012

The next annual congress of the Chemometrics French group will be held on 5 and 6 December...

Location : Villeneuve d'Ascq (Lille) - France.

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