OptiMIR

cra-w

Walloon Agricultural Research Centre

MERGING OF SPECTRAL DATASETS FROM DIFFERENT MIR INSTRUMENTS USED IN THE ROUTINE ANALYSIS OF MILK

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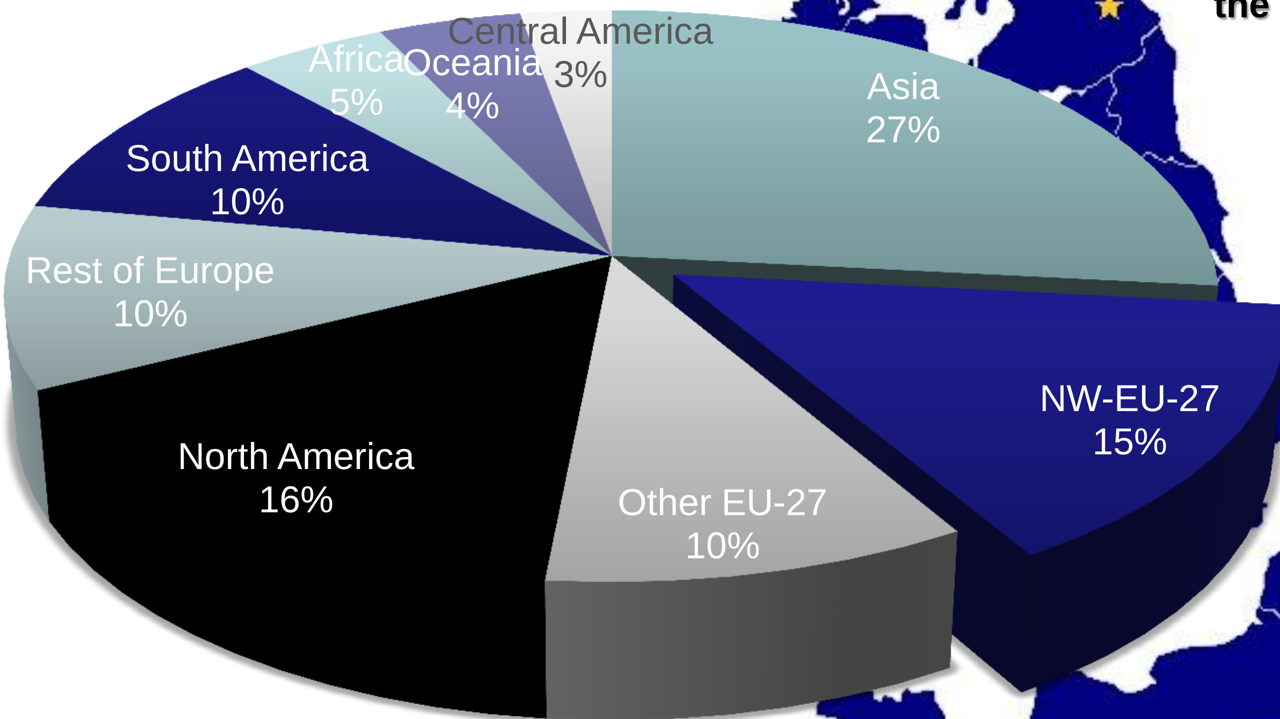
nwe
INTERREG IVB

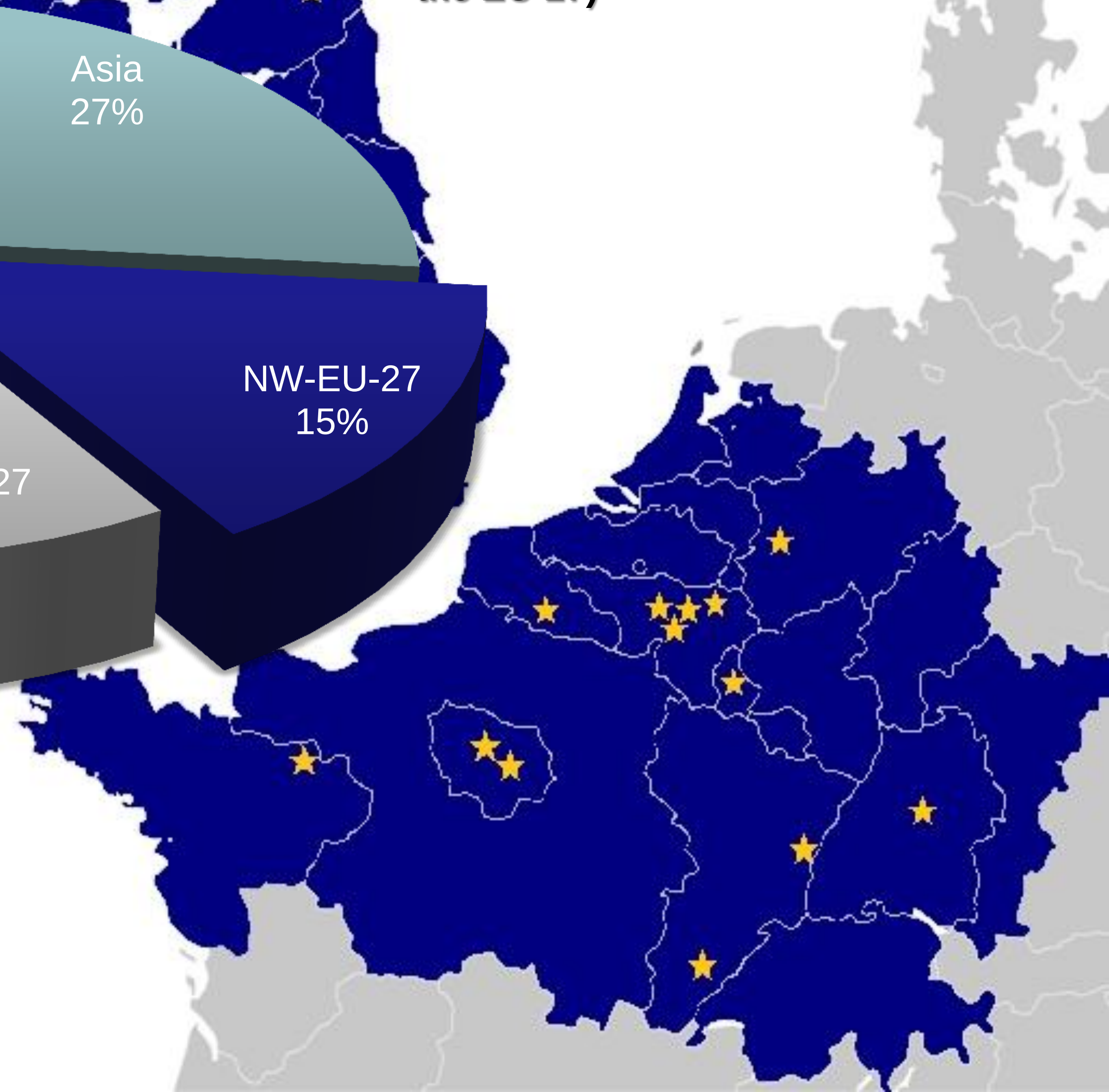
Cork – 28 May 2012

Wallonie

North West Europe

- 60% of the EU-27 milk production
- 150,000 people employed in the dairy sector
- A turnover of € 70 billions (>50% of the EU-27)





INTERREG IVB

The OptiMIR Project

17 partners and 1 sub-contracting partner / 6 countries

Milk recording organizations	Country
AWE asbl	BE
Chambre régionale Agriculture Alsace	FR
ADECL62 (Pas-de-Calais)	FR
CLASEL (Sarthe & Mayenne)	FR
SCL25 (Doubs et territoire de Belfort)	FR
France Conseil Elevage	FR
LKV Baden-Württemberg	DE
LKV Nordrhein-Westfalen	DE
National Milk Recording	UK
Irish Cattle Breeding Federation	IR
CONVIS	LU

Research Units	Country
Institut de l'Elevage	FR
Gembloux Agro-Bio Tech (ULg)	BE
CRA-W (DVPA)	BE
TEAGASC	IR
Scottish Agricultural College	UK
University of Hohenheim	DE

Laboratory	Country
Comité du Lait asbl	BE

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AIMS

To improve the profitability and sustainability of the dairy sector by providing milk producers with innovative standardized management tools based **on association between MIR milk records and cows' status.**

To reduce the costs of production through improved daily herd management.

costs of feeding with energetic balance indicator

veterinary costs with early diagnosis of mastitis

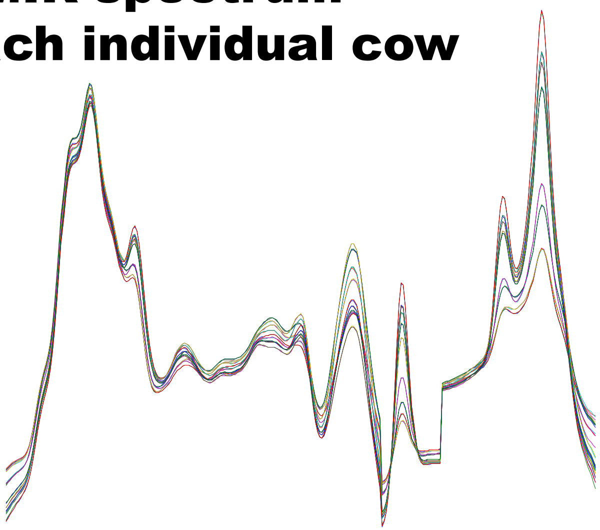
costs of semen straws with insemination predictor

To bring opportunities to access competitive markets by measuring quality traits linked to higher added value (e.g. low-cost measure of food label claims).

To decrease the impact on the environment (quantification of methane and nitrogen production).

