CHALLENGE 2012

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Villeneuve d'ascq, 5-6 Décembre 2012

Polytech'Lille, Université Lille1, FRANCE

Identifiant | Mot de passe | Connexion

NAVIGATION

- Accueil
- Lieu de la conférence
- Conférenciers invités
- Liste de communications acceptées
- Programme CHIMIOMETRIE 2012
- Comités
- Résumé et inscription
- Publication dans CHEMOLAB
- Challenge 2012

PRÉSENTATION

Le **Groupe Français de Chimiométrie (GFC)** sous l'égide de la **Société Française de Statistique (SFdS)** a le plaisir de vous annoncer la tenue de son congrès annuel **CHIMIOMETRIE 2012** qui se déroulera du **5 au 6 décembre 2012** à l'École Polytechnique Universitaire de Lille sur le campus de l'Université Lille 1.

Ce congrès vise à rassembler Universitaires et Industriels pour faire le point sur les avancées de la Chimiométrie, allant de la collecte de l'information aussi efficacement et précisément que possible à partir de plans d'expériences, à l'analyse et à la modélisation des données. Ce congrès, qui depuis de nombreuses années réunit théoriciens et expérimentateurs de tout domaine, a pour vocation de promouvoir l'utilisation de la Chimiométrie au-delà même de l'application des Statistiques dans le domaine de la Chimie. C'est un lieu privilégié de rencontres et d'échanges, qui donne la possibilité aux Universitaires et Industriels, sans restriction disciplinaire, de communiquer en faisant état de leurs expériences, de leurs préoccupations et/ou de leurs besoins actuels et futurs.

En cette année 2012, l'accent sera mis sur les disciplines et les thèmes suivants :

SOCIETE FRANÇAISE DE STATISTIQUE

LASIR

DATES IMPORTANTES

Date limite des soumissions :
22 octobre

Fin des inscriptions à tarif réduit :
20 octobre

Décision du comité scientifique, notifications :

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Challenges - published in ChemoLAB

2004= MEAT (NIR) - Non lin

2005= STARCH (MIR) – Disc

2006= SOILS (NIR) – Large c

2007= WHEAT (NIR) - <<REF – Robustness

2008= none (CAC)

2009= RAPESEED (NIR) – Extrapolation

2010= BEERS (NIR-MIR-Raman) – Discrimination

2011= FEED (NIR) - Calibration Transfer

Data download from:

www.chimiometrie.fr

www.chimiometrie.org

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Challenge 2012

270 spectra in a CAL set with known concentration of a contaminant
276 spectra in a TEST set to be predicted

The goals:

- Obtain the smallest RMSEP
- Obtain the higher rate of good classifications;
  - not contaminated vs contaminated

Send the results including 2 vectors:

1. the quantification
2. the classification: 1 = contaminated 0 = clean

Send the xls file by **November 30** to **dardenne@cra.wallonie.be**
Add a DOC or PPT file with a summary of your approach

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Participants

Florence Kussener, JMP (SAS)

Jean-Claude Boulet, INRA

Nadège Brun, TOTAL

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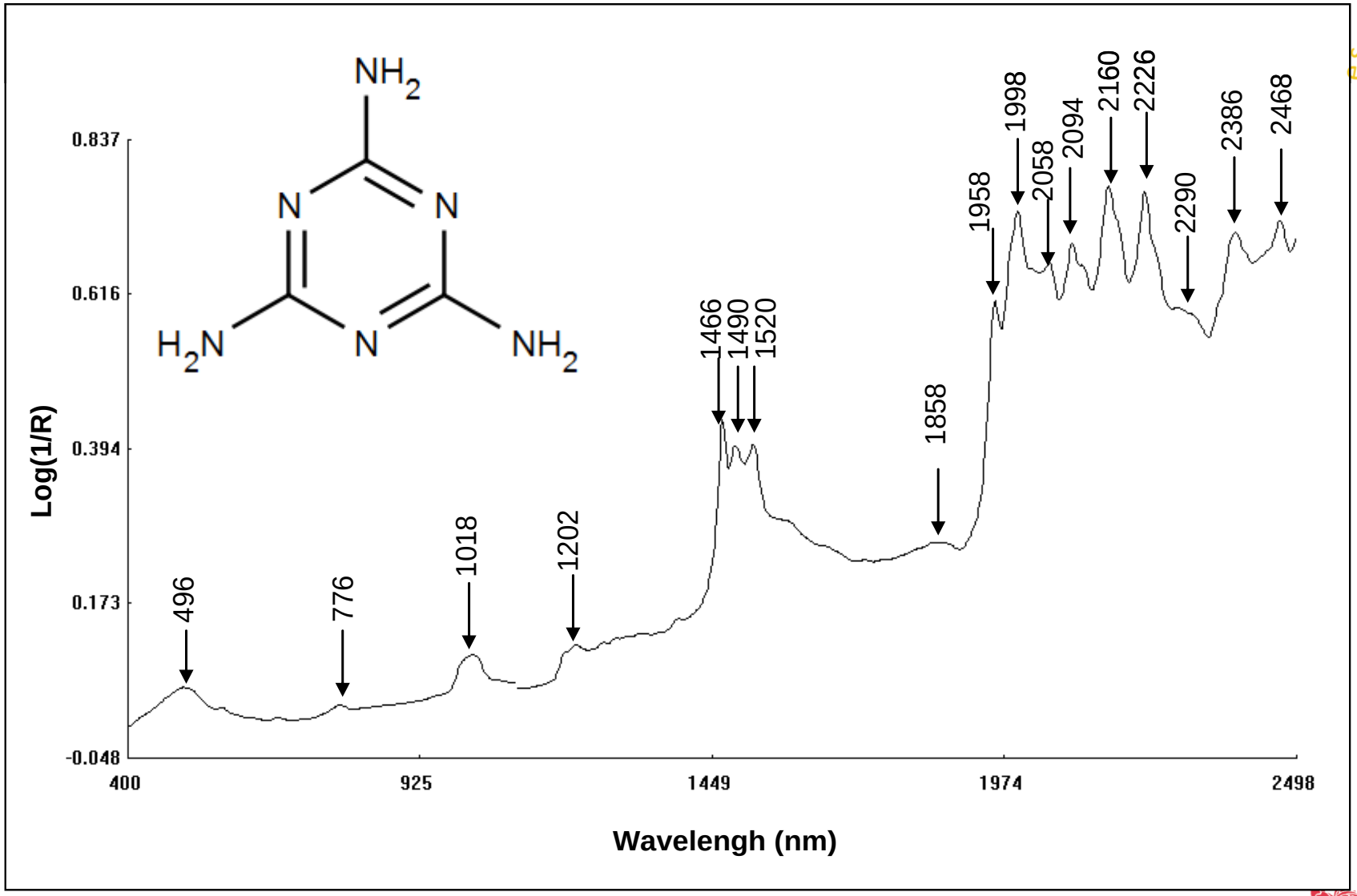
Pure melamine



