TAKE HOME MESSAGES

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NIR 2015 Brazil

Topics	N titles	%
01. Fundamentals / Spectroscopy	4	1.5
02. Chemometrics	31	11.7
03. Instrumental Development	10	3.8
04. Hyperspectral Imaging	30	11.3
05. Portable Instruments: Application,	24	9.0
06. Forensic	6	2.3
07. Wild Live/Ecology/Environmental	25	9.4
08. Agriculture and food	100	37.6
09. Pharmaceutical	9	3.4
10. Petrochemical/Polymers	7	2.6
11. Biochemical/ Biomedical Applicati	7	2.6
12. Others	13	4.9
	266	

WILD LIFE

OP11 In vivo sex identification of the endangered Mississippi Gopher Frog (Lithobates sevosa) using Near Infrared Reflectance Spectroscopy

Carrie Vance, Katie Graham, Andrew Kouba, Scott Willard
Mississippi State University-Biochemistry, Molecular Biology, Plant Pathology and Entomology - United States

OP14 Simulation method design to link the spectral properties of dense microalgal culture to cell physiology

Ryad Bendoula, Sarah Bellini, Jean-Michel Roger – France
Irstea - UMR ITAP

AGRICULTURE AND FOOD

OP18 The impossible made possible: providing a detailed topological map of chemical classification parameters for pork carcasses with on-line slaughter line instrumentation

Klavs Sørensen, Søren Balling Engelsen

University of Copenhagen - Department of Food Science - Spectroscopy & Chemometrics - Denmark

OP19 Evolution of Vis/NIR bulk optical properties of apple skin and flesh during fruit maturation

Robbe Van Beers, Ben Aernouts, Rodrigo Watté, Ann Schenk, Bart Nicolai, Wouter Saeys

KU Leuven Department of Biosystems, MeBioS, Leuven - Belgium

HANDHELD INSTRUMENTS

OP32 Evaluation of portable NIR instruments for discrimination of 6 similar tropical wood species by PLS-DA

Maria Cecilia Bergo, T.C.M. Pastore, V.T.R. Coradin, D.C. da Silva, L.F. Soares, Jez W.B. Braga

Chemistry Institute, University of Brasília, Brasília - Brazil

OP36 Near-infrared spectroscopy using a supercontinuum laser - application to long-wavelength transmission spectra of barley seeds

Tine Ringsted, S. Dupont, J, Ramsay, S.R. Keiding, S. B. Engelsen

University of Copenhagen - Faculty of Sciences - Department of Food Science, Spectroscopy and Chemometrics - Denmark

IMAGING

OP39 Quality control of herbal medicines through Hyperspectral imaging: species discrimination and adulteration detection

Ilze Vermaak, Maxleene Sandasi, Sidonie Tankeu, Alvaro Viljoen
Tshwane University of Technology -South Africa

OP44 Intuitive, semi-supervised training of the segmentation of hyperspectral images

Jeroen van Roy, Niels Wouters, Bart De Ketelaere, Wouter Saeys
KU Leuven, Department of Biosystems, MeBioS - Belgium

CHEMOMETRICS

OP52 New tools to solve large complexity in large scale soil NIR libraries thought the use of memory-based learning

Leonardo Ramirez-Lopez, Antoine Stevens

Swiss Federal Institute of Technology (ETH) Zurich - Switzerland

FUNDAMENTALS/BIOCHEMICAL

OP54 Retrieving Beer-Lambert law absorbance of highly scattering materials by combining Light Polarization Spectroscopy and the Representative Layer Theory

