NIR MICROSPECTROMETERS - CASE STUDIES

HELIOSPIR, CIRAD, IRSTEA

SAMPLE AND REFERENCE DATA: CIRAD AGAP, CIRAD SELMET

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Avec les contributions de Vincent Baeten (CRA-W), Denis Bastianelli (CIRAD), Jean Michel Roger (IRSTEA), Nathalie Gorretta (IRSTEA), Pierre Dardenne, Laurent Bonnal (CIRAD), Bernard Barthes (IRD), Vincent Larat (ADISSEO), Sébastien Lurol (CTIFL), Anne Clément Vidal (CIRAD), Sylvie Roussel (ONDALYS), Michaël Bonin (FONDIS ELECTRONICS)

PRODUCT	Wood
Use of set	Calibration
Y	Extractives
N samples	FOSS cup 53

SPECTROMETER	COMPANY	ORIGIN	RANGE	
ASD_1	BONSAI	CRAW	350-2500	X
ASD_2	BONSAI	CIRAD	350-2500	X
VECTOR	BRUKER	CIRAD	800-2800	X
TANGO	BRUKER	CIRAD	800-2700	X
MICRONIR2200_1	JDSU	CIRAD	1150-2150	X
MICRONIR2200_2	JDSU	IRD	1150-2150	X
MICRONIR1700_1	VIAVI	CRAW	900-1700	X
MICRONIR1700_2	VIAVI	CRAW	900-1700	X
MICRONIR1700_3	VIAVI	FONDIS	900-1700	
TELLSPEC	TELLSPEC	ADISSEO	900-1700	
NANONIR	TI	CIRAD	900-1700	X
NIRONE22_2	SPECTRAL ENGINE	ADISSEO	1750-2150	X
NIRONE22_1	SPECTRAL ENGINE	CRAW	1750-2150	X
NIRONE20	SPECTRAL ENGINE	CRAW	1550-1950	X
SCIO	SCIO	CRAW	750-1050	X
F750	FELIX	CTIFL	400-1140	

Choix / disponibilité et opportunité

On a plutot dupliquer les appareils

PRODUCT	Sugarcane
Use of set	Calibration
Y	Sugars, CP, ADF, IVDMO FOSS cup
N samples	60

SPECTROMETER	COMPANY	ORIGIN	RANGE	
ASD_1	BONSAI	CRAW	350-2500	
ASD_2	BONSAI	CIRAD	350-2500	X
VECTOR	BRUKER	CIRAD	800-2800	X
TANGO	BRUKER	CIRAD	800-2700	X
MICRONIR2200_1	JDSU	CIRAD	1150-2150	X
MICRONIR2200_2	JDSU	IRD	1150-2150	
MICRONIR1700_1	VIAVI	CRAW	900-1700	
MICRONIR1700_2	VIAVI	CRAW	900-1700	
MICRONIR1700_3	VIAVI	FONDIS	900-1700	X
TELLSPEC	TELLSPEC	ADISSEO	900-1700	X
NANONIR	TI	CIRAD	900-1700	X
NIRONE22_2	SPECTRAL ENGINE	ADISSEO	1750-2150	X
NIRONE22_1	SPECTRAL ENGINE	CRAW	1750-2150	
NIRONE20	SPECTRAL ENGINE	CRAW	1550-1950	
SCIO	SCIO	CRAW	750-1050	X
F750	FELIX	CTIFL	400-1140	X

Choix / disponibilité et opportunité

Diversisification des appareils

			PRODUCT	Wood	Sugarcane	Forage, foods	Chemicals
			Use of set	Calibration	Calibration	Transfert calibration	
			Y	Extractives	Sugars, CP, ADF, IVDMO	-	-
				FOSS cup	FOSS cup	Seal. FOSS cup	FOSS cup
			N samples	53	60	23	8
SPECTROMETER	**COMPANY**	**ORIGIN**	**RANGE**				
ASD_1	BONSAI	CRAW	350-2500	X		X	X
ASD_2	BONSAI	CIRAD	350-2500	X	X	X	X
VECTOR	BRUKER	CIRAD	800-2800	X	X	X	X
TANGO	BRUKER	CIRAD	800-2700	X	X	X	X
MICRONIR2200_1	JDSU	CIRAD	1150-2150	X	X	X	X
MICRONIR2200_2	JDSU	IRD	1150-2150	X		X	X
MICRONIR1700_1	VIAVI	CRAW	900-1700	X		X	X
MICRONIR1700_2	VIAVI	CRAW	900-1700	X		X	X
MICRONIR1700_3	VIAVI	FONDIS	900-1700		X	X	X
TELLSPEC	TELLSPEC	ADISSEO	900-1700		X	X	X
NANONIR	TI	CIRAD	900-1700	X	X	X	X
NIRONE22_2	SPECTRAL ENGINE	ADISSEO	1750-2150	X	X	X	X
NIRONE22_1	SPECTRAL ENGINE	CRAW	1750-2150	X		X	X
NIRONE20	SPECTRAL ENGINE	CRAW	1550-1950	X		X	X
SCIO	SCIO	CRAW	750-1050	X	X	X	X
F750	FELIX	CTIFL	400-1140		X	X	X