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480 SM spectra with contamination (0.1, 0.25, 0.5, 1, 2, 3, 4, 5%)
233 SM spectra clean

CAL SET (only soya meal)

240 with 4 concentrations (0.10,0.25, 0.50,1.00%)

+30 randomly selected from the clean set

270 spectra

+ Noise on Y
0.15 noise
N(0, 0.15)
M=0.41→36%

TEST SET

T1 = 40 randomly selected from the 240 with high contamination (2,3,4,5%)

T2 = 50 randomly selected from the clean set

T3 = 43 soyameal spl from another origin + another instrument

T4 = 78 wheat gluten (39 in duplicates)

T5 = 65 maize gluten

Total : 276

Foss XDS

Foss 6500
Clean & Conta.
Melamine
Cyanuric Acid

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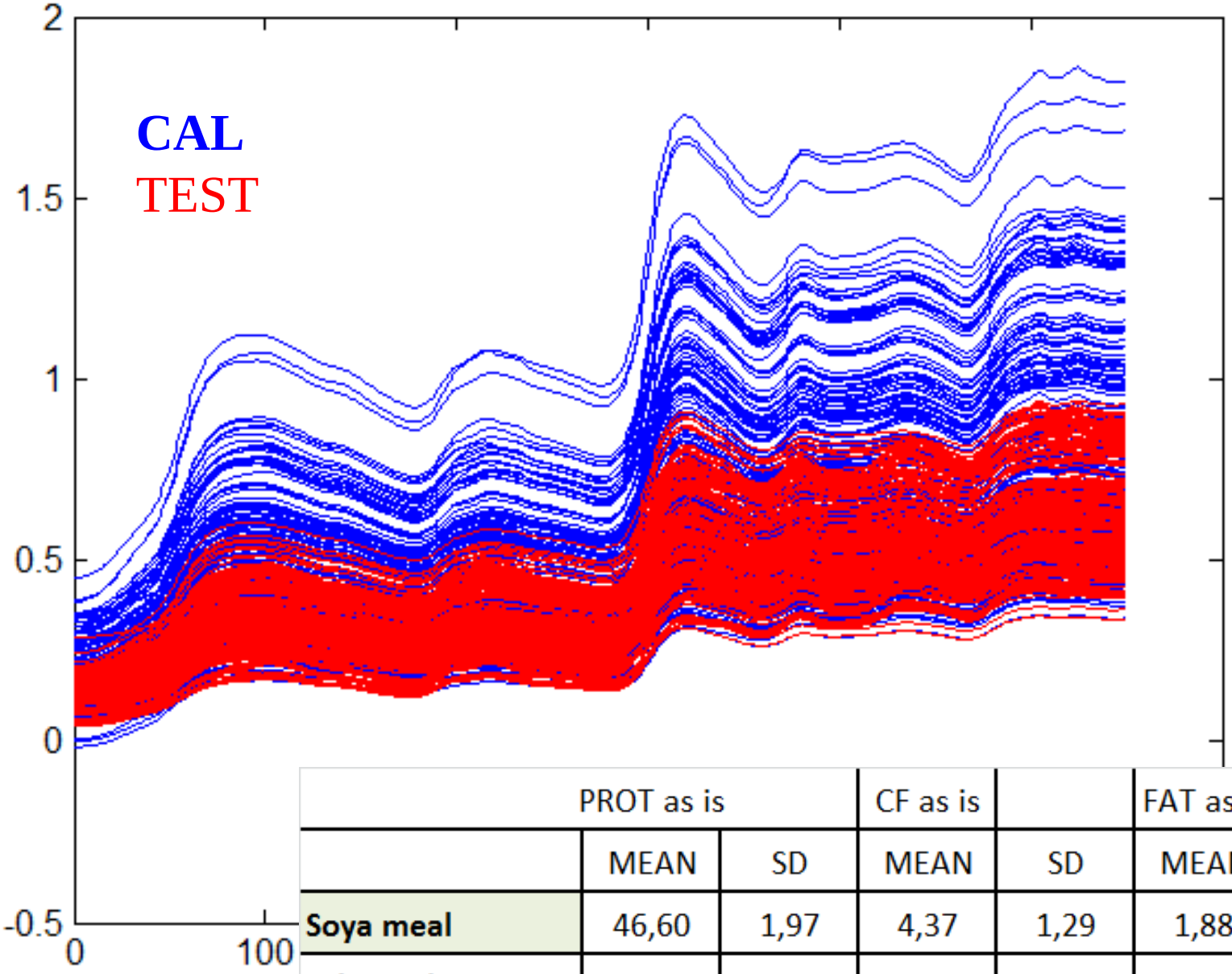