Alexia Gobrecht, Ryad Bendoula, Jean-Michel Roger, Véronique Bellon-Maurel

Irstea - UMR ITAP - France

AGRICULTURE & FOOD

PASQUINI C. & al. : 1 oral and 15 posters

PIMENTEL M.F. & al. : 1 oral and 15 posters

Jean-Michel Roger, Irstea

Soren Engelsen, U. Copenhagen

Wouters Saeys, U. Leuven

NIR News

Some considerations about NIR spectroscopy: Closing speech at NIR-2009

Pierre Dardenne, ICNIRS Chairman
Walloon Agricultural Research Centre (CRA-W), Quality of Agricultural Products Department, Chaussée de Namur n°24, 5030 Gembloux, Belgium. E-mail: dardenne@cra.wallonie.be

	Calibration results	
	PRODUCT	Wheat
1	Parameters	PROT
2	Units	%DM
3	SEL-Reproductibility	0.25
4	N	65
5	Outliers	0
6	Min	6.39
7	Mean	10.9
8	Max	15.08
9	SD	1.59
10	R2C	0.96
11	R2CV	0.94
12	SEC	0.33
13	SECV	0.38
14	NIR_repeatabilty	0.19
15	RPDC	4.82
16	RPDCV	4.18
17	Number of terms	4
18	Segments of CV	4
	Loo,Rnd, Sys, Block,..	blocks
19	WL-Range/step	1100-2498/2
20	Pretreatment (s)	SNVD-144

Validation results	
PRODUCT	Wheat
Parameters	PROT
Units	%DM
N	20
Outliers	1
Min	6
Mean	10
Max	4
SD	1.41
R2P	0.95
RMSEP	0.45
SEP	0.41
RSD	0.35
NIR_repeatabilty	0.19
RPDP (SDyCal/SEP)	3.95
BIAS	-0.11
INTERCEPT	0.11
SLOPE	0.89
AveGH	5.6
AveNH	2.5

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ISO 12099:2010

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

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3 hypothesis tests:

BIAS ≠ 0 ?

SLOPE ≠ 1 ?

SEP ≠ SECV ?

ISO 17025

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IN CASE OF A PERFECT GAUSSIAN DISTRIBUTION OF THE RESIDUALS

JUST REMOVED OUTLIERS ONCE
WHEN (Yref-Ynirs)/SEC >>3

Bcoefficients are not very much affected by several outliers
The stats seem better but the prediction performance will be equal or even weaker

% of OUTLIERS REMOVED	RMSEP
0	1
1	0.96
2	0.93
3	0.91
4	0.89
5	0.87
10	0.79
15	0.72
20	0.66
25	0.61

NEW FIGURE OF MERIT :
MEDIAN ABSOLUTE DEVIATION

$$MAD = MEDIAN(|x - MEDIAN(x)|)$$

$$SD = 1.48 * MAD$$

For Gaussian distribution

B. Godin *et al.*, *J. Near Infrared Spectrosc.* **23**, 1–14 (2015)
Received: 4 November 2014 ■ *Revised: 27 January 2015* ■ *Accepted: 29 January 2015* ■ *Publication: 17 February 2015*

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JNIRS JOURNAL OF NEAR INFRARED SPECTROSCOPY

Prediction of chemical characteristics of fibrous plant biomasses from their near infrared spectrum: comparing local versus partial least square models and cross-validation versus independent validations