Mid-Infrared (MIR) spectra of milk
=
Mirror of cow's status

Milk MIR spectrum
for each individual cow



- **FERTILITY**
  Ex. : Pregnancy
- **FEEDING**
  Ex. : Energy Balance
- **ANIMAL HEALTH**
  Ex. : Mastitis
- **ENVIRONNEMENTAL IMPACT**
  Ex. : CH_4

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To pool the resources of Milk Recording Organizations to have a **common transnational database** coupling:

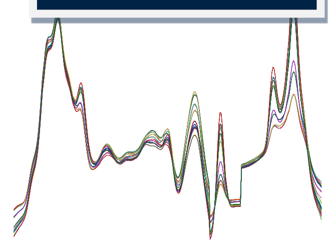
- Physiological data of the cows
- with the related Milk Recording data
- and the standardized Spectrum Information (1060 values for each wavelength for a Foss instrument / record)

Pregnancy diagnosis
AI events
Heats
Mastitis
Acidosis
Individual feeding
Methane measurement
...

+

Milk Recording Data including

MIR Spectrum



=

COMMON TRANSNATIONAL DATABASE

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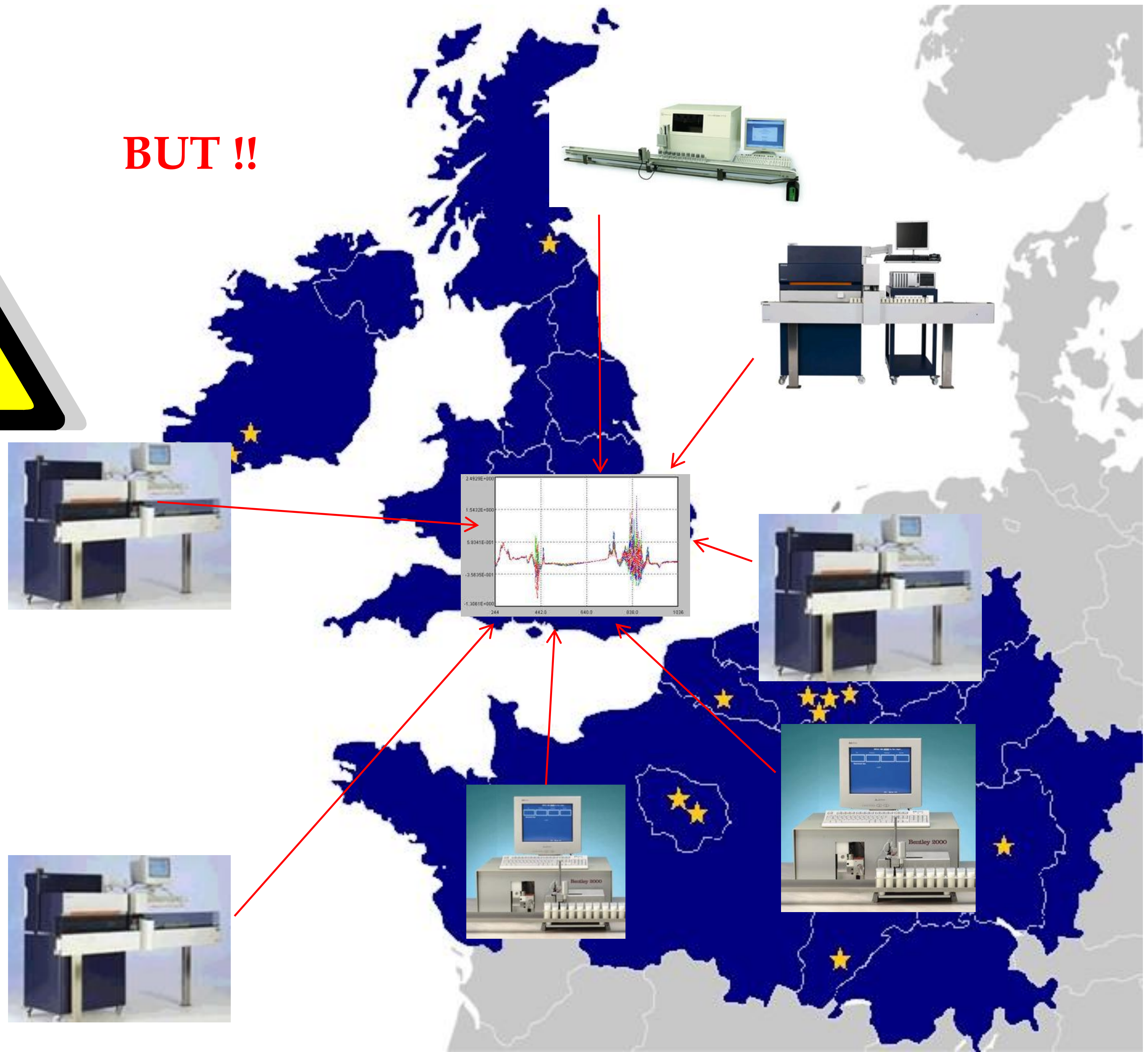
Wallonie

OptiMIR

BUT !!



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Because of differences between the instrumental responses of different MIR spectrometers, and because of changes in the instrumental response of a spectrometer over time, the use of calibration models developed at a certain time on a certain instrument with MIR spectra obtained on the same instrument after a period of time, or on another instrument, will usually lead to erroneous results.

Inconvenient to recalibrate instruments or may want to utilize a historical database.

Standardization procedures are needed

A decision needs to be made which instrument will be declared as **MASTER** instrument, the remaining instruments will be used as **SLAVE** instruments.

An own unique **standardization model for every master-slave** combination needs to be designed, describing the shift between the particular slave instrument and the master instrument

In order to be able to perform data standardization between the master and a slave instrument, an equal amount of measurements have to be done with both instruments.

New measurements will be later standardized using the standardization models built.

STANDARDIZATION APPROACHES

Find a transformation that maps the response of the slave instrument onto the master instrument

Direct and piece-wise direct standardization

…

Process the data from both instruments in a way that makes the differences disappear

baselining and derivatizing

multiplicative scatter correction, FIR filtering

orthogonal signal correction

prediction augmented classical least squares

generalized least squares

explicit deresolution

…

PIECE-WISE DIRECT STANDARDIZATION (PDS)

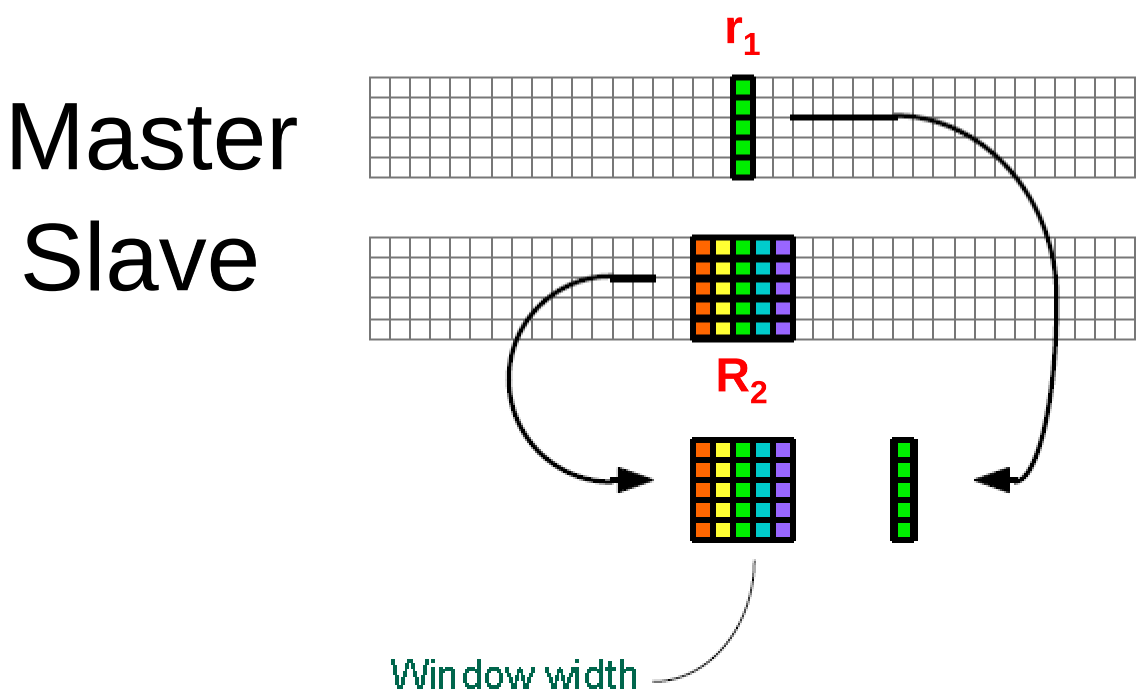
Proposed by Wang et al.

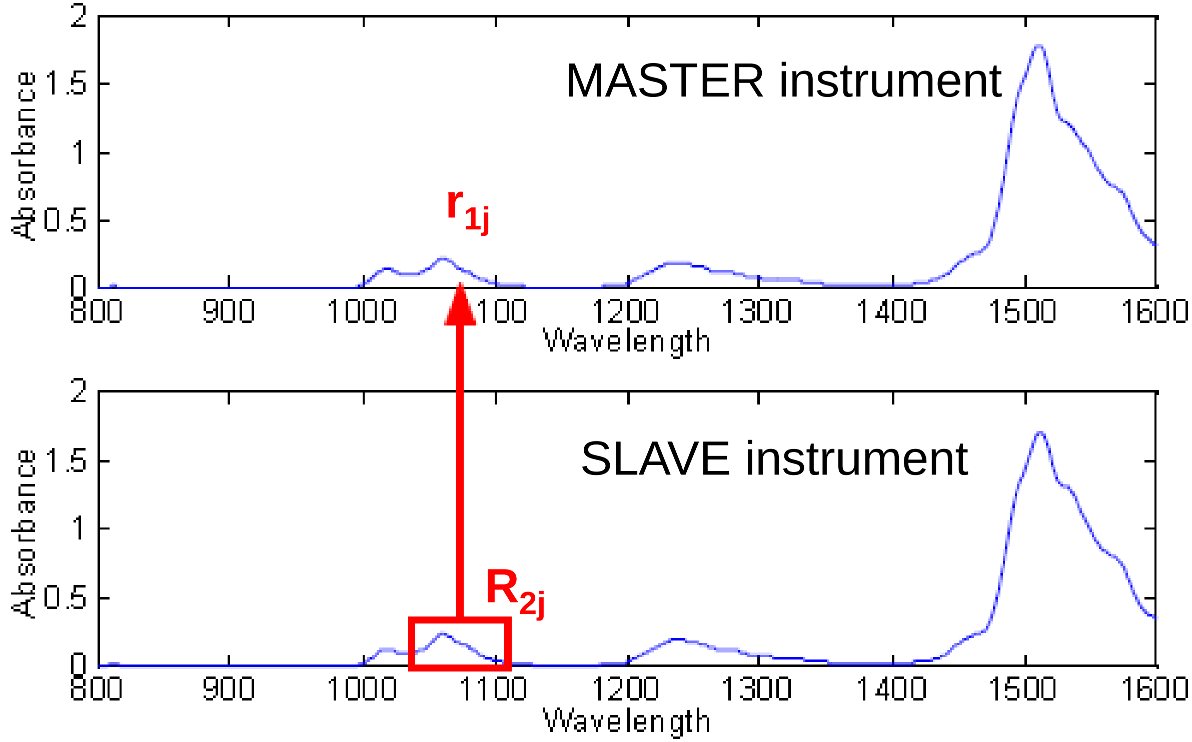
This method transfers the MIR spectra from the instrument on which they were collected ('slave') to the instrument on which the calibration model was developed ('master').

