

# CHALLENGE 2018

Data provided by CRA-W

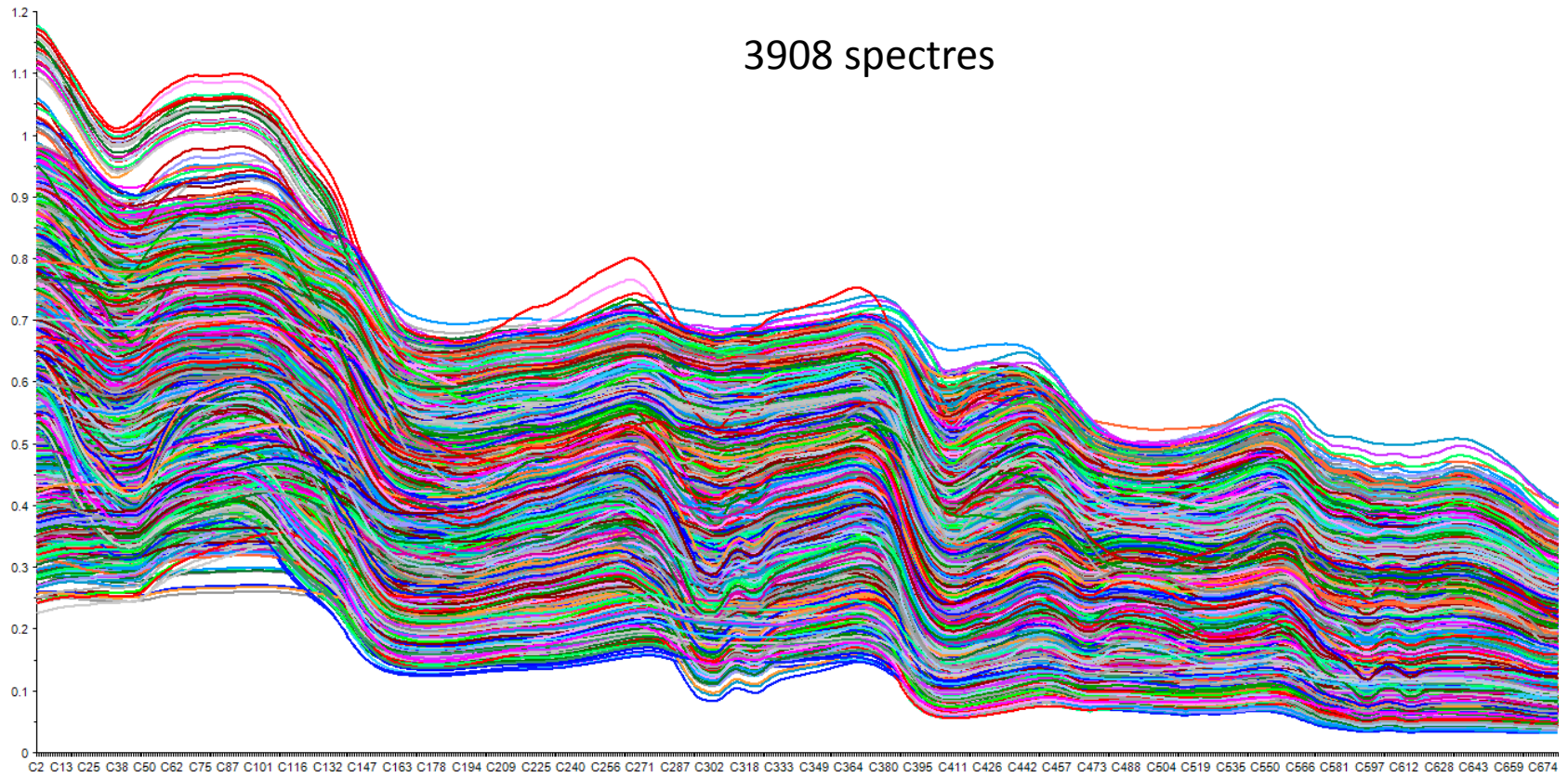
3 prix à distribuer :