Bruno Godin,* Richard Agneessens, Jérôme Delcarte and Pierre Dardenne

NIR 2015 Brazil

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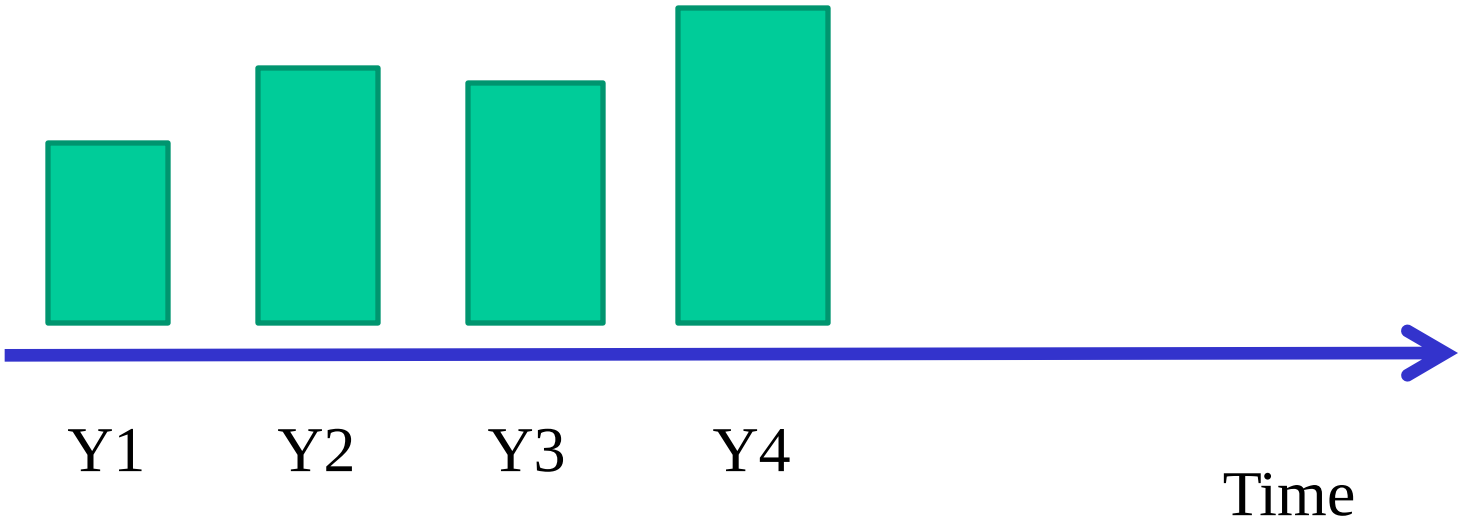
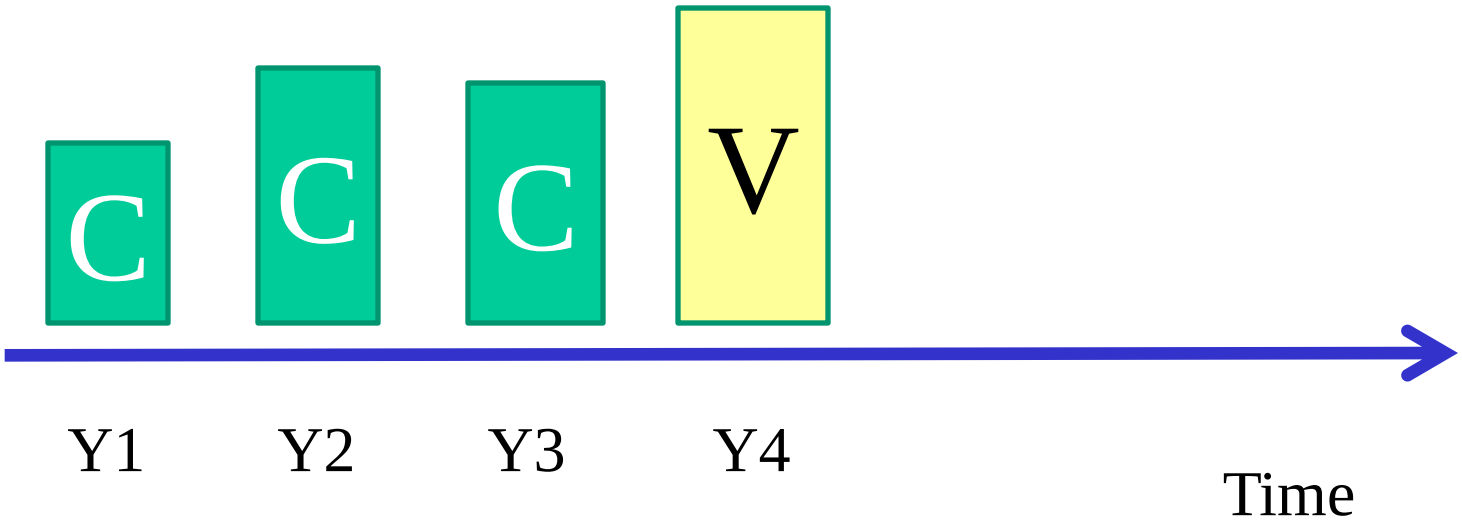
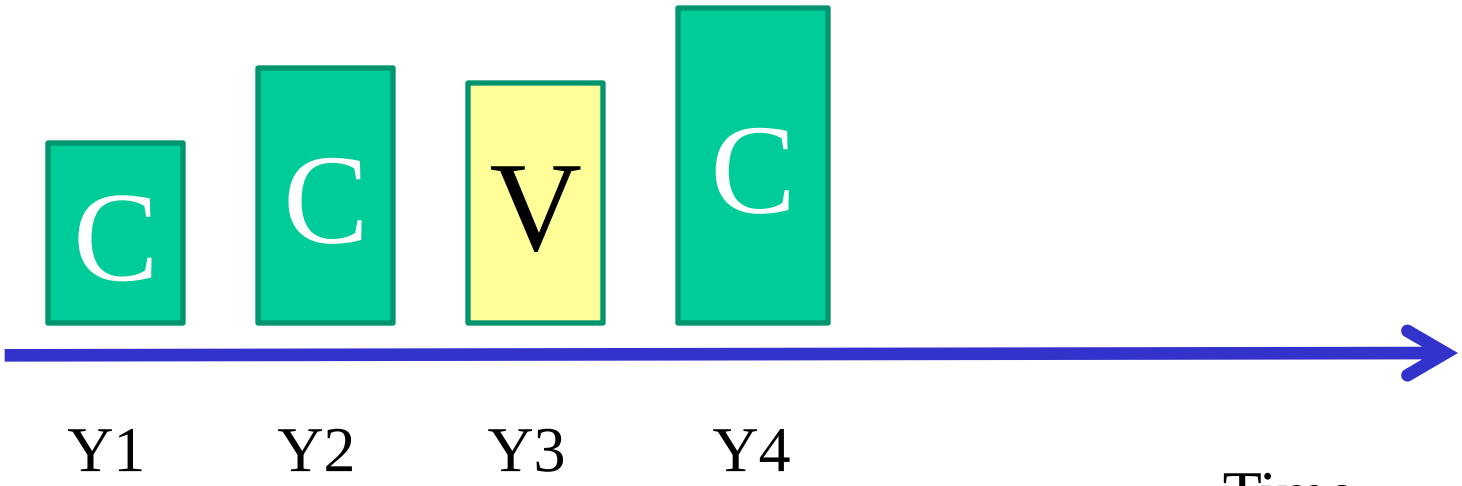
INDEPENDENT VALIDATION