PDS is based on the fact that the spectral information contained in a certain wavelength on the master instrument is highly correlated to the spectra of neighbor wavelengths on the slave instrument.

PIECE-WISE DIRECT STANDARDIZATION (PDS)

The PDS method is based on the fact that the spectral variation of spectroscopic data is limited to small regions. In PDS, the response **r_1** of the standardization samples measured at wavelength **j** on the 'master' instrument is related to the wavelengths located in a small window (**R_2**) around j (neighbouring) measured on the 'slave' instrument:

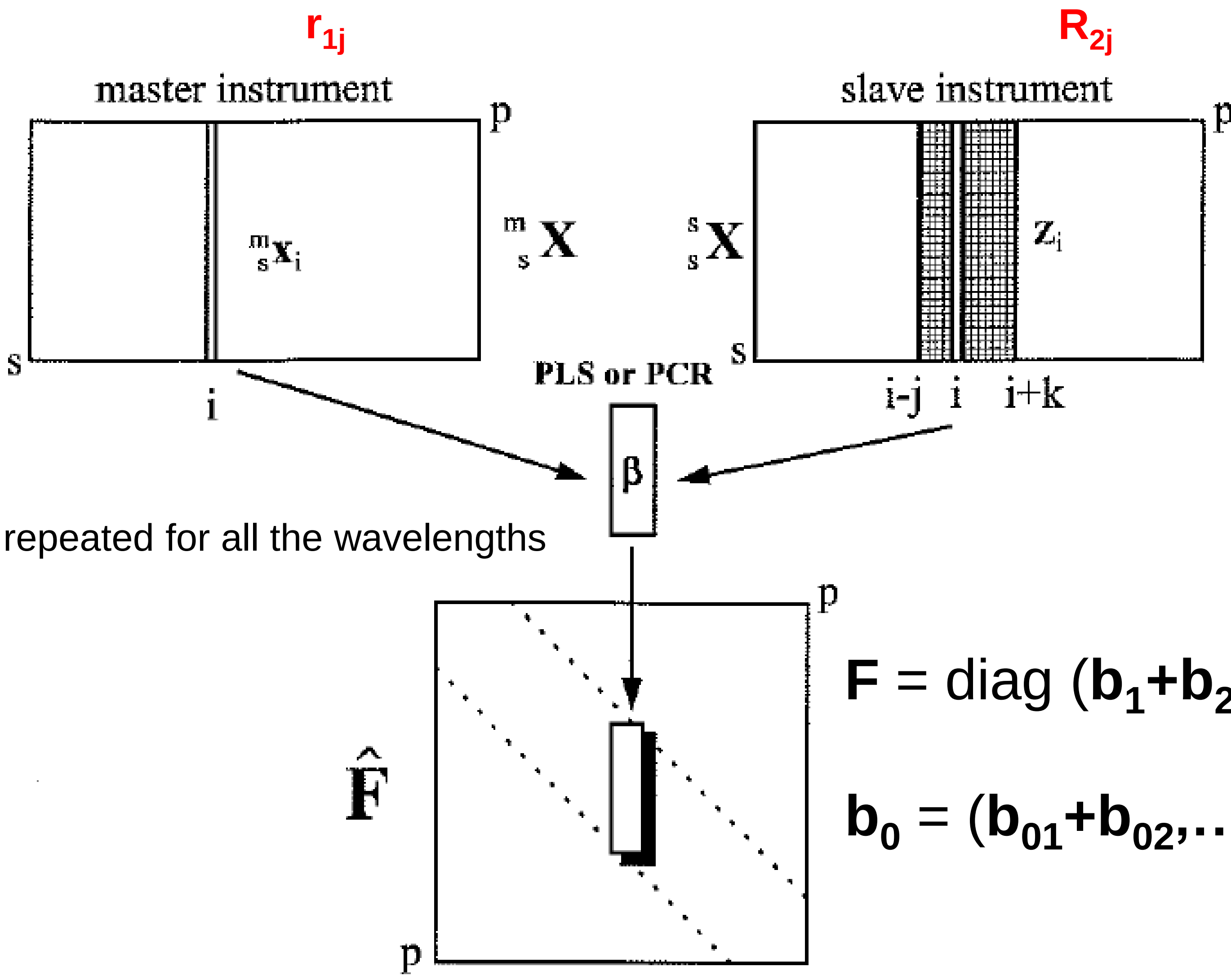




$$r_{1j} = R_{2j}\, b_j + b_{0j}$$

Where $\mathbf{R_{2j}}$ is the localized response matrix of the transfer samples and $\mathbf{b_j}$ is the vector of transformation coefficients for the j^{th} wavelength and $\mathbf{b_{0j}}$ is the offset term.

The regression vectors (b) can be calculated by PCR or PLS method



$F = \text{diag}\,(b_1 + b_2, \ldots, b_i, \ldots, b_n)$

$b_0 = (b_{01} + b_{02}, \ldots, b_{0i}, \ldots, b_{0n})$

Source: PhD thesis H. Swierenga, Univ. Wageningen, NL (2000)

The F matrix and the b_0 vector are used to correct new spectra measured in the slave instrument, **$r_{2,unk}$**

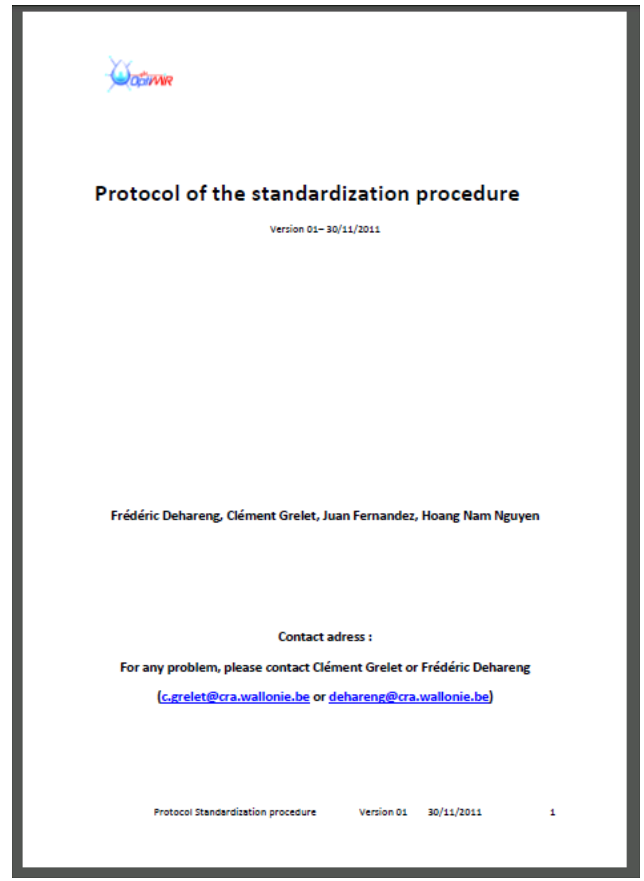
$$(\mathbf{R}_{\mathbf{2,unk}})_{\mathbf{std}} = r_{2,unk}\,\mathbf{F}+\mathbf{b}_{\mathbf{0}}$$

SOME RESULTS

OptiMIR Standardization of February – March 2012

- 25 laboratories
- 50 instruments
- 600 samples

Master FOSS (Battice Foss05009)



Protocol of the standardization procedure

Version 01– 30/11/2011

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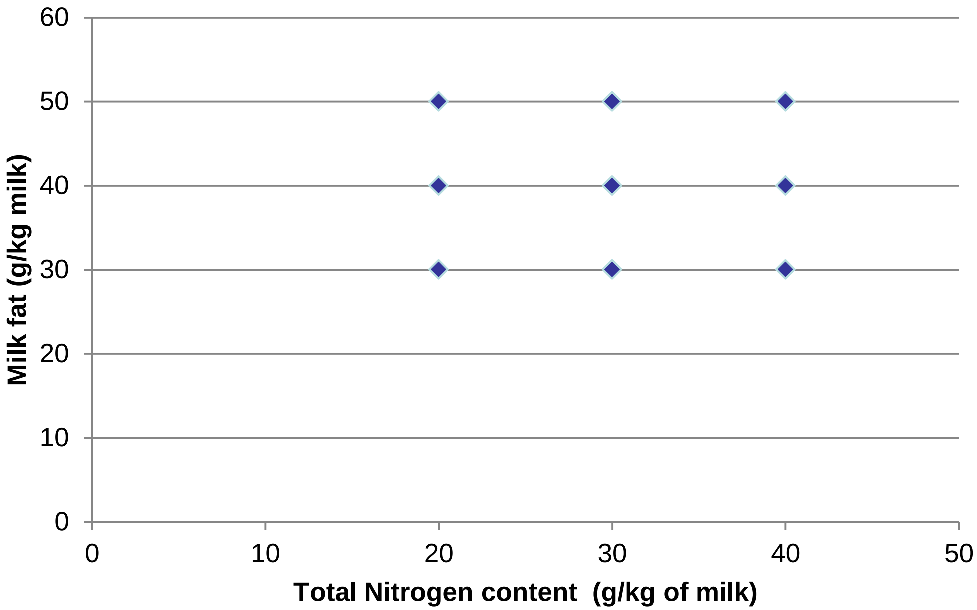
Protocol Standardization procedure Version 01 30/11/2011 1