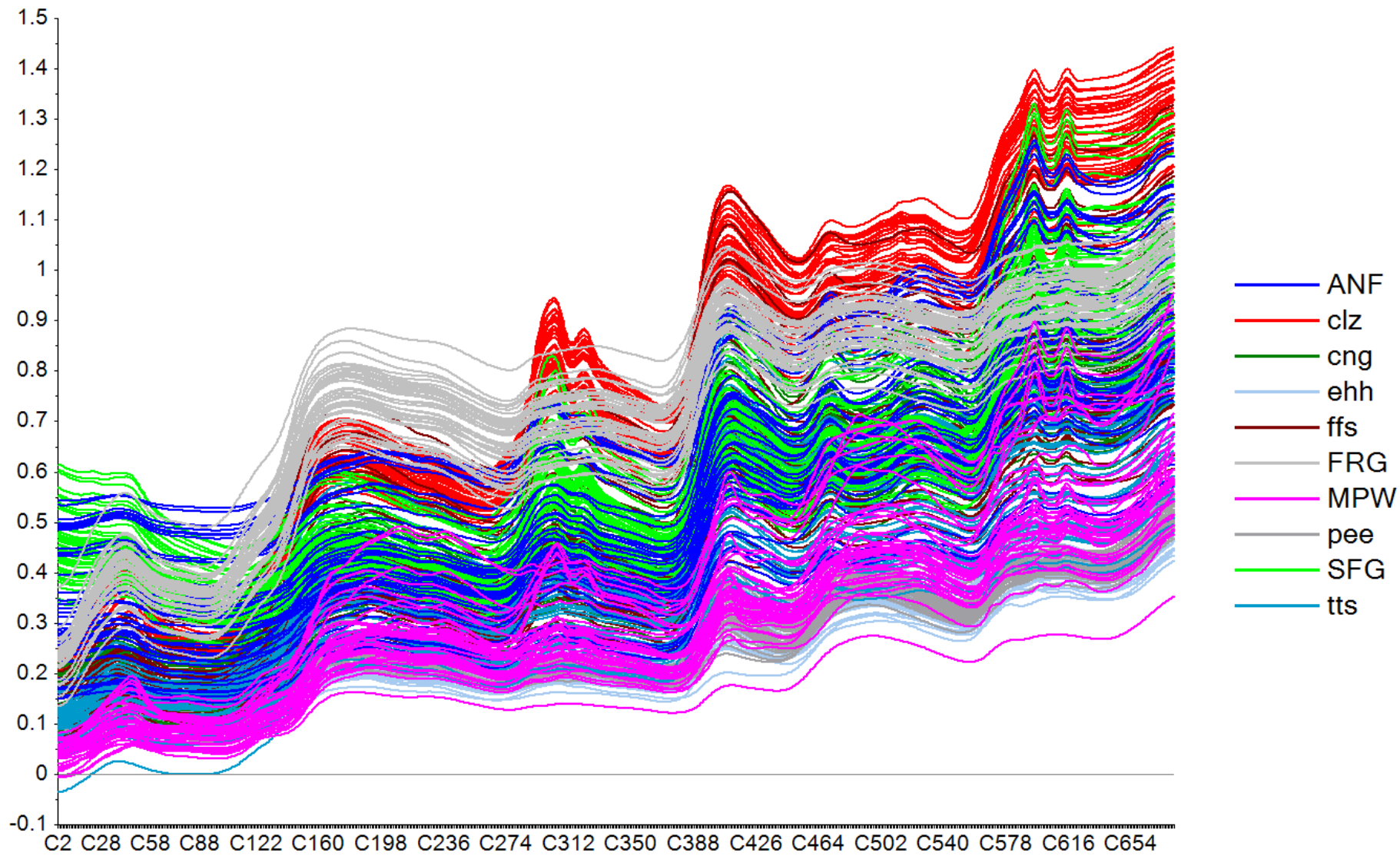
une licence Pirouette offerte par Infometrix,