INDEPENDENT VALIDATION



INDEPENDENT VALIDATION

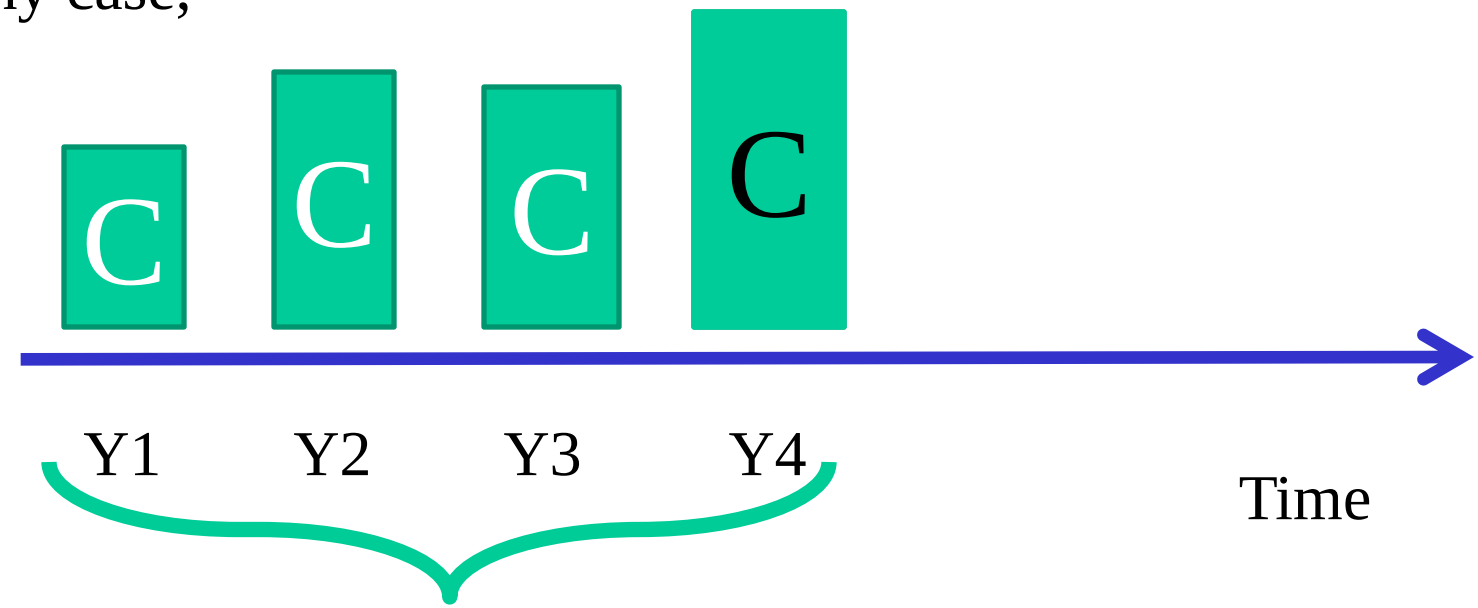


4 segments Cross Validation

Software must have this feature of defining the CV segments

INDEPENDENT VALIDATION