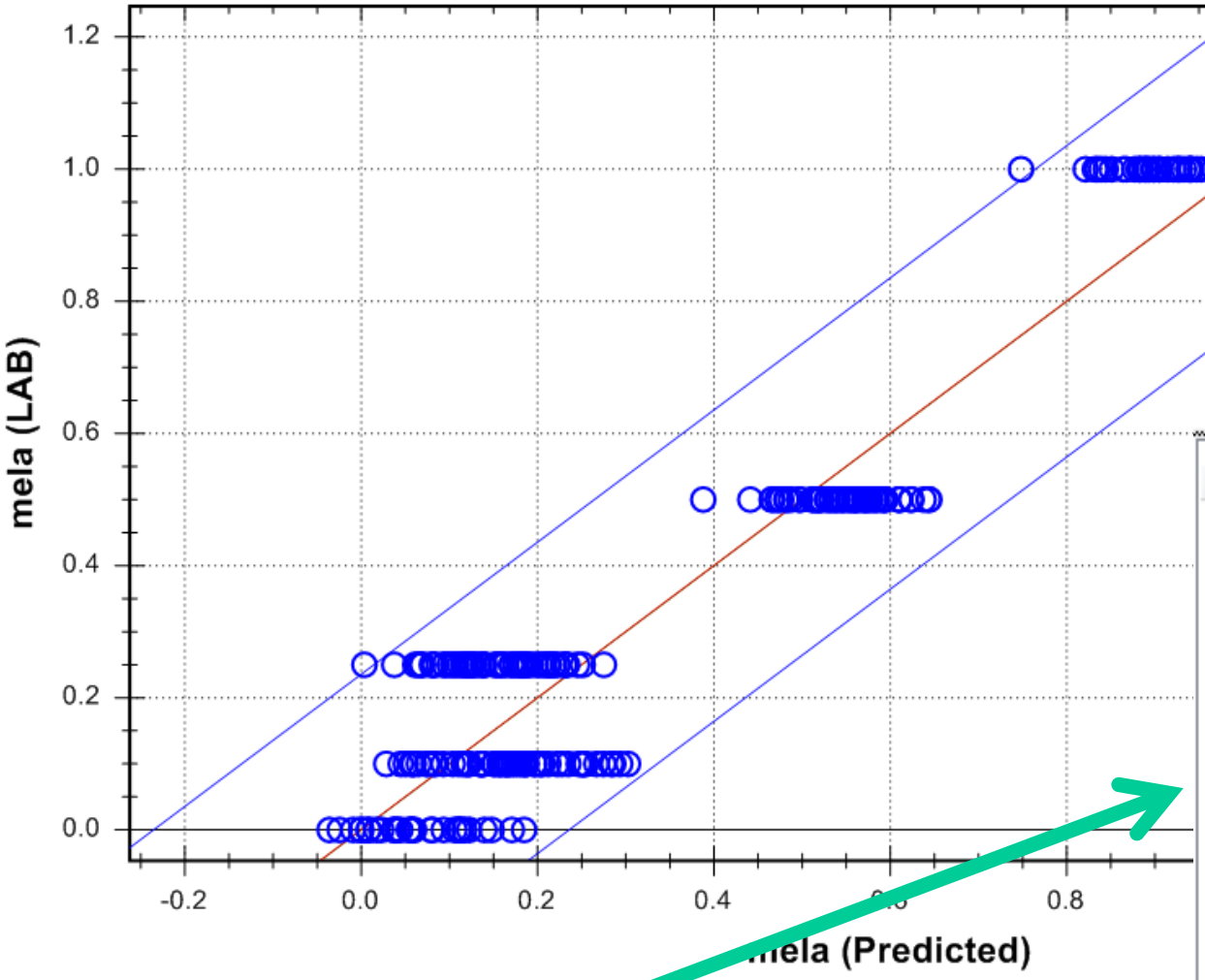


	PROT as is		CF as is		FAT as is	
	MEAN	SD	MEAN	SD	MEAN	SD
Soya meal	46,60	1,97	4,37	1,29	1,88	1,59
Wheat gluten	80,54	2,23	_	_	_	_
maize gluten meal	61,64	2,99	1,53	0,72	1,85	0,83

Calibration (SEC) with unmodified Y values



Statistic	Value
Number of Samples	270
Samples used for St..	270
Slope	1.000
Intercept	0.000
Bias	0.000
SEC	0.095
SEP	0.094
SEP(C)	0.094
RSQ	0.929
Predicted Average	0.411
Actual Average	0.411
Predicted SD	0.341
Actual SD	0.354

0.1 = 1000 ppm

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Multiple Linear Regression – Manual Step up

Segment 1 1300 - 2398, 2

Constituent	N	Mean	SD	SEC	1-VR	SECV	1-VR
mela	270	0.4111	0.3540	0.0828	0.9442	0.0835	0.9442