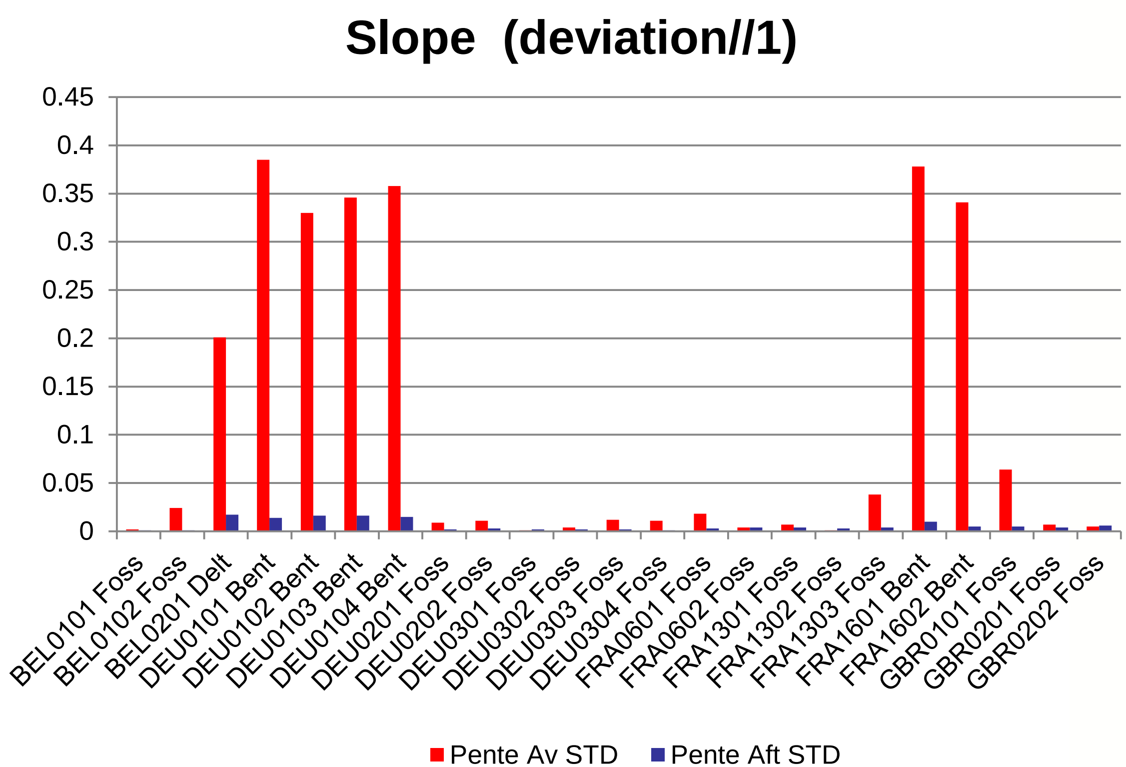


+ raw milk sample
+ sucrose sample
+ standard sample (blank)

STANDARDIZATION - MODEL

(February 2012)

		BEFORE STD	AFTER STD
	Brand	Pente Master//Slave	P Master//Slave
BEL0101	Foss	1.002	1.001
BEL0102	Foss	0.976	1.001
BEL0201	Delta	0.799	0.983
DEU0101	Bentley	0.615	1.014
DEU0102	Bentley	0.670	1.016
DEU0103	Bentley	0.654	1.016
DEU0104	Bentley	0.642	1.015
DEU0201	Foss	0.991	1.002
DEU0202	Foss	0.989	0.997
DEU0301	Foss	1.001	0.998
DEU0302	Foss	1.004	0.998
DEU0303	Foss	0.988	0.998
DEU0304	Foss	0.989	1.001
FRA0601	Foss	1.018	0.997
FRA0602	Foss	0.996	0.996
FRA1301	Foss	1.007	0.996
FRA1302	Foss	1.001	0.997
FRA1303	Foss	1.038	0.996
FRA1601	Bentley	0.622	1.010
FRA1602	Bentley	0.659	1.005
GBR0101	Foss	1.064	0.995
GBR0201	Foss	1.007	0.996
GBR0202	Foss	1.005	0.994



Master FOSS

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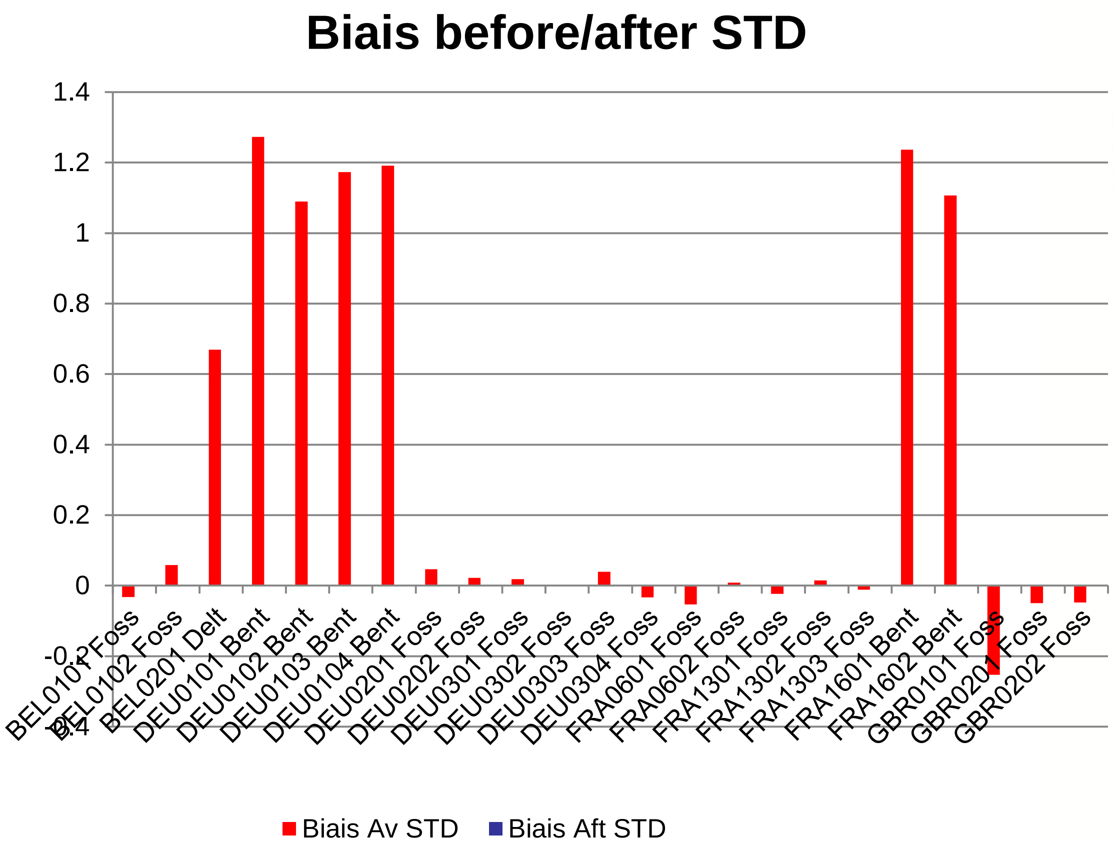
STANDARDIZATION - MODEL

(February 2012)

		BEFORE STD	AFTER STD
	Brand	Biais Master//Slave	Biais Master//Slave
BEL0101	Foss	-0.0324	0.0000
BEL0102	Foss	0.0583	0.0000
BEL0201	Delta	0.6689	0.0000
DEU0101	Bentley	1.2731	0.0000
DEU0102	Bentley	1.0893	0.0000
DEU0103	Bentley	1.1728	0.0000
DEU0104	Bentley	1.1917	0.0000
DEU0201	Foss	0.0466	0.0000
DEU0202	Foss	0.0217	0.0000
DEU0301	Foss	0.0185	0.0000
DEU0302	Foss	-0.0007	0.0000
DEU0303	Foss	0.0391	0.0000
DEU0304	Foss	-0.0332	0.0000
FRA0601	Foss	-0.0534	0.0000
FRA0602	Foss	0.0082	0.0000
FRA1301	Foss	-0.0232	0.0000
FRA1302	Foss	0.0144	0.0000
FRA1303	Foss	-0.0115	0.0000
FRA1601	Bentley	1.237	0.0000
FRA1602	Bentley	1.1067	0.0000
GBR0101	Foss	-0.2532	0.0000
GBR0201	Foss	-0.0496	0.0000
GBR0202	Foss	-0.0479	0.0000