une licence CART offerte par Salford Systems- Minitab,

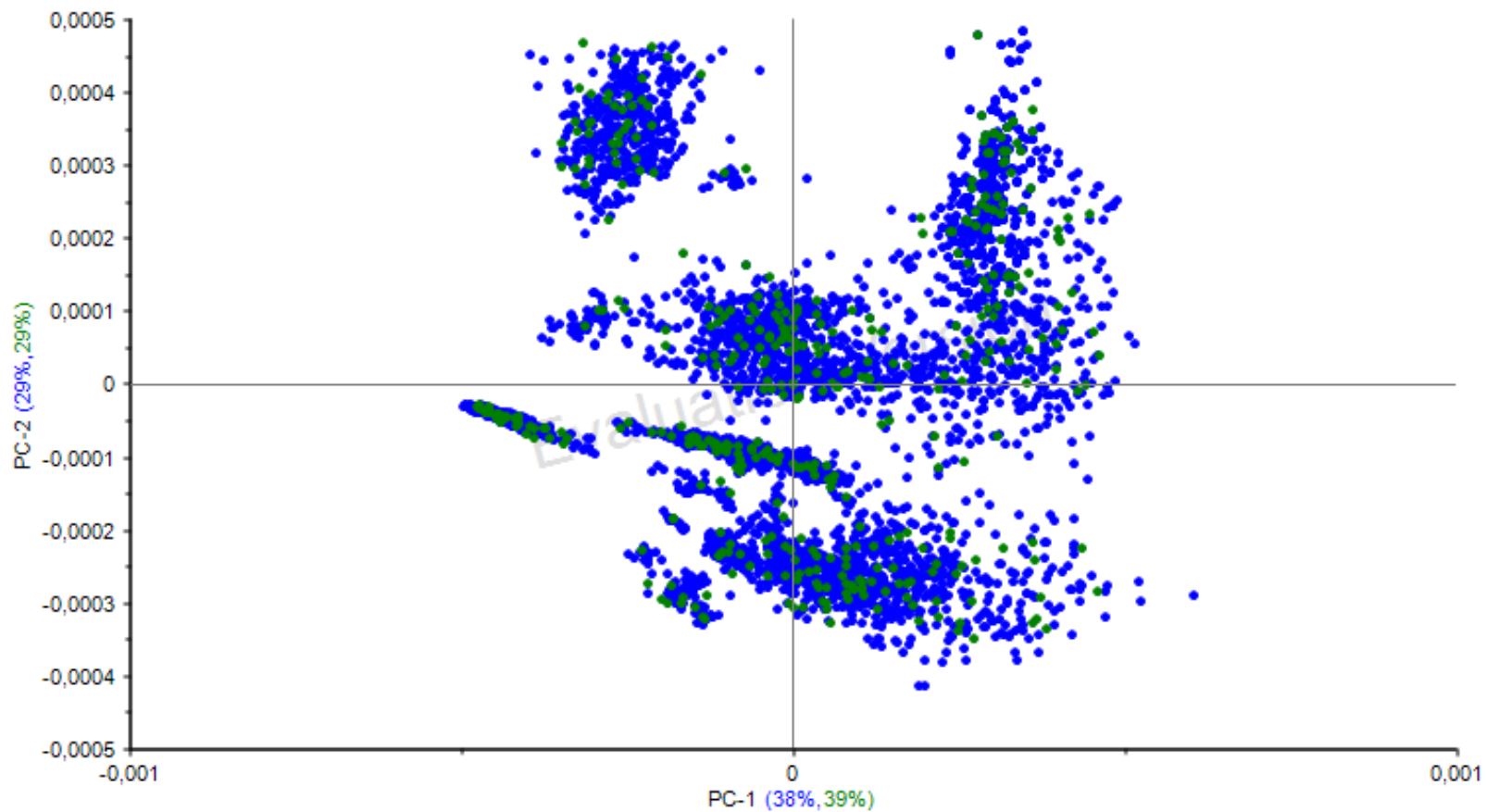
une licence JMP

# 3908 spectres





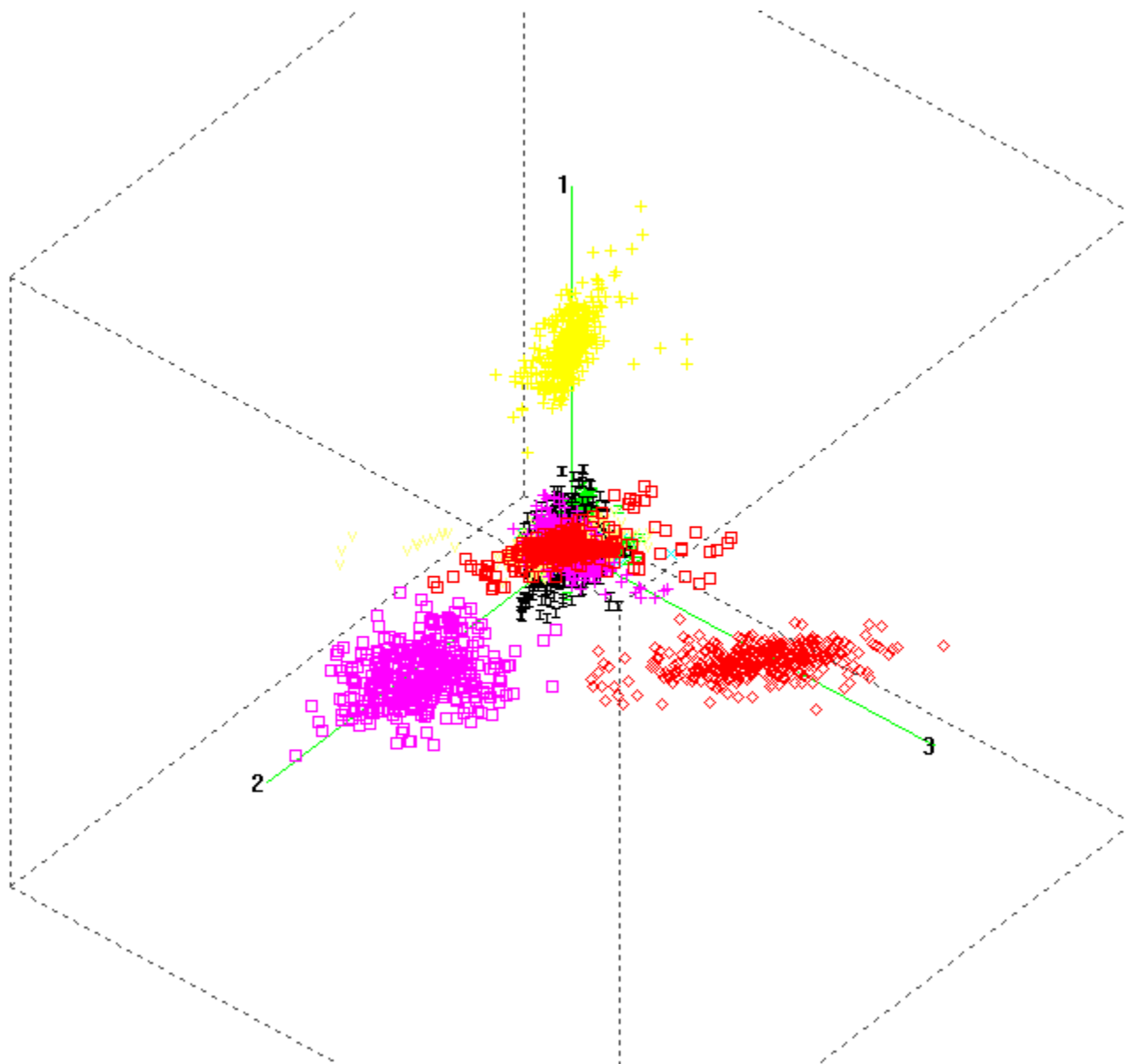
Scores



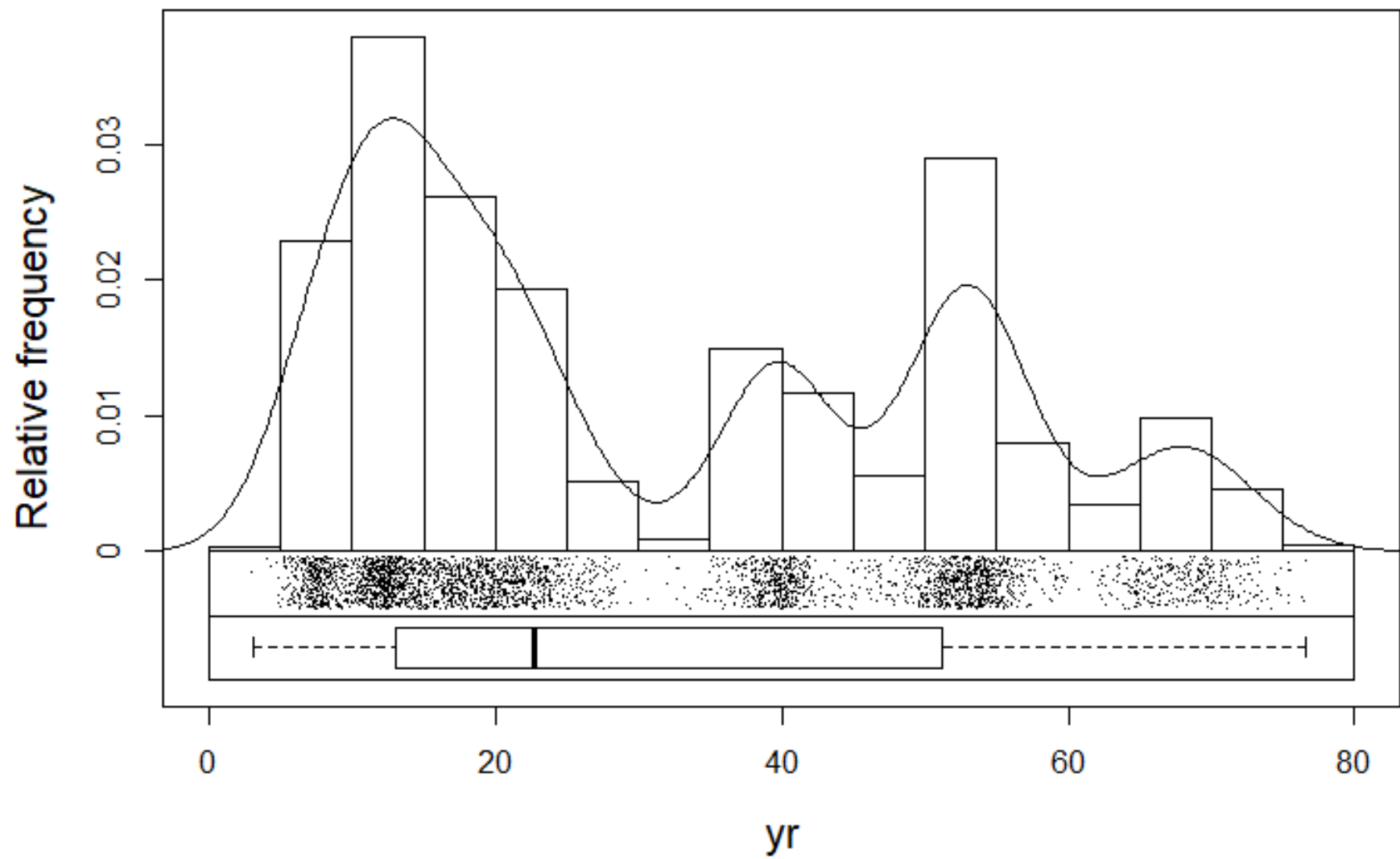
# DATA 10 PRODUCTS DISCRIM PLS-DA 16 factors - no error in CV (2blocks) - Winisi

	<i>rapeseed(ung)</i>	<i>grass silage</i>	<i>maïs wp</i>	<i>corn gluten</i>	<i>full fat soya</i>	<i>soya meal</i>	<i>sun flower seed(gr)</i>	<i>animal feed</i>	<i>wheat (ung)</i>	<i>milk powder &amp; whey</i>
	CLZ	EHH	PEE	CNG	FFS	TTS	SFG	ANF	FRG	MPW
<b>rapeseed(ung)</b>	378	0	0	0	0	0	0	0	0	0
<b>grass silage</b>	0	380	0	0	0	0	0	0	0	0
<b>maïs wp</b>	0	0	367	0	0	0	0	0	0	0
<b>corn gluten</b>	0	0	0	358	0	0	0	0	0	0
<b>full fat soya</b>	0	0	0	0	417	0	0	0	0	0
<b>soya meal</b>	0	0	0	0	0	457	0	0	0	0
<b>sun flower seed(gr)</b>	0	0	0	0	0	0	452	0	0	0
<b>animal feed</b>	0	0	0	0	0	0	0	351	0	0
<b>wheat (ung)</b>	0	0	0	0	0	0	0	0	371	0
<b>milk powder &amp; whey</b>	0	0	0	0	0	0	0	0	0	377
Totals	378	380	367	358	417	457	452	351	371	377
Misses	0	0	0	0	0	0	0	0	0	0
Uncertain	0	5	10	0	2	0	0	8	0	1