5dp → PLS instead of MLR

Mean 0.411 Range 0.00 - 1.00

	SEC	RSQ	F	SECV	1-VR
1	0.348	0.031	9.62	0.348	0.030
2	0.203	0.670	518.94	0.204	0.666
3	0.087	0.940	1209.55	0.087	0.939

WITHOUT NOISE

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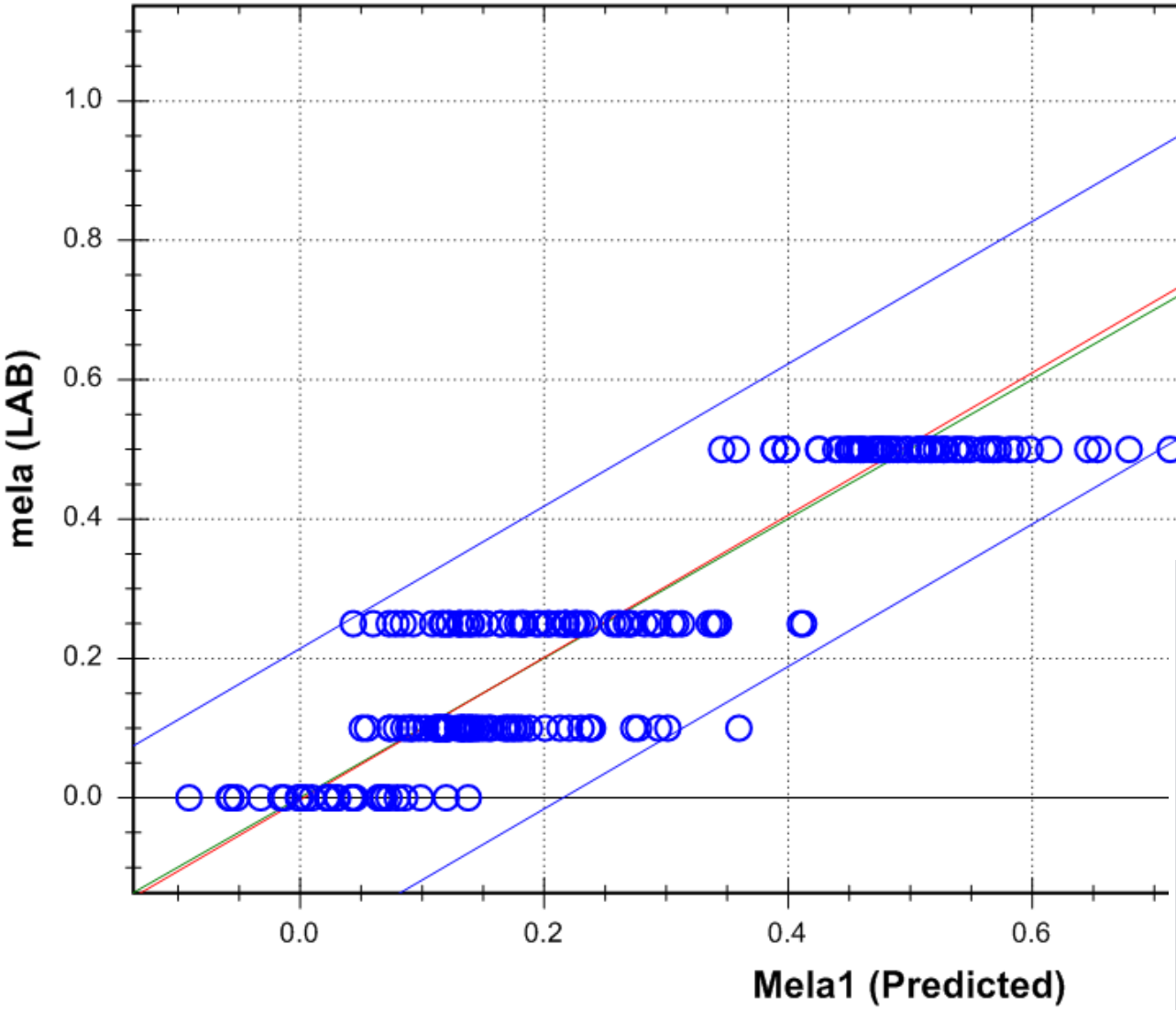

Statistic	Value
Number of Samples	270
Samples used for St..	270
Slope	1.022
Intercept	-0.003
Bias	0.005
SEC	0.087
SEP	0.087
SEP(C)	0.087
RSQ	0.940
Predicted Average	0.406
Actual Average	0.411
Predicted SD	0.336
Actual SD	0.354