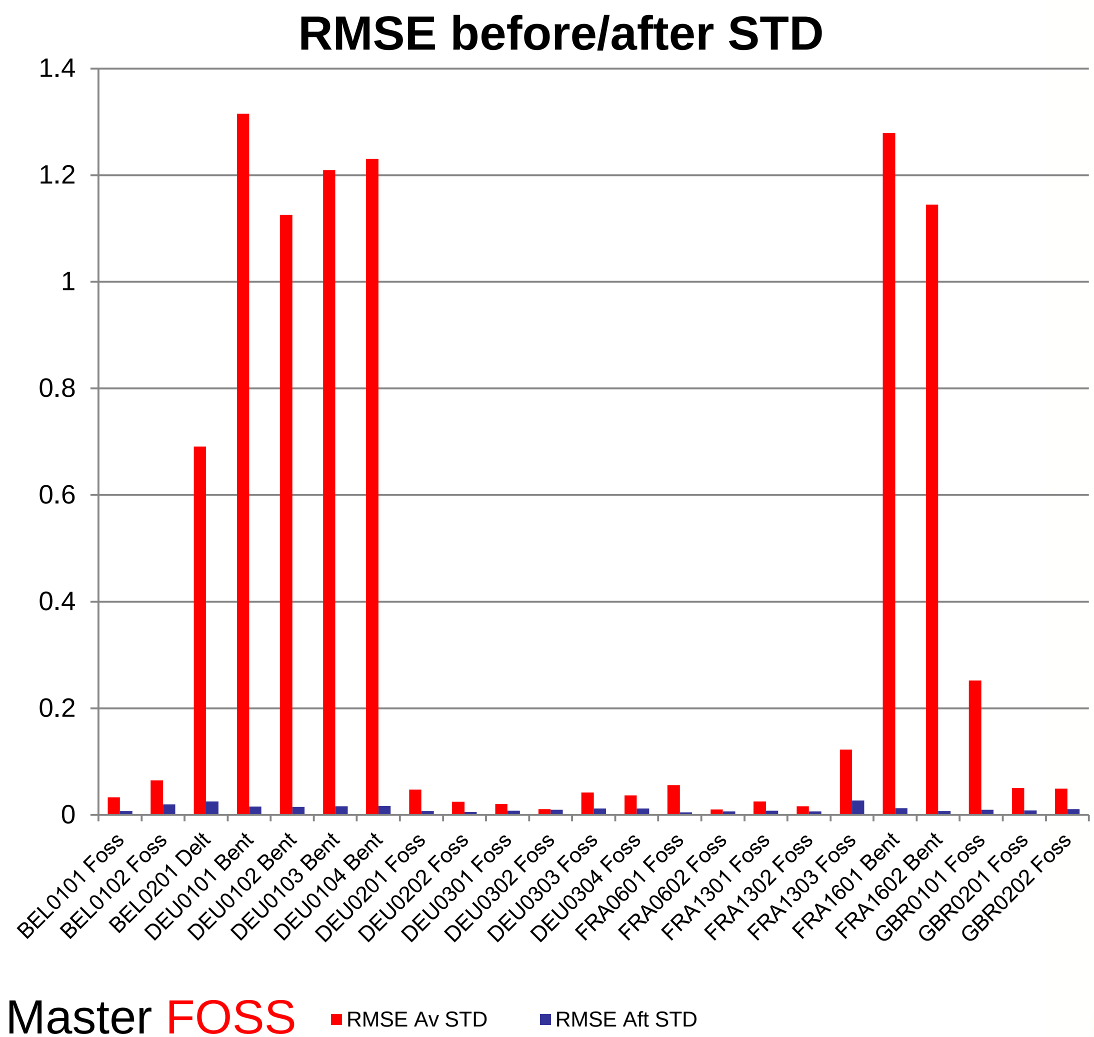


Master FOSS

STANDARDIZATION - MODEL

(February 2012)

		BEFORE STD	AFTER STD
	Brand	RMSE Master//slave	RMSE Master//slave
BEL0101	Foss	0.0331	0.0073
BEL0102	Foss	0.0648	0.0198
BEL0201	Delta	0.6908	0.0249
DEU0101	Bentley	1.315	0.0154
DEU0102	Bentley	1.1253	0.0152
DEU0103	Bentley	1.2096	0.0163
DEU0104	Bentley	1.2303	0.0168
DEU0201	Foss	0.0474	0.0074
DEU0202	Foss	0.0245	0.0055
DEU0301	Foss	0.0201	0.0078
DEU0302	Foss	0.0108	0.0098
DEU0303	Foss	0.0421	0.0117
DEU0304	Foss	0.0364	0.0117
FRA0601	Foss	0.0557	0.0047
FRA0602	Foss	0.0103	0.0064
FRA1301	Foss	0.0250	0.0076
FRA1302	Foss	0.0159	0.0064
FRA1303	Foss	0.1226	0.0272
FRA1601	Bentley	1.2788	0.0123
FRA1602	Bentley	1.1446	0.0073
GBR0101	Foss	0.2521	0.0097
GBR0201	Foss	0.0506	0.0084
GBR0202	Foss	0.0489	0.0108



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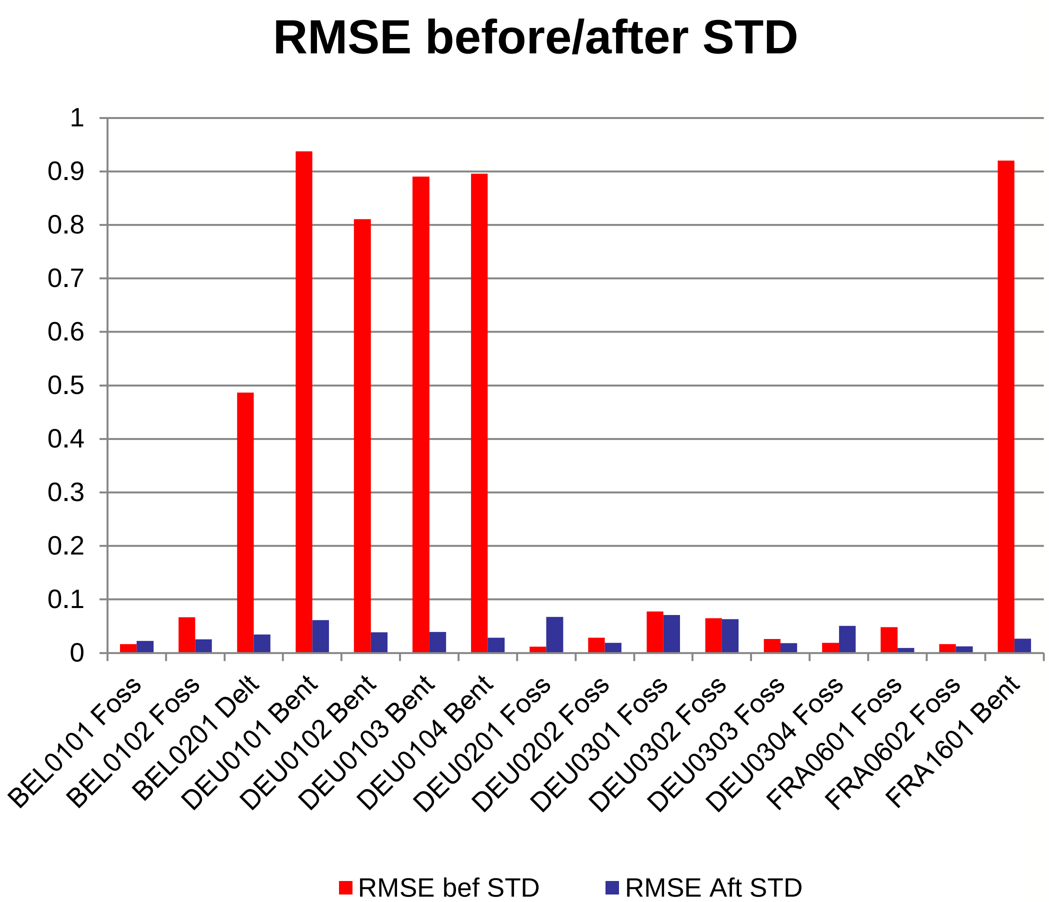
STANDARDIZATION - VALIDATION

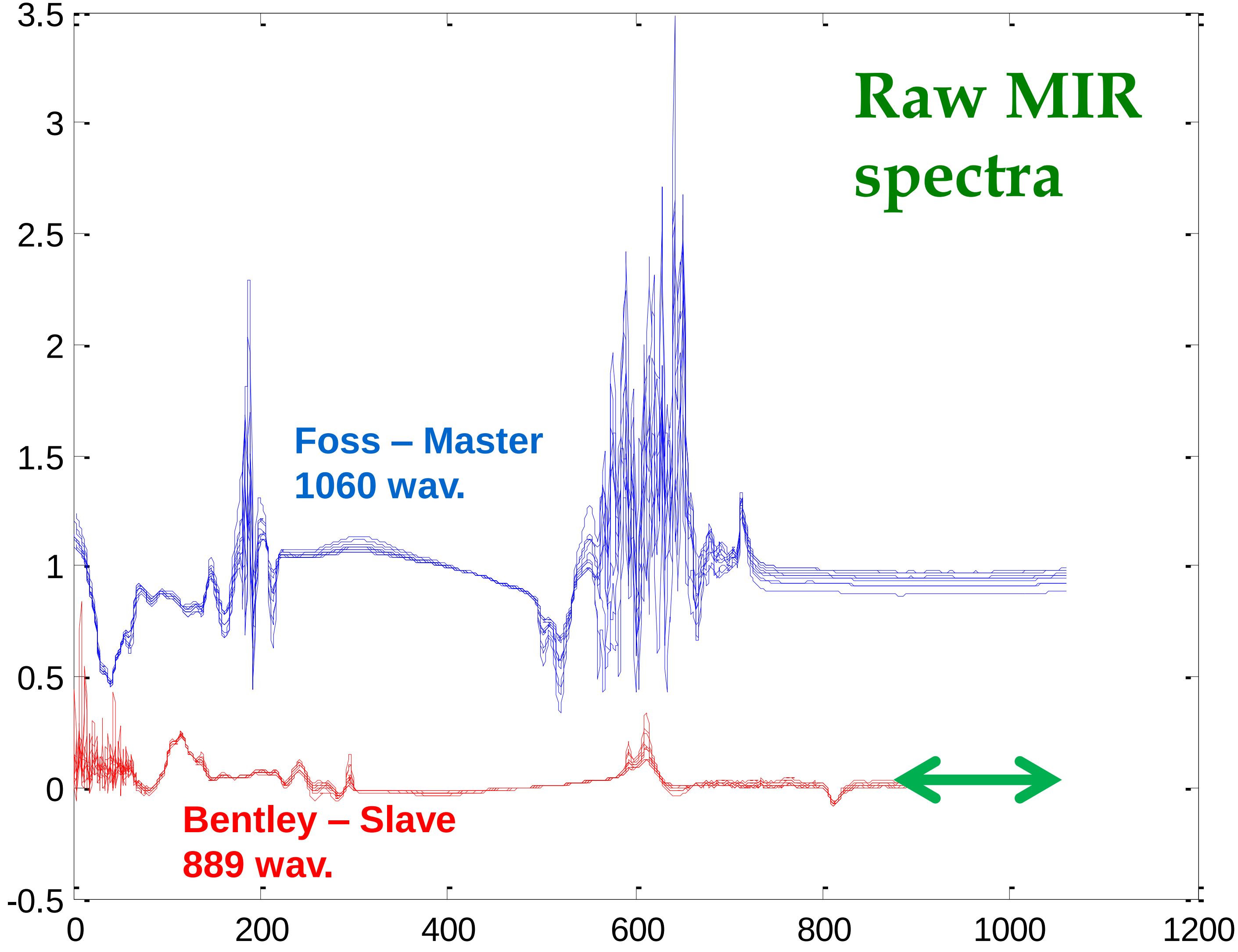
(March 2012)