In any case,



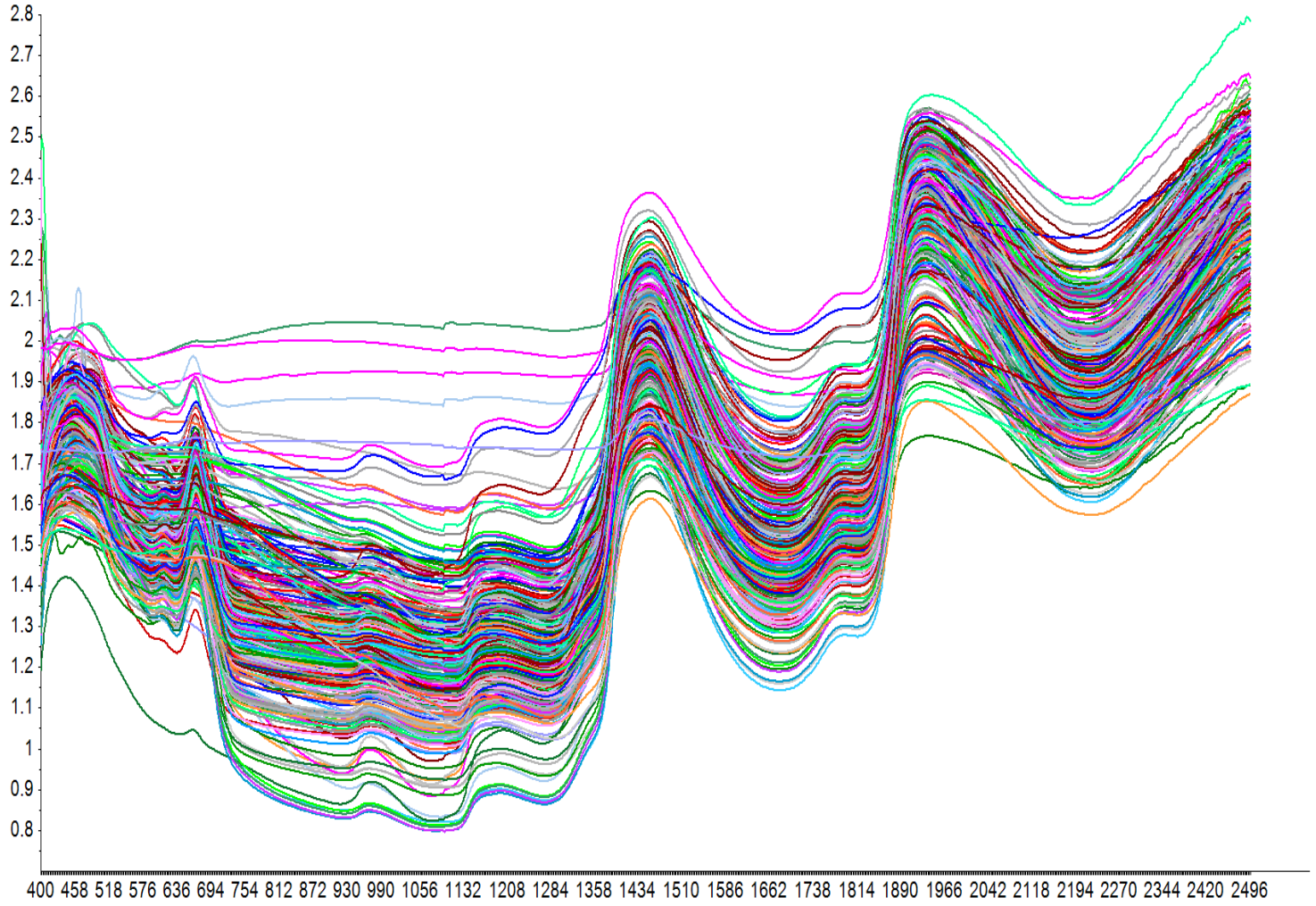
FINAL MODEL FOR ROUTINE

EXPRESSION OF REFERENCE VALUES

DM OR ASIS

DM or ASIS: no problem with “dry” products

DM or ASIS ?? When high water content ?