>Calibration set = 0.1 % = 1000 ppm

Ref values without noise

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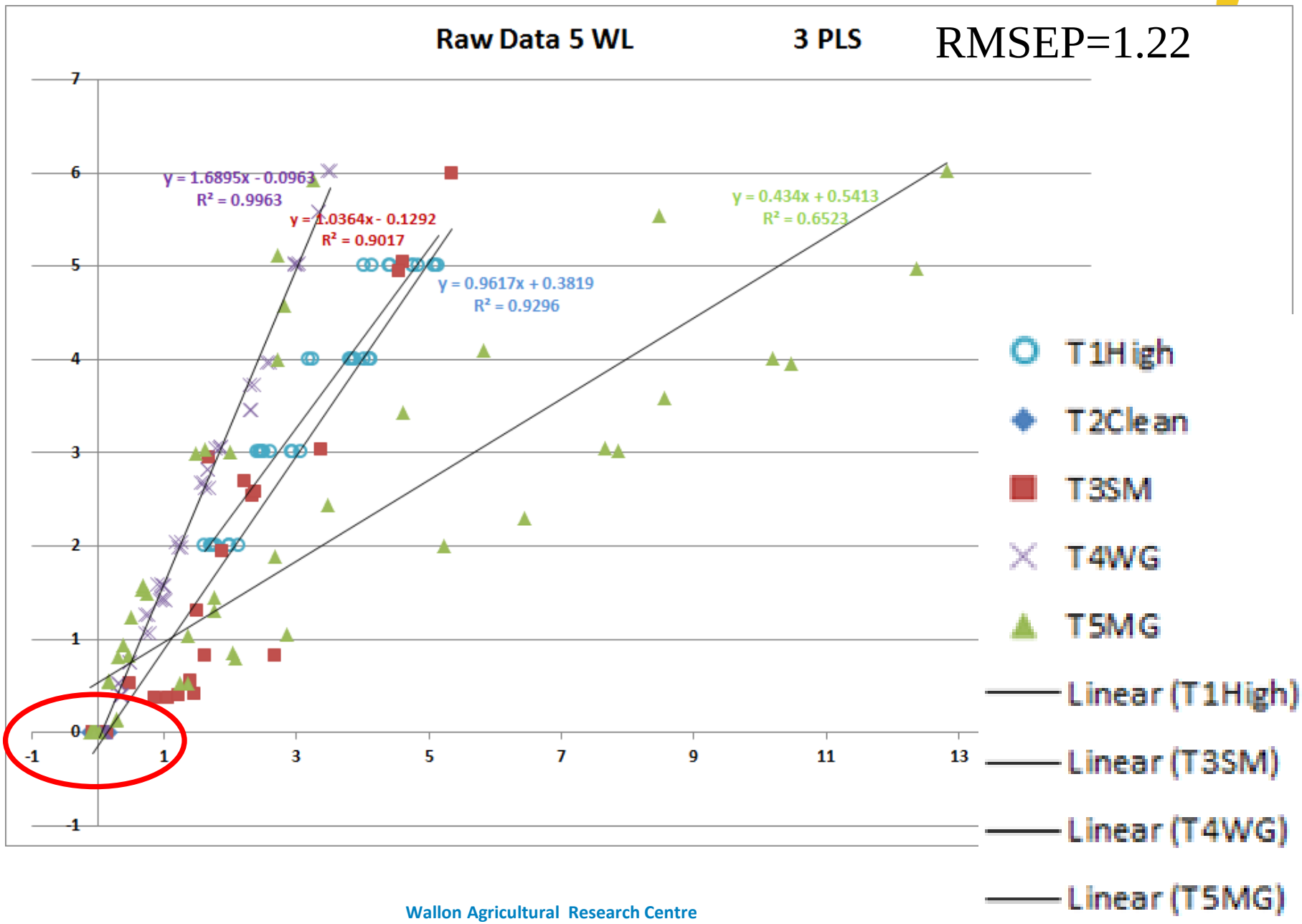

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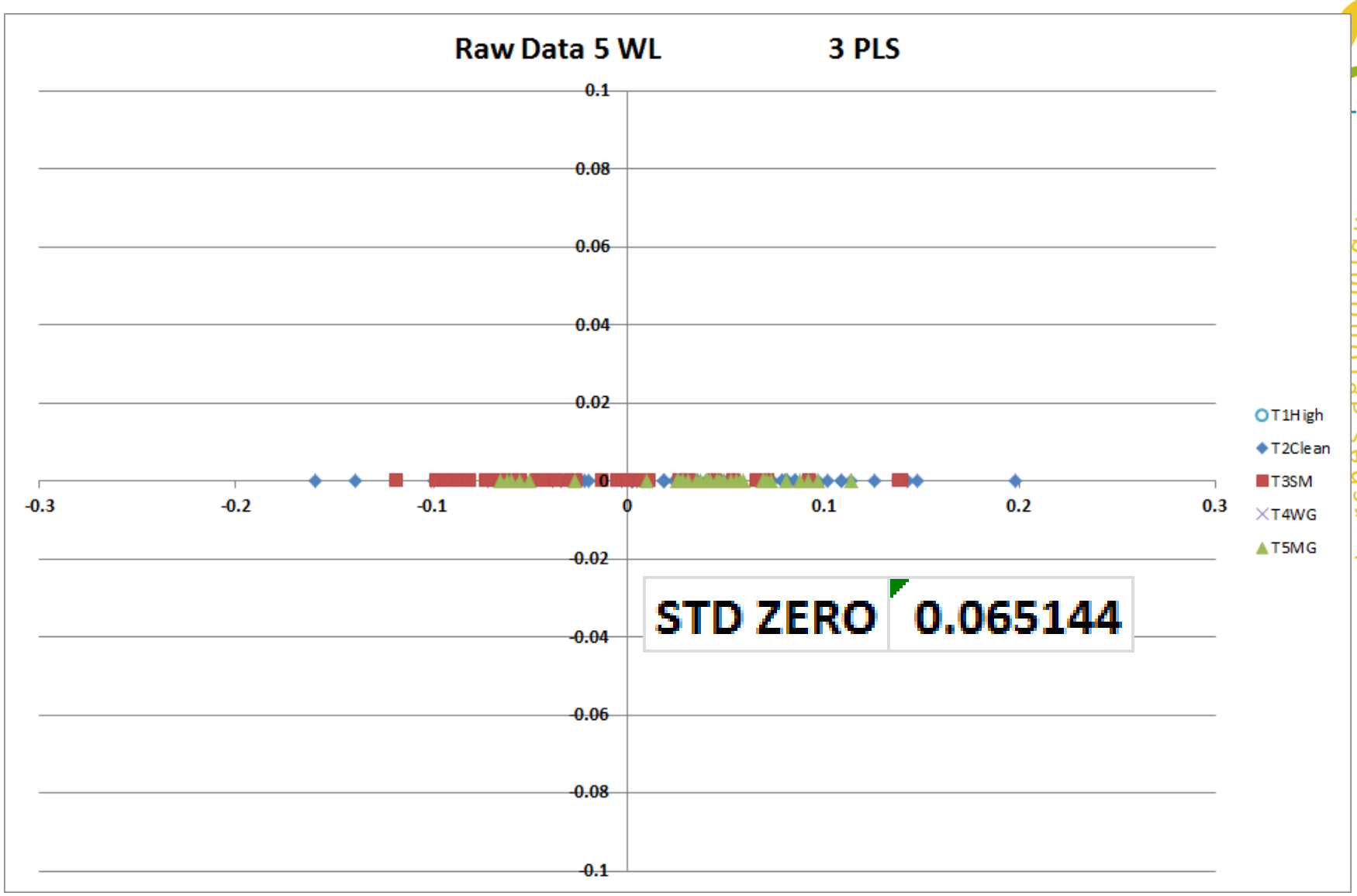