	Brand	BEFORE STD RMSE Master//slave	AFTER STD RMSE Master//slave
BEL0101	Foss	0.0166	0.0226
BEL0102	Foss	0.067	0.0257
BEL0201	Delta	0.4864	0.0344
DEU0101	Bentley	0.9375	0.0614
DEU0102	Bentley	0.8107	0.0385
DEU0103	Bentley	0.8902	0.0395
DEU0104	Bentley	0.8957	0.0286
DEU0201	Foss	0.0116	0.0671
DEU0202	Foss	0.0288	0.0192
DEU0301	Foss	0.0778	0.0709
DEU0302	Foss	0.0652	0.0629
DEU0303	Foss	0.0263	0.0182
DEU0304	Foss	0.0189	0.0505
FRA0601	Foss	0.0485	0.0095
FRA0602	Foss	0.0165	0.0126
FRA1601	Bentley	0.9205	0.0266
Mean		0.3324	0.0368



Master FOSS

STANDARDIZATION - EXAMPLE



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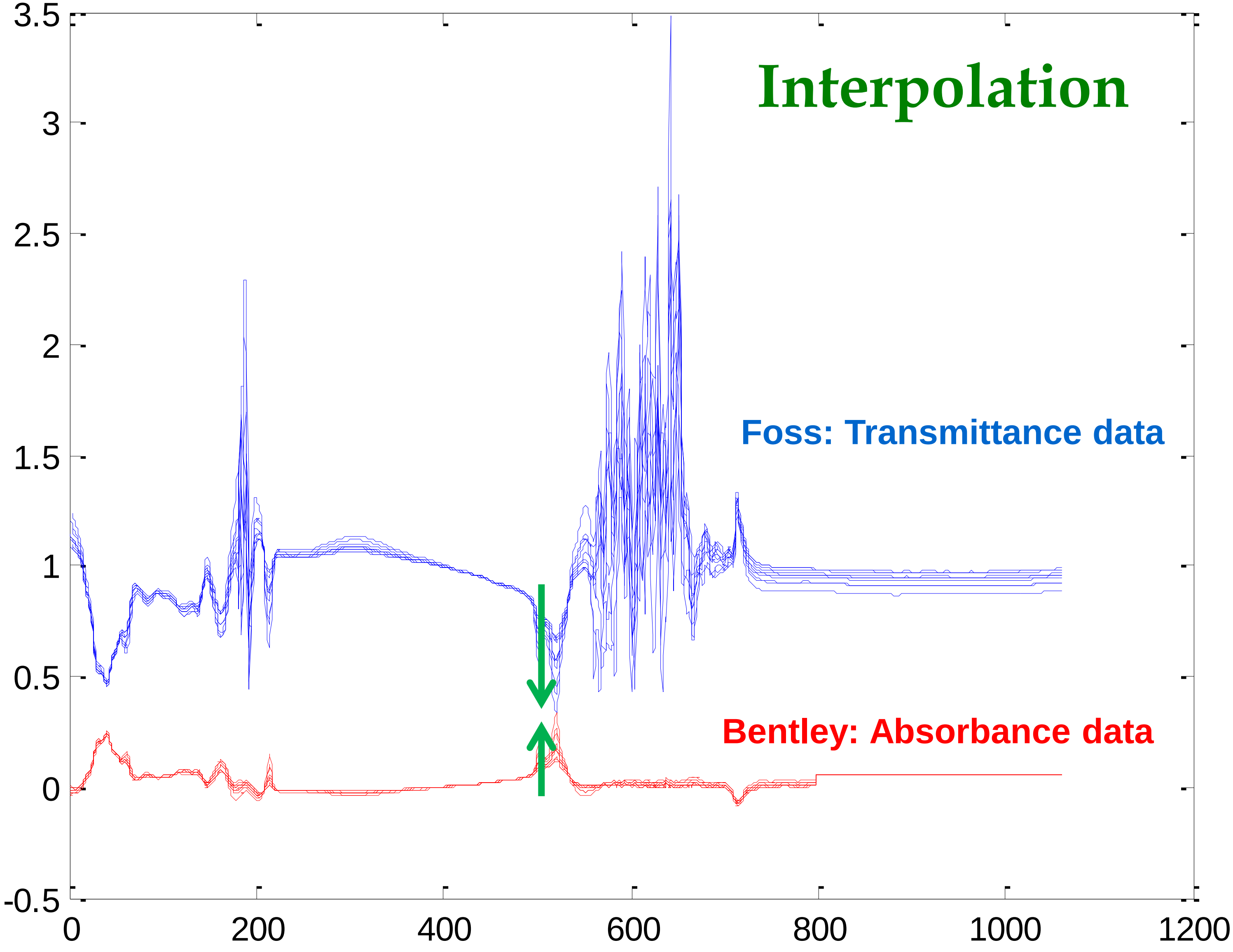
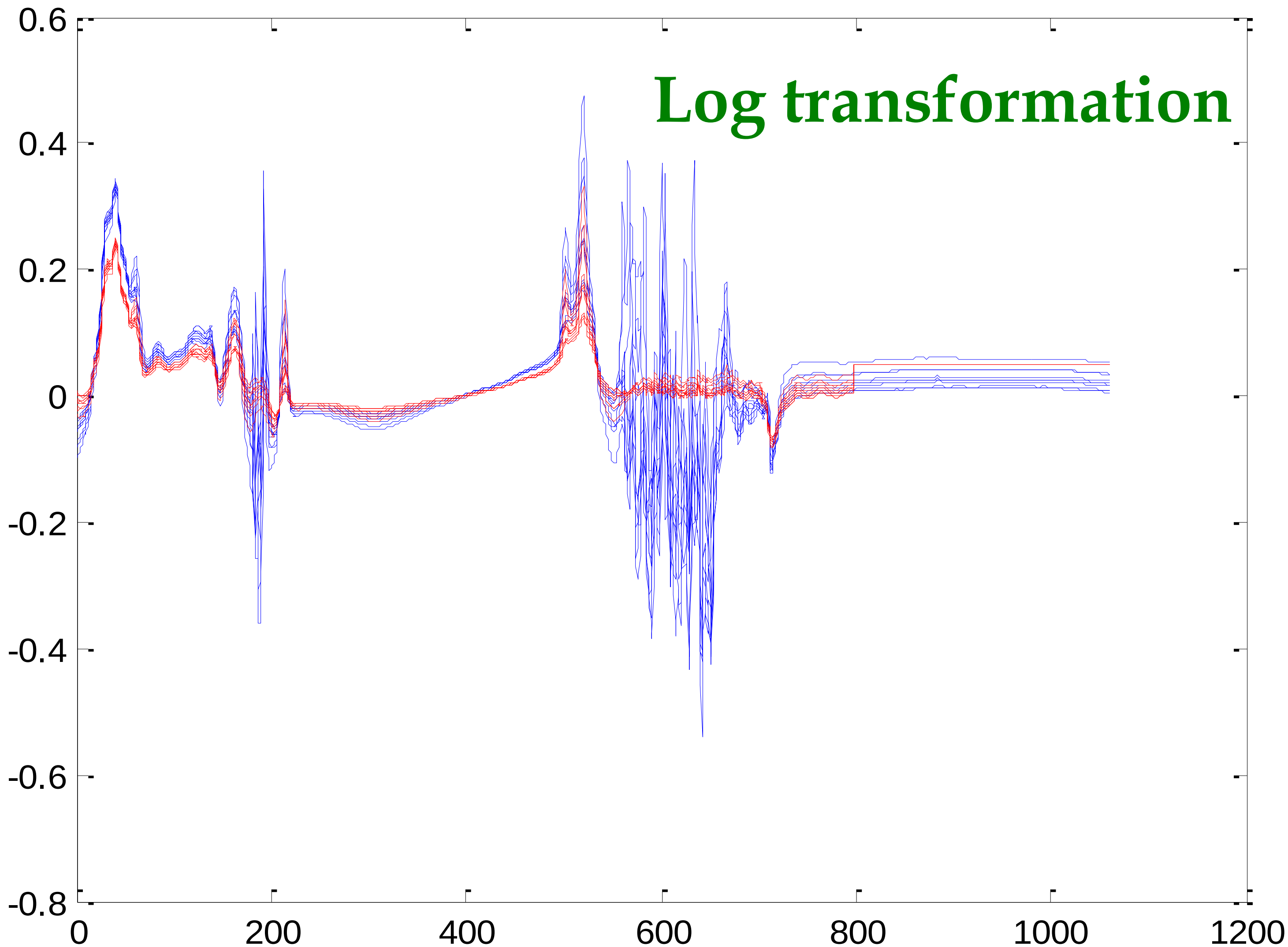
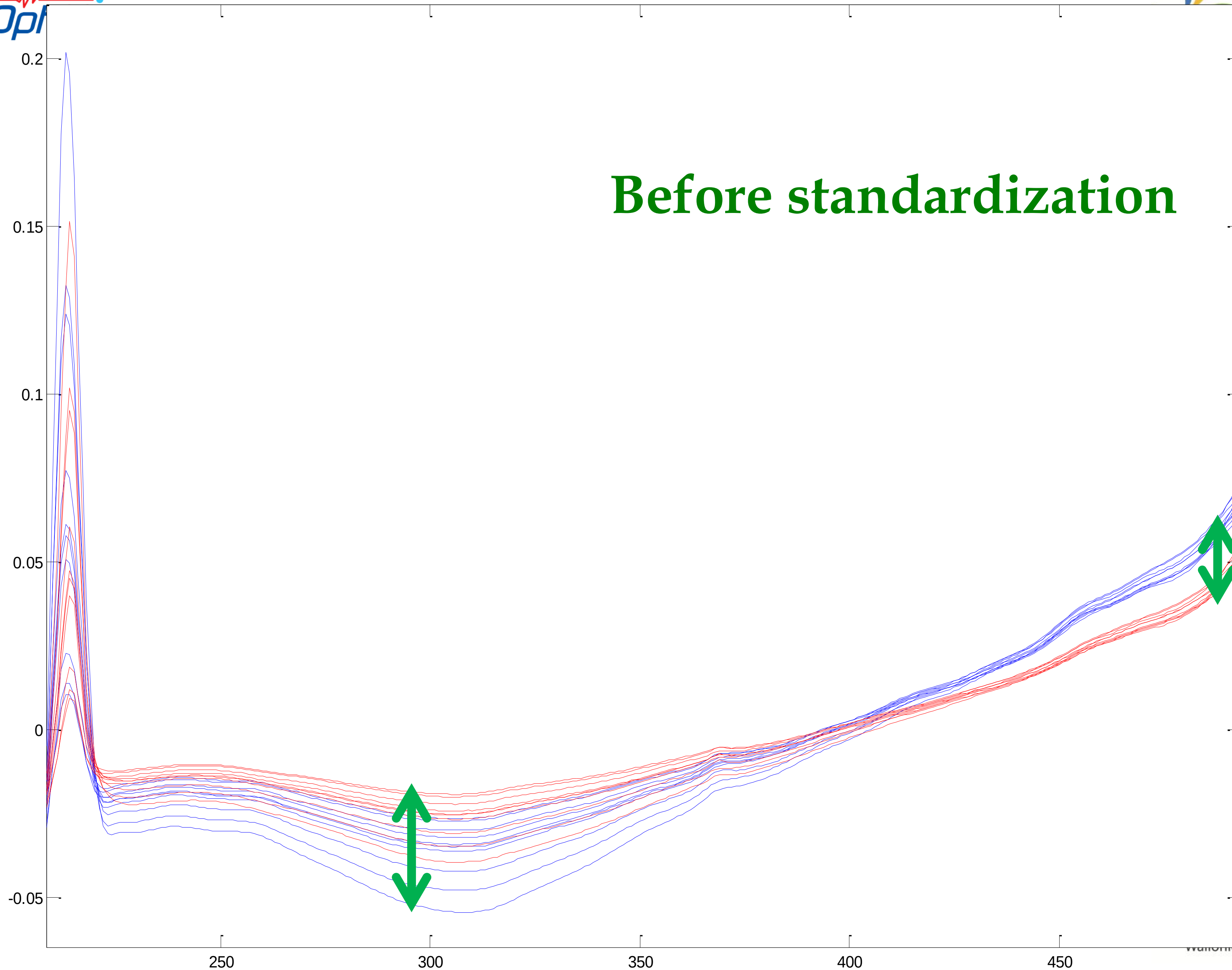
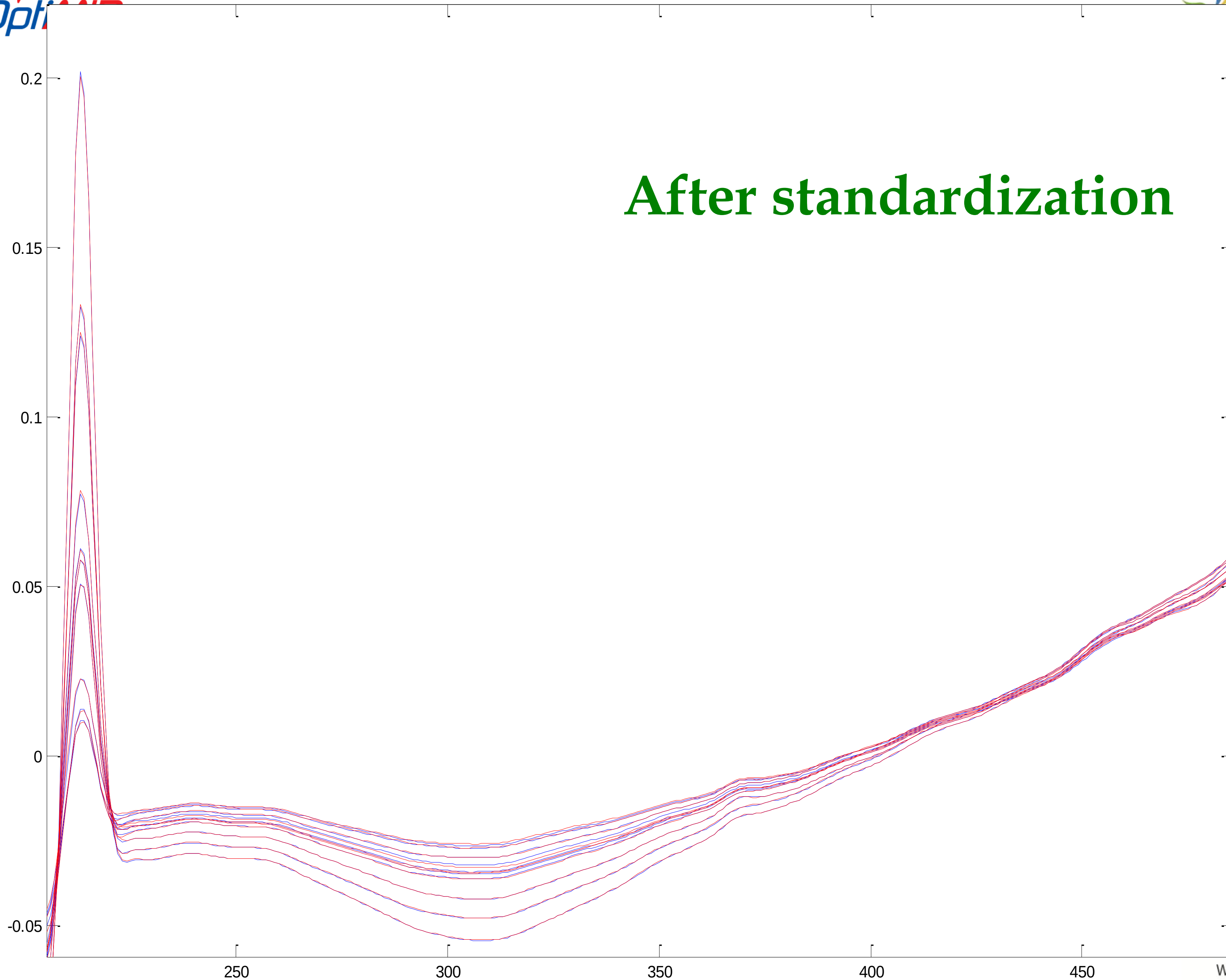
STANDARDIZATION - EXAMPLE