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D7-EQ-696
INGOT
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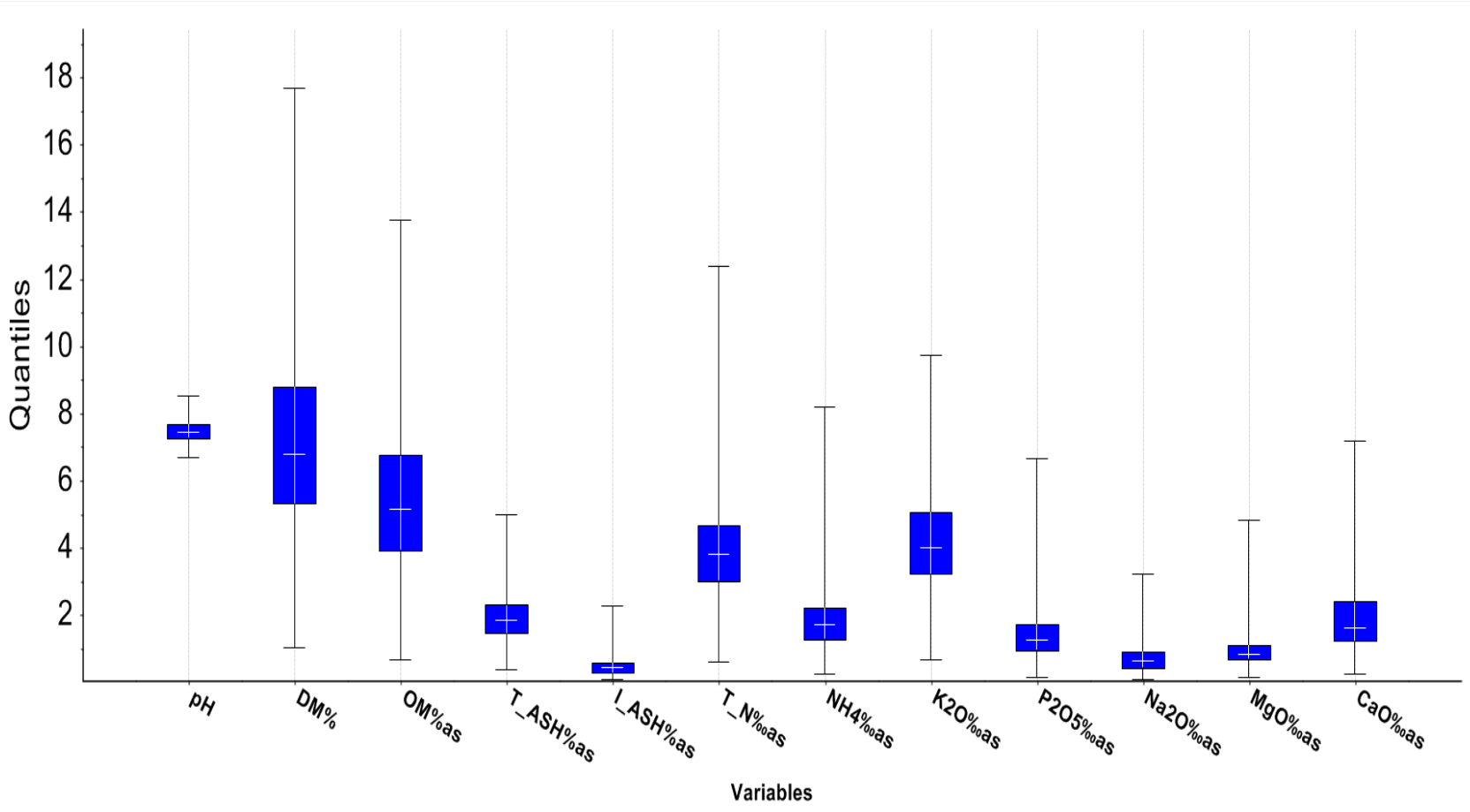
Rapid Content Analyzer
XDS
near-infrared

MANURE



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CORRELATION MATRIX (n=328)

	pH	DM%	OM%as	T_ASH%as	I_ASH%as	T_N‰as	NH4‰as	K2O‰as	P2O5‰as	Na2O‰as	MgO‰as	CaO‰as
pH	1.00	0.06	0.01	0.26	-0.08	0.27	0.30	0.19	0.37	0.38	0.18	0.27
DM%	0.06	1.00	0.99	0.84	0.44	0.74	0.45	0.71	0.76	0.46	0.66	0.72
OM%as	0.01	0.99	1.00	0.76	0.38	0.71	0.42	0.68	0.73	0.40	0.62	0.67
T_ASH%as	0.26	0.84	0.76	1.00	0.56	0.70	0.48	0.74	0.74	0.61	0.72	0.79
I_ASH%as	-0.08	0.44	0.38	0.56	1.00	0.02	-0.15	0.19	0.11	-0.03	0.10	0.17
T_N‰as	0.27	0.74	0.71	0.70	0.02	1.00	0.86	0.70	0.79	0.68	0.62	0.70
NH4‰as	0.30	0.45	0.42	0.48	-0.15	0.86	1.00	0.56	0.60	0.61	0.48	0.52
K2O‰as	0.19	0.71	0.68	0.74	0.19	0.70	0.56	1.00	0.57	0.46	0.52	0.51
P2O5‰as	0.37	0.76	0.73	0.74	0.11	0.79	0.60	0.57	1.00	0.68	0.64	0.77
Na2O‰as	0.38	0.46	0.40	0.61	-0.03	0.68	0.61	0.46	0.68	1.00	0.50	0.58
MgO‰as	0.18	0.66	0.62	0.72	0.10	0.62	0.48	0.52	0.64	0.50	1.00	0.85
CaO‰as	0.27	0.72	0.67	0.79	0.17	0.70	0.52	0.51	0.77	0.58	0.85	1.00