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65 Mais Gluten predicted + GH based on 30 Clean # : 5 dp Log(1/R)

				>7	>4					>7	>4					>7	>4
Posit	Sample Numbe	REF	mela	GH-mela	NH-mela	Positic	Sample Numb	REF	mela	GH-mela	NH-mela	Positi	Sample Numb	REF	mela	GH-mela	NH-mela
1	T5MG__094	0.00	-0.04	2.58	0.48	26	T5MG__119	3.02	8.06	7376.12	7180.28	51	T5MG__144	1.23	0.49	30.08	17.86
2	T5MG__095	2.00	5.37	3253.86	3124.86	27	T5MG__120	0.00	-0.08	2.01	0.96	52	T5MG__145	3.03	1.64	316.29	275.44
3	T5MG__096	3.05	7.86	7043.32	6851.92	28	T5MG__121	1.49	0.73	66.34	47.81	53	T5MG__146	0.00	0.00	0.41	0.06
4	T5MG__097	3.95	10.75	13228.21	12964.88	29	T5MG__122	3.01	2.04	489.63	438.66	54	T5MG__147	1.04	1.37	205.73	174.43
5	T5MG__098	6.02	13.17	19905.54	19581.54	30	T5MG__123	3.99	2.77	900.07	830.86	55	T5MG__148	2.44	3.54	1424.05	1338.43
6	T5MG__099	0.00	-0.05	3.13	0.83	31	T5MG__124	4.58	2.87	968.33	896.57	56	T5MG__149	3.43	4.73	2544.45	2429.50
7	T5MG__100	0.00	-0.06	3.06	0.68	32	T5MG__125	0.00	-0.09	2.23	1.25	57	T5MG__150	5.54	8.70	8670.86	8457.39
8	T5MG__101	0.00	-0.11	4.15	1.09	33	T5MG__126	0.00	-0.09	2.17	1.21	58	T5MG__151	0.00	-0.04	0.89	0.02
9	T5MG__102	0.00	-0.13	4.48	1.40	34	T5MG__127	0.00	-0.09	2.21	1.19	59	T5MG__152	0.00	-0.06	1.31	0.15
10	T5MG__103	0.14	0.27	5.53	2.75	35	T5MG__128	0.00	-0.09	2.26	1.29	60	T5MG__153	0.00	-0.07	1.56	0.21
11	T5MG__104	0.85	2.08	471.47	424.09	36	T5MG__129	0.83	0.45	26.41	14.98	61	T5MG__154	0.00	-0.08	1.68	0.24
12	T5MG__105	0.80	2.13	492.93	444.22	37	T5MG__130	0.81	0.28	11.88	4.55	62	T5MG__155	1.89	2.74	845.92	780.51
13	T5MG__106	4.01	10.47	12532.79	12276.61	38	T5MG__131	0.94	0.36	18.23	8.89	63	T5MG__156	1.45	1.79	359.53	317.32
14	T5MG__107	0.00	-0.03	2.73	0.67	39	T5MG__132	2.99	1.51	270.33	232.54	64	T5MG__157	1.31	1.79	355.09	313.28
15	T5MG__108	0.52	1.39	201.07	171.20	40	T5MG__133	0.00	-0.06	1.86	0.75	65	T5MG__158	4.10	5.97	4091.09	3944.82
16	T5MG__109	1.05	2.91	932.71	865.25	41	T5MG__134	0.55	0.16	4.96	0.79						
17	T5MG__110	3.59	8.79	8808.25	8594.03	42	T5MG__135	1.53	0.66	54.61	37.84						
18	T5MG__111	4.97	12.70	18482.90	18171.29	43	T5MG__136	5.12	2.77	898.71	829.56						
19	T5MG__112	0.00	-0.06	3.21	0.73	44	T5MG__137	5.93	3.32	1289.58	1206.78						
20	T5MG__113	0.00	-0.07	3.77	0.94	45	T5MG__138	0.00	-0.08	2.06	1.15						
21	T5MG__114	0.00	-0.09	3.95	1.00	46	T5MG__139	0.00	-0.06	1.90	0.75						
22	T5MG__115	0.00	-0.10	4.52	1.29	47	T5MG__140	0.00	-0.08	2.07	1.02						
23	T5MG__116	0.13	0.27	5.26	2.27	48	T5MG__141	0.00	-0.07	2.11	1.02						
24	T5MG__117	0.52	1.27	167.21	140.38	49	T5MG__142	0.54	0.15	4.73	0.71						
25	T5MG__118	2.30	6.61	4950.30	4790.38	50	T5MG__143	1.58	0.68	58.53	41.13						