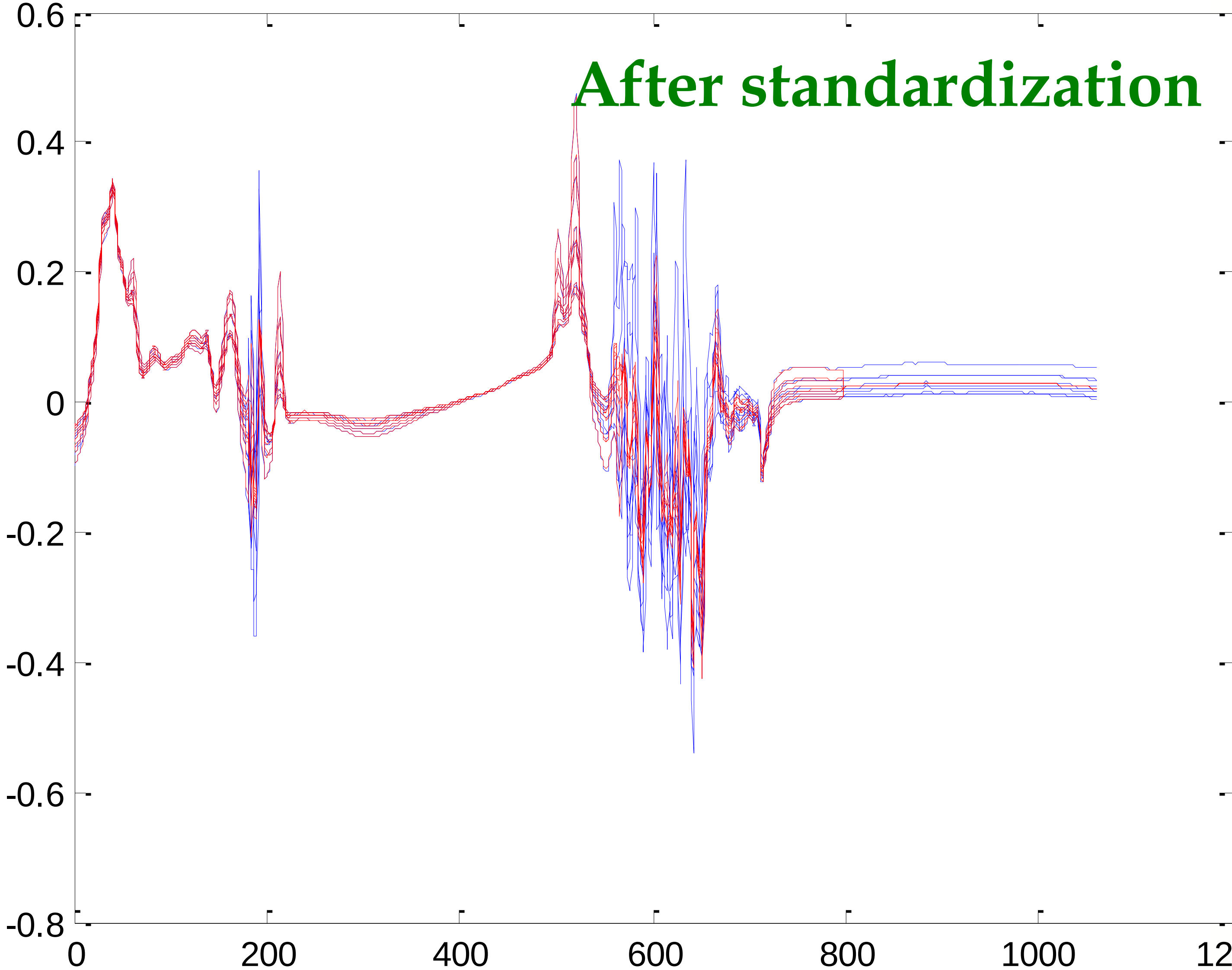
Log transformation




Before standardization
0.2
0.15
0.1
0.05
0
-0.05
250
300
350
400
450

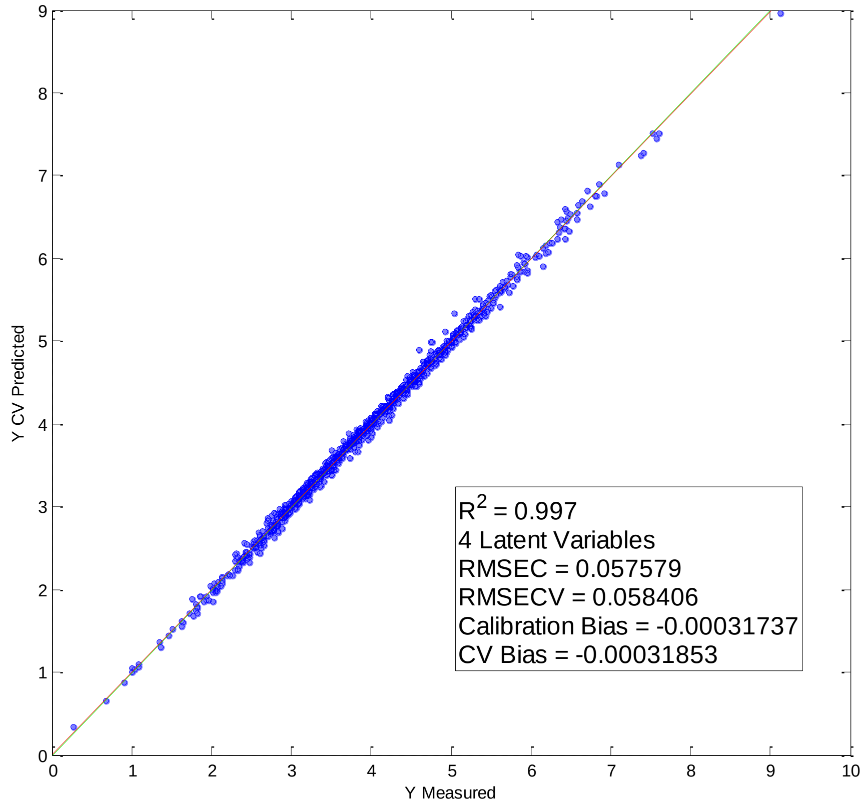


After standardization
0.2
0.15
0.1
0.05
0
-0.05
250
300
350
400
450

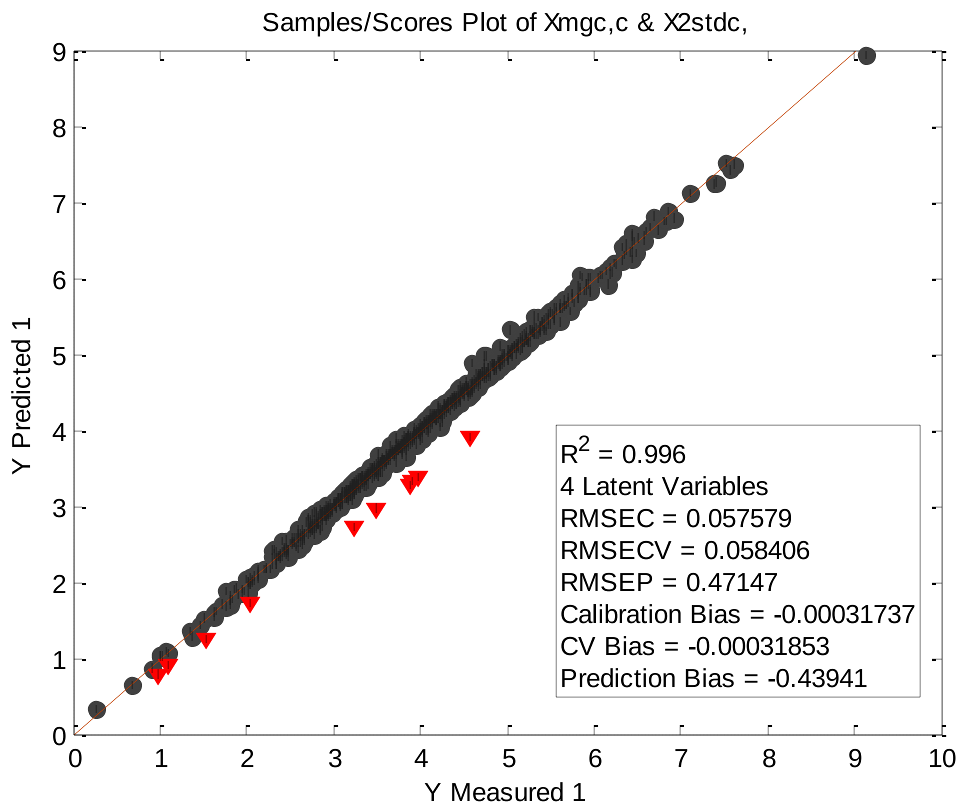

After standardization
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
200
400
600
800
1000
1200

1236 spectra with reference values

Fat content equation



DELTA slave
(CRA-W Delta)



RMSEP: 0.4715

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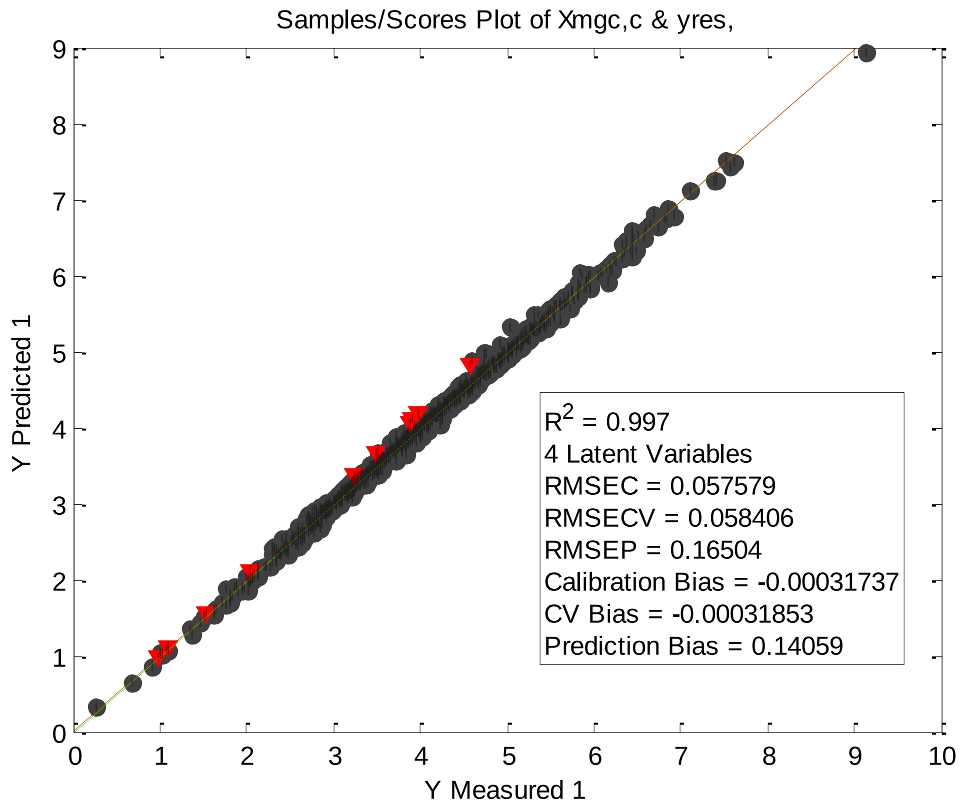
DELTA slave

(CRA-W Delta)



RMSEP: 0.1650

CONCLUSIONS

The standardization correction using PDS seems to work correctly during time for the different slave instruments available, including different brands.

The use of this standardization method is a crucial step for the OptiMIR project because it will allow the use of only one single equation by property for all the different instruments.

Useful to pool the resources of milk recording organizations and research centres and MIR milk spectra to be used as indicator of the cows' status.

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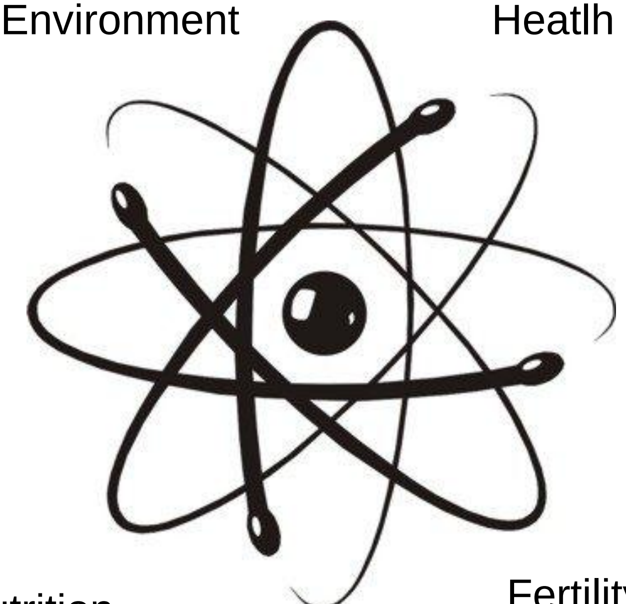
SAC



teagasc

Agriculture and Food Development Authority

INSTITUT DE L'ELEVAGE

gembloux agro bio tech

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http://www.optimir.eu

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