	<i>rapeseed(ung)</i>	<i>grass silage</i>	<i>maïs wp</i>	<i>corn gluten</i>	<i>full fat soya</i>	<i>soya meal</i>	<i>sun flower seed(gr)</i>	<i>animal feed</i>	<i>wheat (ung)</i>	<i>milk powder &amp; whey</i>		
	CLZ	EHH	PEE	CNG	FFS	TTS	SFG	ANF	FRG	MPW	Min PRO	Max PRO
<b>rapeseed(ung)</b>	378	0	0	0	0	0	0	0	0	0	14	33
<b>grass silage</b>	0	380	0	0	0	0	0	0	0	0	5	32
<b>maïs wp</b>	0	0	367	0	0	0	0	0	0	0	4	13
<b>corn gluten</b>	0	0	0	358	0	0	0	0	0	0	59	77
<b>full fat soya</b>	0	0	0	0	417	0	0	0	0	0	35	48
<b>soya meal</b>	0	0	0	0	0	457	0	0	0	0	47	59
<b>sun flower seed(gr)</b>	0	0	0	0	0	0	452	0	0	0	9	25
<b>animal feed</b>	0	0	0	0	0	0	0	351	0	0	46	60
<b>wheat (ung)</b>	0	0	0	0	0	0	0	0	371	0	7	17
<b>milk powder &amp; whey</b>	0	0	0	0	0	0	0	0	0	377	3	41
Totals	378	380	367	358	417	457	452	351	371	377		
Misses	0	0	0	0	0	0	0	0	0	0		
Uncertain	0	5	10	0	2	0	0	8	0	1		



### Histogram of yr





<b>PREDICTION WITH 10 PLS MODELS</b>				
			<b>RMSEP</b>	<b>Factor</b>
<b>rapeseed(ung)</b>	<b>CLZ</b>	<b>42</b>	<b>0.605</b>	<b>9</b>
<b>grass silage</b>	<b>EHH</b>	<b>42</b>	<b>0.985</b>	<b>11</b>
<b>maïs wp</b>	<b>PEE</b>	<b>40</b>	<b>0.471</b>	<b>10</b>
<b>corn gluten</b>	<b>CNG</b>	<b>40</b>	<b>0.776</b>	<b>8</b>
<b>full fat soya</b>	<b>FFS</b>	<b>45</b>	<b>0.92</b>	<b>8</b>
<b>soya meal</b>	<b>TTS</b>	<b>50</b>	<b>0.908</b>	<b>12</b>
<b>sun flower seed(g</b>	<b>SFG</b>	<b>50</b>	<b>0.437</b>	<b>9</b>
<b>animal feed</b>	<b>ANF</b>	<b>40</b>	<b>0.893</b>	<b>9</b>
<b>wheat (ung)</b>	<b>FRG</b>	<b>40</b>	<b>0.359</b>	<b>11</b>
<b>mikk powder &amp; w</b>	<b>MPW</b>	<b>40</b>	<b>0.778</b>	<b>10</b>
		<b>429</b>	<b>0.7467</b>	

# 19 réponses →

	1	Nadege Brun, IS	PLS - UNSC - Global
	1	Jean-Francois Bardeau	Global PLS + WL Regions sel.
	1	Sébastien Génété	PLS Global Classique
	1	Jean-Claude Boulet, INRA	Stacked-PLS ( sel var )
	2	Benoit Jaillais, INRA	Kmeans - 8 Classes - PLS
	2	Caroline Peltier	12 Classes + PLS
	2	Johan Cailletaud, Ulg Pharma	9 classes + PLS
	2	Yoann Gut, Servier	8 Classes + PLS
	2	Jean Michel Roger, IRSTEA	5 classes + PLS
XX	2	Brian Rohrback, Infometrics	4 classes dbscan + PLS
	3	Philippe Courcoux, ONIRIS	Random Forest
	3	Pierre-Alexandre Mattei	Wavelets + Random Forest
	4	Abdelmajid Boukhlof, OPEX	PLS locale
XX	4	Ludovic Duponchel, LASIR	LWR Bootstrap
	4	Matthieu Lesnoff, CIRAD	Local spectra + pls
XX	4	Ali Gahkani, Aunir	LWR
	5	Maxime Metz, Opex	NNET
	5	Belal Gaci, Opex	SVR
XX	5	Alvaro Uceda, Aunir	Gaussian Process Reg.