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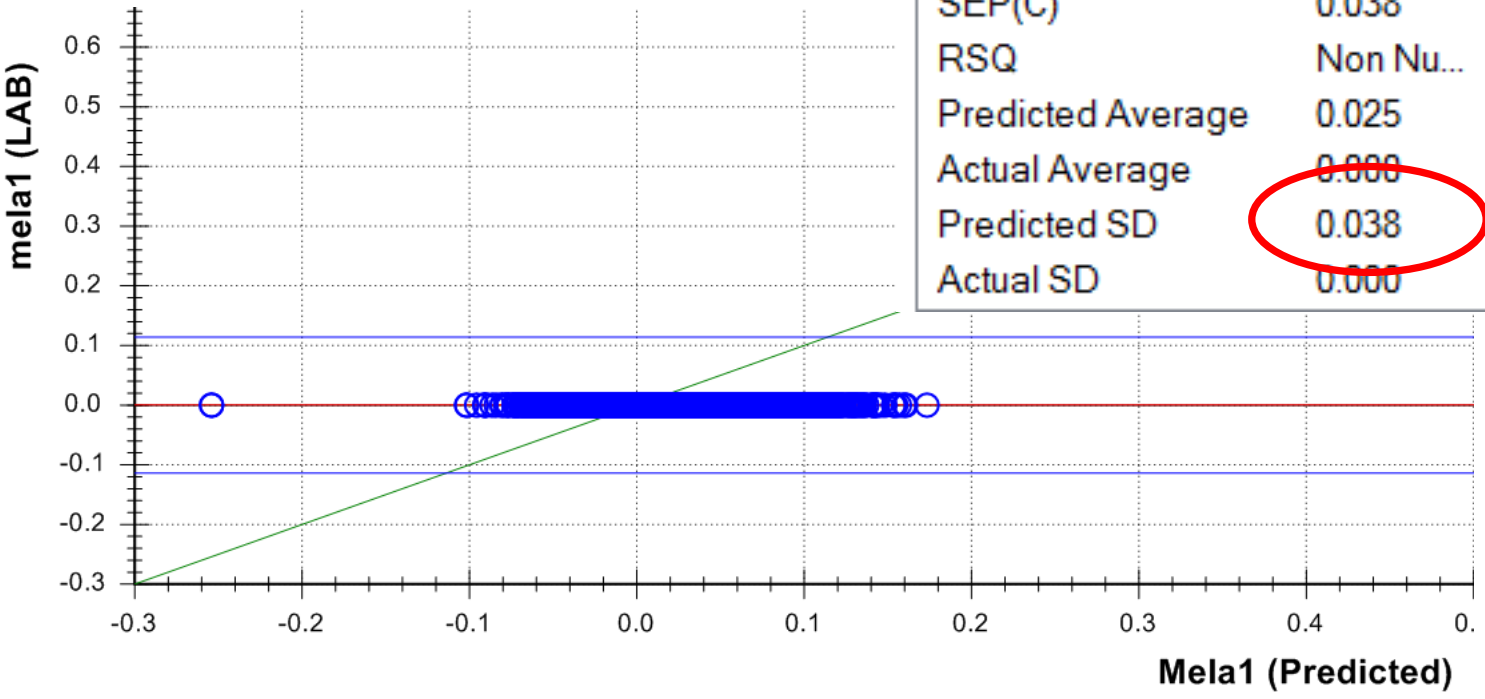
Wheat flour data set :

Statistic	Value
Number of Samples	5269
Samples used for St...	5269
Slope	0.000
Intercept	0.000
Bias	-0.025
SEC	0.000
SEP	0.046
SEP(C)	0.038
RSQ	Non Nu...
Predicted Average	0.025
Actual Average	0.000
Predicted SD	0.038
Actual SD	0.000