Local PLS LOO CV

	CAL on ASIS Basis	
	RMSEPCV	RSQCV
pH	0.24	0.43
DM%	1.02	0.86
OM%as	0.83	0.86
T_ASH%as	0.38	0.70
I_ASH%as	0.21	0.51
T_N‰as	0.84	0.84
NH4‰as	0.60	0.77
K2O‰as	0.81	0.63
P2O5‰as	0.40	0.84
Na2O‰as	0.30	0.66
MgO‰as	0.38	0.54
CaO‰as	0.68	0.66

	CAL on ASIS Basis		Recalculated on DM basis		
	RMSEPCV	RSQCV		RMSEPCV	RSQCV
pH	0.24	0.43			
DM%	1.02	0.86			
OM%as	0.83	0.86	OM%dm	4.57	0.39
T_ASH%as	0.38	0.70	T_ASH%dm	5.56	0.49
I_ASH%as	0.21	0.51	I_ASH%dm	2.49	0.48
T_N‰as	0.84	0.84	T_N‰dm	14.85	0.53
NH4‰as	0.60	0.77	NH4‰dm	11.37	0.60
K2O‰as	0.81	0.63	K2O‰dm	15.33	0.55
P2O5‰as	0.40	0.84	P2O5‰dm	5.37	0.61
Na2O‰as	0.30	0.66	Na2O‰dm	5.09	0.53
MgO‰as	0.38	0.54	MgO‰dm	4.56	0.33
CaO‰as	0.68	0.66	CaO‰dm	8.65	0.38

	CAL on ASIS Basis		Recalculated on DM basis			CAL on DM basis	
	RMSEPCV	RSQCV		RMSEPCV	RSQCV	RMSEPCV	RSQCV
pH	0.24	0.43					
DM%	1.02	0.86					
OM%as	0.83	0.86	OM%dm	4.57	0.39	4.24	0.44
T_ASH%as	0.38	0.70	T_ASH%dm	5.56	0.49	4.75	0.61
I_ASH%as	0.21	0.51	I_ASH%dm	2.49	0.48	2.38	0.52
T_N‰as	0.84	0.84	T_N‰dm	14.85	0.53	15.25	0.50
NH4‰as	0.60	0.77	NH4‰dm	11.37	0.60	11.77	0.57
K2O‰as	0.81	0.63	K2O‰dm	15.33	0.55	14.37	0.60
P2O5‰as	0.40	0.84	P2O5‰dm	5.37	0.61	5.20	0.64
Na2O‰as	0.30	0.66	Na2O‰dm	5.09	0.53	5.00	0.53
MgO‰as	0.38	0.54	MgO‰dm	4.56	0.33	4.39	0.36
CaO‰as	0.68	0.66	CaO‰dm	8.65	0.38	8.19	0.42

Look at the intercorrelations

PROTEIN (Total N) vs AA

Total FAT vs FA

…….

Beta Carotene (ppm) vs Color

TAKE HOME MESSAGES

REPORT MODELS CORRECTLY

VALIDATE PROPERLY (CV stinks)

DO NOT REMOVE (too many) OUTLIERS

BE CAREFUL WITH INTERNAL CORRELATONS

THANK YOU FOR YOUR ATTENTION

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http://chimio2016.sciencesconf.org/

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