Calibration Transfer from dispersive to FT instruments

Dardenne P., Lecler B., Mouteau A., Baeten V. ; *Centre wallon de Recherches agronomiques, Gembloux, Belgium*

Many research centres and industries have developed during the last decades important data sets (thousands of spectra) associated with reference methods. When new instruments arrive the market, there is an evident interest to be able to use the "historical" information and avoid new calibration developments and costly reference method analyses. This work presents a methodology to transfer data sets from a dispersive instrument to a FT instrument. The transferability and the performances of the PLS models are evaluated on the basis of a collaborative study.

Calibration Transfer : Steps of transfer spectral data between an instrument H to a target instrument T:

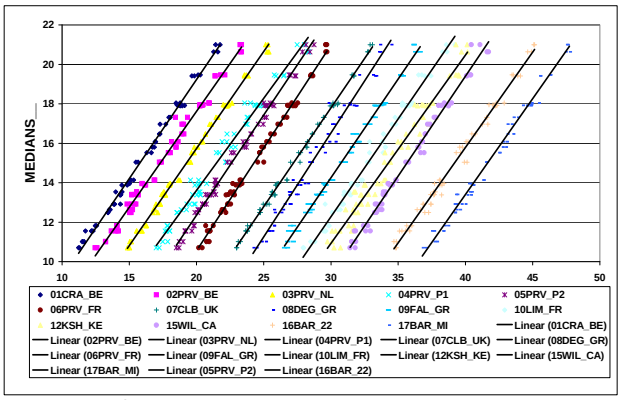
1. Scan on both instruments 30 sealed cups (type H)
2. Convert the data from T in nanometer
3. Generate a correction matrix between H and T
4. Transform the data base (DB) from H to T
5. Scan 20 times one average sample on instrument T with cup H and 20 times with cup T
6. Average the 20 readings and calculate the difference
7. Remove the difference from the DB
8. Transform the DB in cm-1
9. Add few spectra of the products directly scanned on T
10. Recalibrate within the T software (OPUS)

Stats of the "INGOT®" Models

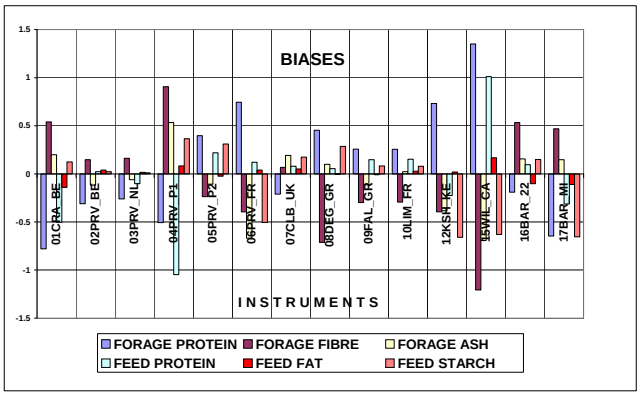
GRASS SILAGE AND FORAGE (DM basis)							PLS
Constituent	N	Mean	MIN	MAX	SECV	R2CV	TERMS
Moisture	6624	6.9	1	13	0.75	0.85	14
PROTEIN	**7680**	**15.5**	**2**	**31**	**0.88**	**0.97**	**14**
FIBRE	**6349**	**26.6**	**12**	**41**	**0.92**	**0.96**	**15**
ASH	**8019**	**10.6**	**4**	**18**	**0.86**	**0.87**	**16**
NDF	2379	47.7	26	70	1.86	0.94	14
ADF	1658	27.8	13	43	1.24	0.94	15
ADL	1522	3.5	0	9	0.48	0.92	14
OMDauf	2126	69.6	37	80	2.62	0.94	14
COMPLETE FEED (Asis Basis)							
Protein	**19565**	**19.5**	**4**	**35**	**0.82**	**0.98**	**12**
Fibre	5571	5.8	0	16	0.73	0.95	17
Fat	**8965**	**5.0**	**0**	**15**	**0.47**	**0.98**	**16**
Ash	13646	7.0	0	14	1.13	0.80	18
Starch	**1326**	**24.4**	**0**	**67**	**1.61**	**0.99**	**11**

Collaborative study: 30 dried and ground grass silages and 27 ground complete feed samples have been prepared in CRA-W, Gembloux, BE. Each sample was carefully split in 20 bags of 120 gr (forage) and 150 gr (feed). Before sealing the bags in a vacuum device, the content of each bag have been scanned in duplicate on a BRUKER MPA instrument to check the homogeneity before shipment ((30+27)spl*20*2=2280 spectra). We collected 16 sets of 60 forage spectra and 54 feed spectra from 16 different BRUKER instruments, 14 MPA, 1 Matrix I and 1 FT22N spread in 10 countries and 3 continents. The data of 2 instruments were removed due to technical problems. The results are based on 14 instruments. The next table sum up the **results**: RMS are mostly affected by biases. SEPC (standard deviation of the residuals) are very good with the same order as the standard deviations of the replicates. Biases are significant and models need tp be corrected for some instruments. There was quite wide variation in the STD of Replicates indicating variation in the carfullness in the way the cups are filled. Slopes can be significant (<>1) but they

	FORAGE			FEED		
	ASH	PROTEIN	FIBRE	FAT	PROTEIN	STARCH
SCEV of calbration models	0.86	0.88	0.92	0.47	0.82	0.73
STD of bags before shipment (one instr.)		0.301		0.157	0.292	
STD of REPLICATES (within Instruments)	0.376	0.298	0.530	0.158	0.424	0.694
RMS vs Medians (quadratic average)	0.459	0.684	0.709	0.144	0.562	0.702
SEPC vs Medians corrected for bias (qua. Ave.)	0.321	0.342	0.456	0.123	0.358	0.603
Average of absolute values of the Biases	0.250	0.507	0.455	0.060	0.292	0.293
STD of Biases	**0.336**	**0.609**	**0.564**	0.081	**0.452**	**0.379**
Average R2	0.960	0.987	0.962	0.998	0.993	0.996



Protein in forage predicted with the same model – 14 instrument responses vs medians



Biases for 14 instruments calculated from the medians of the 14 instruments

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Centre wallon de Recherches agronomiques
Chaussée de Namur, 24 – 5030 GEMBLOUX - Tél :++ 32 (0) 81 62 03 50 - Fax : ++ 32 (0) 81 62 03 88
dptqual@cra.wallonie.be - http://cra.wallonie.be