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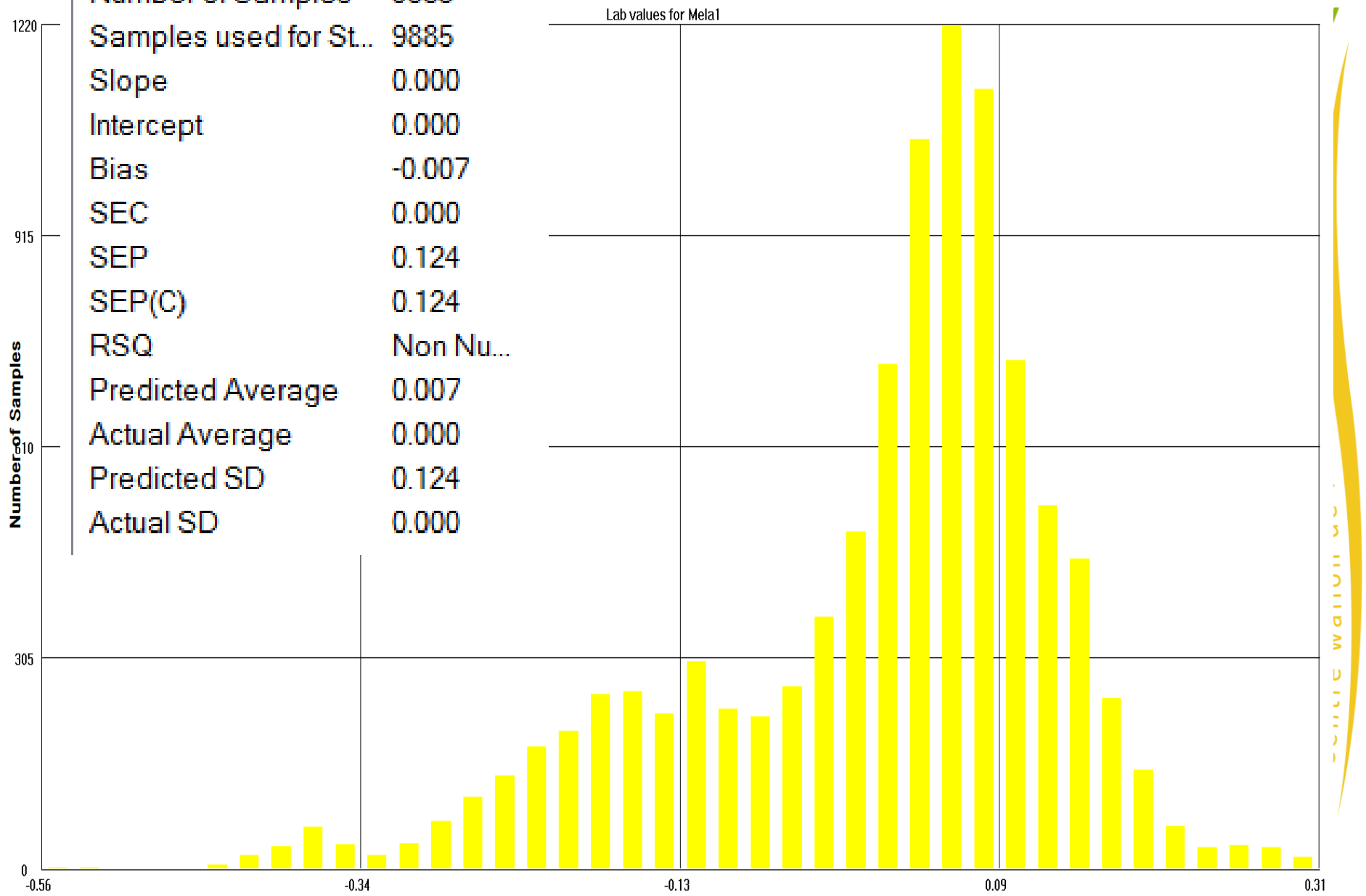
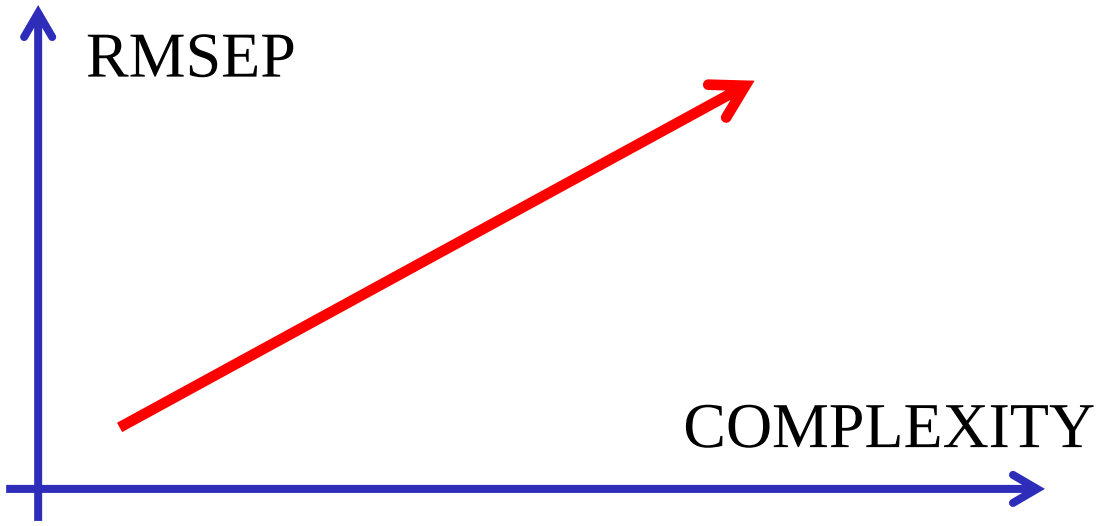
HIGH PROTEIN FEED INGREDIENTS

Number of Samples	9885
Samples used for St...	9885
Slope	0.000
Intercept	0.000
Bias	-0.007
SEC	0.000
SEP	0.124
SEP(C)	0.124
RSQ	Non Nu...
Predicted Average	0.007
Actual Average	0.000
Predicted SD	0.124
Actual SD	0.000



		RMSEP	% err.
Florence	ANN	2.36	40.2
Jean-Claude	Independant Interference Reduction risques 1er et 2ieme espèce	1.81	16.3
Nadege	Classical PLS - SG2 - Windows (IPLS)	1.41	5.4
Pierre	MLR (best 3) -> PLS 3F with 5 Log(1/R)	1.22	0.7



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SOMETIMES IT IS OBVIOUS THAT SHEER BRUTE FORCE IS NOT GOING TO WORK!

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www.icnirs.org

ICNIRS

The International Council for Near Infrared Spectroscopy

Established in 1986 to promote the advance of NIR technology

1 2

Next events

NIR platfor... detection

27 March 2013

We are pleased... platform worksh...

Location : Gembl...

16th ICNIRS Conference

1 - 07 June 2013

Dear Colleagues,On behalf of the organizing committee of ICNIRS 2013, we are pleased to invite you to join us...

Location : Montpellier - France

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