XX : find 54 duplicates (not repetitions) identical spectra in VAL and CAL

**MAD = median ( | Res<sub>i</sub> – median(Res) | )**

**MAD\*1.48 = SEP for a Gaussian distribution and  $\infty$**

**MADb = median ( | Res<sub>i</sub> | )**

**MADb\*1.48 = RMSEP includes the bias**

**PLACE AUX 5 MEILLEURS RESULTATS**



# CRAW RESULTS

	<b>RMSEP</b>	<b>Median*1.48</b>
<b>LOCAL WINISI (B.Lecle</b>	<b>0.71</b>	<b>0.64</b>
<b>10 PLS MODELS(1/pro</b>	<b>0.78</b>	<b>0.63</b>
<b>LOCAL JUAN</b>	<b>0.72</b>	<b>0.62</b>
<b>LCCRS - Franco Juan</b>	<b>0.69</b>	<b>0.57</b>

# LCCRS The Local Calibration by Customized Radii Selection (LCCRS)



Analytica Chimica Acta

Volume 933, 24 August 2016, Pages 50–58

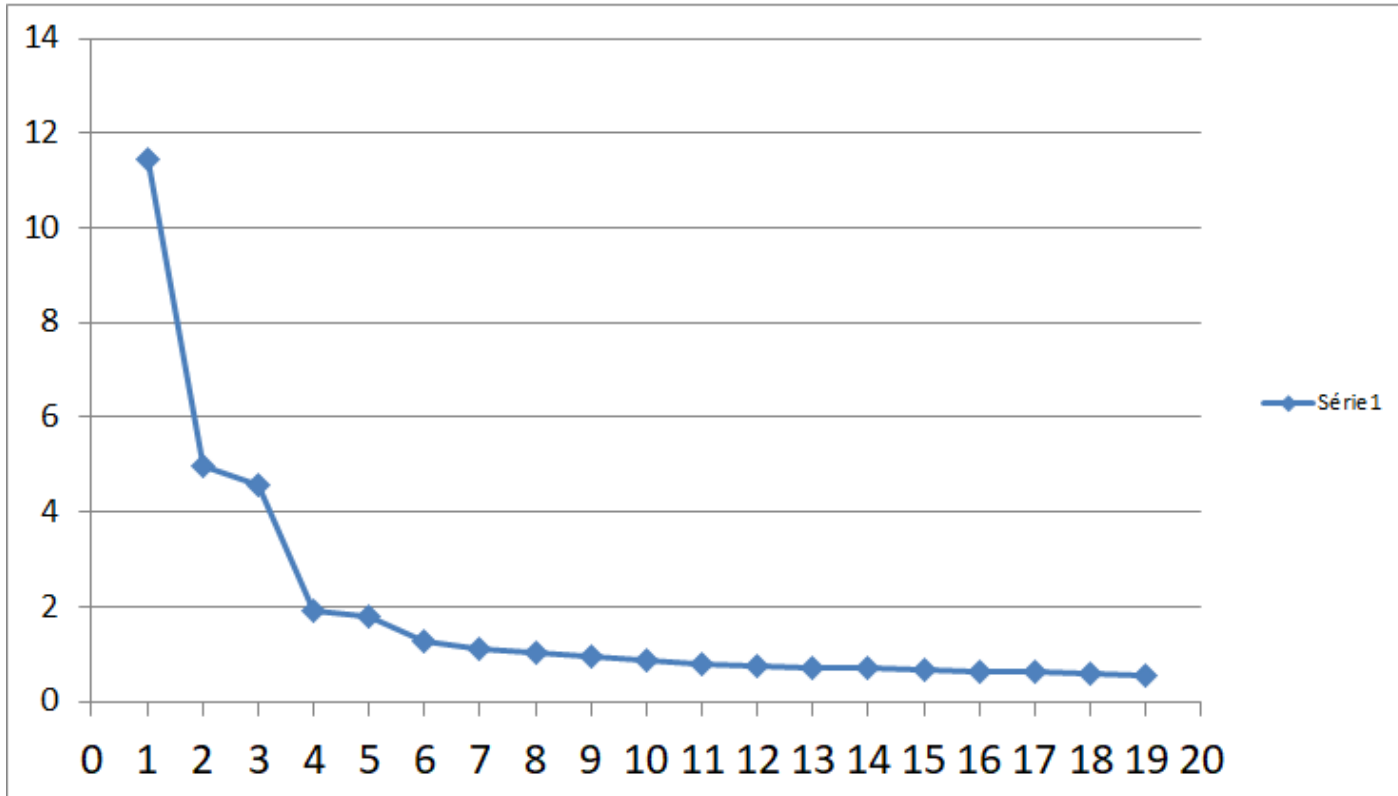


## Regression models based on new local strategies for near infrared spectroscopic data

F. Allegrini<sup>a</sup>,  , J.A. Fernández Pierna<sup>b</sup>, W.D. Fragoso<sup>c</sup>, A.C. Olivieri<sup>a</sup>, V. Baeten<sup>b</sup>, P. Dardenne<sup>b</sup>

The selection of the samples is made by establishing a **standardized radio** around the projection of the unknown sample in the PLS scores space. This radius changes its size until an appropriate number of samples to perform the local calibration is included. Prediction of the unknown sample is performed **by weighting the values based on the size of the regression coefficients and the X residuals** obtained during individual (one by one factor) PLS models.

# MAD 19 participants



1	Nadege Brun, IS	PLS - UNSC - Global
1	Jean-Francois Bardeau	Global PLS + WL Regions sel.
1	Sébatien Génété	PLS Global Classique
1	Jean-Claude Boulet, INRA	Stacked-PLS ( sel var )
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	RMSEP	Median*1.48
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LOCAL JUAN	0.72	0.62
LCCRS - Franco Juan	0.69	0.57

5	Maxime Metz, Opex	NNET	0.829	0.682
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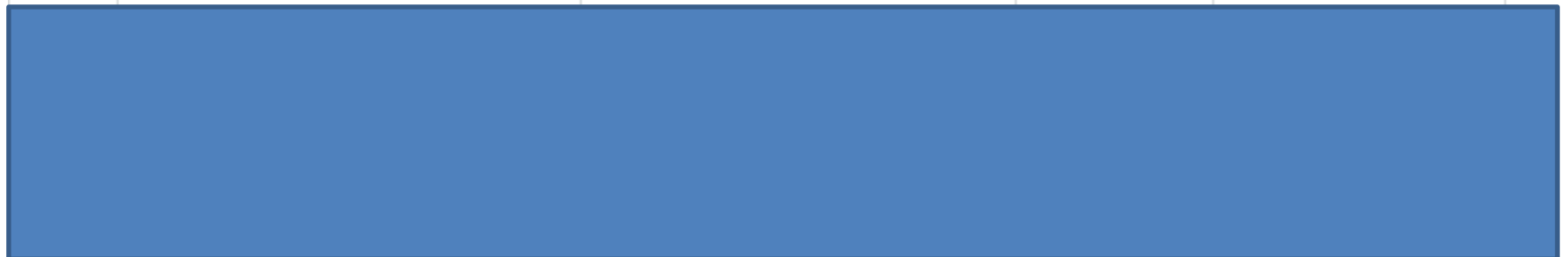
	<b>RMSEP</b>	<b>Median*1.48</b>
<b>LOCAL WINISI (B.Lecle</b>	<b>0.71</b>	<b>0.64</b>
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<b>LCCRS - Franco Juan</b>	<b>0.69</b>	<b>0.57</b>

<b>5</b>	<b>Maxime Metz, Opex</b>	<b>NNET</b>	<b>0.829</b>	<b>0.682</b>
<b>4</b>	<b>Belal Gaci, Opex</b>	<b>SVR</b>	<b>0.811</b>	<b>0.612</b>



	RMSEP	Median*1.48
LOCAL WINISI (B.Lecle	0.71	0.64
10 PLS MODELS(1/pro	0.78	0.63
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LCCRS - Franco Juan	0.69	0.57

5	Maxime Metz, Opex	NNET	0.829	0.682
4	Belal Gaci, Opex	SVR	0.811	0.612
3	Matthieu Lesnoff, CIRA	Local spectra + pls	0.785	0.607



	RMSEP	Median*1.48
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5	Maxime Metz, Opex	NNET	0.829	0.682
4	Belal Gaci, Opex	SVR	0.811	0.612
3	Matthieu Lesnoff, CIRA	Local spectra + pls	0.785	0.607
2	Ali Gahkani, Aunir	LWR	0.716	0.591



	RMSEP	Median*1.48
LOCAL WINISI (B.Lecle	0.71	0.64
10 PLS MODELS(1/pro	0.78	0.63
LOCAL JUAN	0.72	0.62
LCCRS - Franco Juan	0.69	0.57

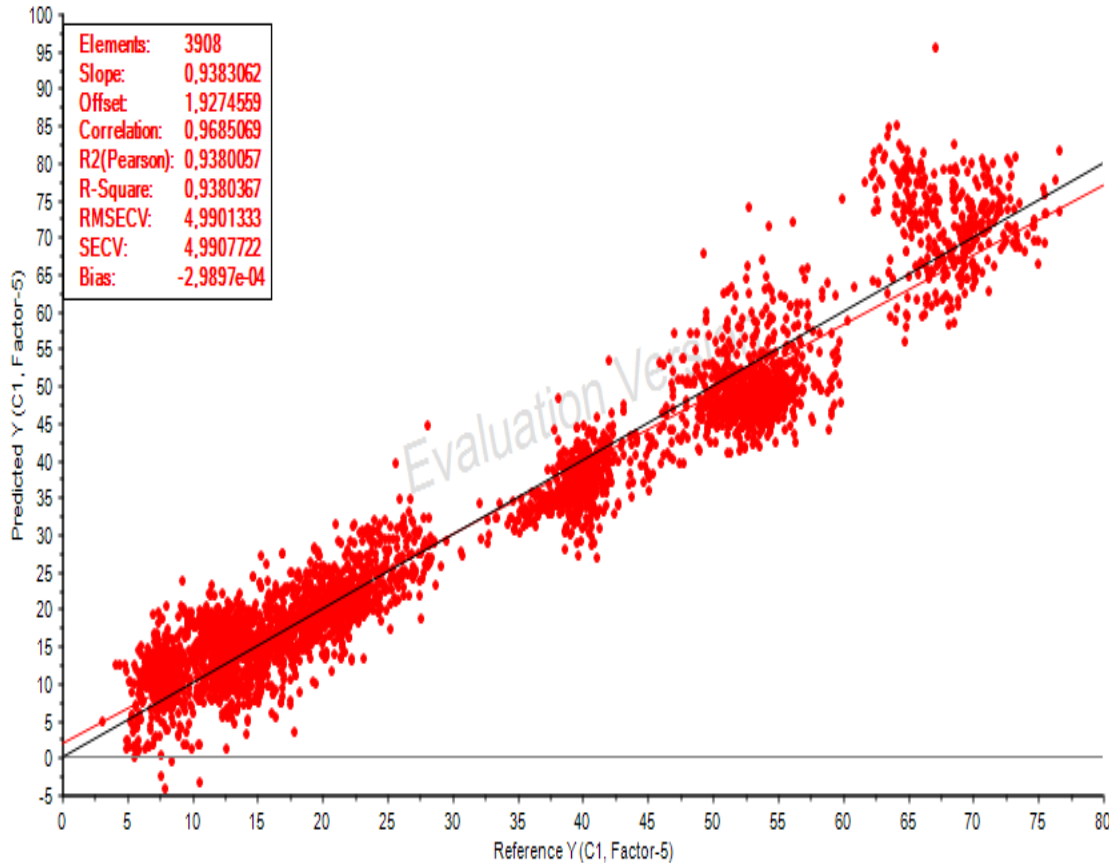
5	Maxime Metz, Opex	NNET	0.829	0.682
4	Belal Gaci, Opex	SVR	0.811	0.612
3	Matthieu Lesnoff, CIRA	Local spectra + pls	0.785	0.607
2	Ali Gahkani, Aunir	LWR	0.716	0.591
1	Alvaro Uceda, Aunir	Gaussian Process Re	0.687	0.540



# 5 Factors PLS

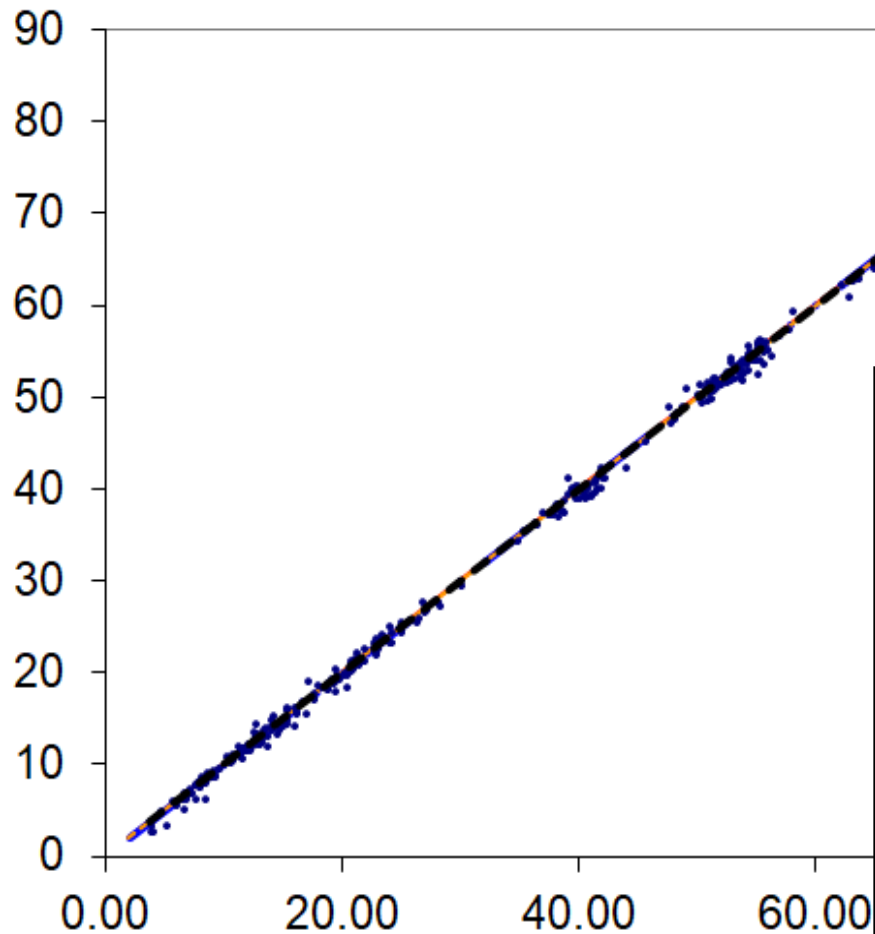
# UNSCRAMBLER

Predicted vs. Reference



Elements:	3908
Slope:	0,9383062
Offset:	1,9274559
Correlation:	0,9685069
R2(Pearson):	0,9380057
R-Square:	0,9380367
RMSECV:	4,9901333
SECV:	4,9907722
Bias:	-2,9897e-04

Alvaro



45°

REF = f (Alvaro )			
	REF		Alvaro
N=		375	
Average=	32.30		32.39
Min=	2.77	2.00	3.80
Max=	75.86	77.00	75.40
SD=	20.848		20.89
Medians=	24.71		24.94
SD_medians=	23.59		23.99
N outliers removed =		0	Robust(medians)
RMSEP=		0.687	0.540
Median ABS errors=			0.360
SEPC=		0.683	0.533
RSDyx=		0.682	0.515
BIAS=		0.083	0.229
Slope=		0.998	
Intercept=		-0.004	
RSQ=		0.999	0.999
RPD=		30.604	40.474