PARAMETERS

Context: Lambda user

Regression: PLS

Cross-validation: 2 random groups, repeted 20 times

Pretreatments: no, normalization, -logX, SNV, D1, D2, 5-25 points, combination

Full range for each equipement

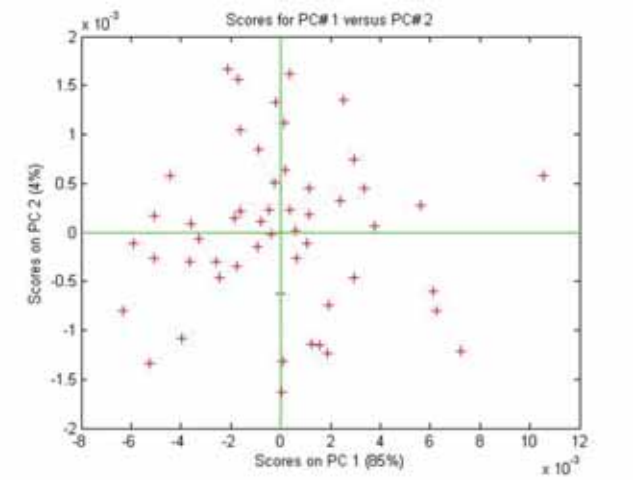
ASD Full range (reference 350-2500 nm)

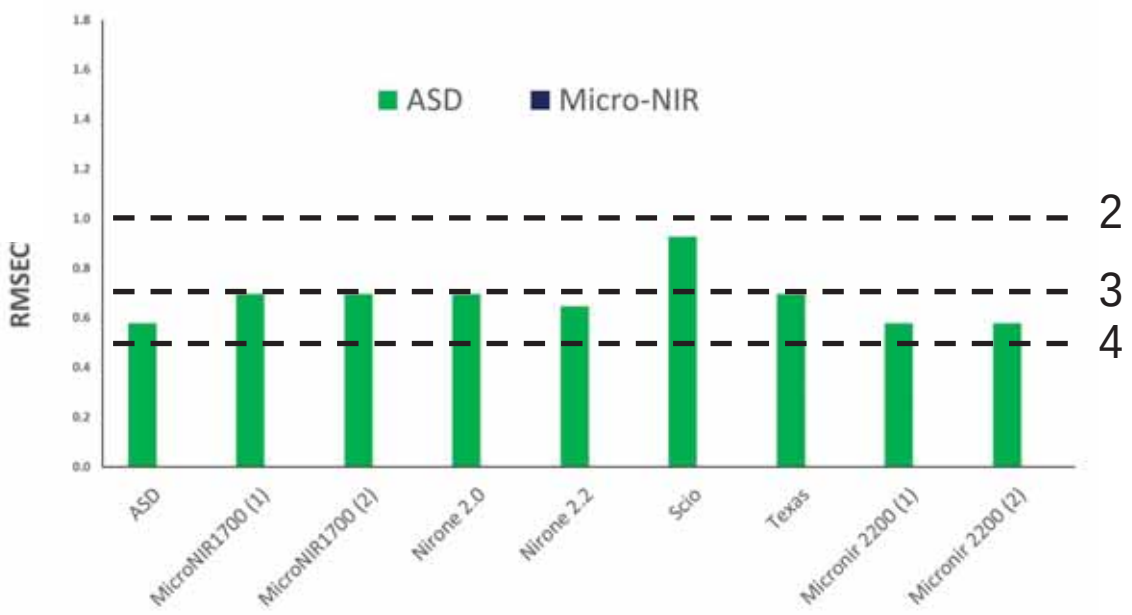
ASD with range of each equipement

WOOD RESULTS

Wood powder
Extractive contents

	ASD
Equipment	**RMSECV**
ASD Full	
MicroNIR1700 (1)	0.70
MicroNIR1700 (2)	0.70
Nirone 2.0	0.70
Nirone 2.2	0.65
Scio	0.93
Texas	0.70
Micronir 2200 (1)	0.58
Micronir 2200 (2)	0.58

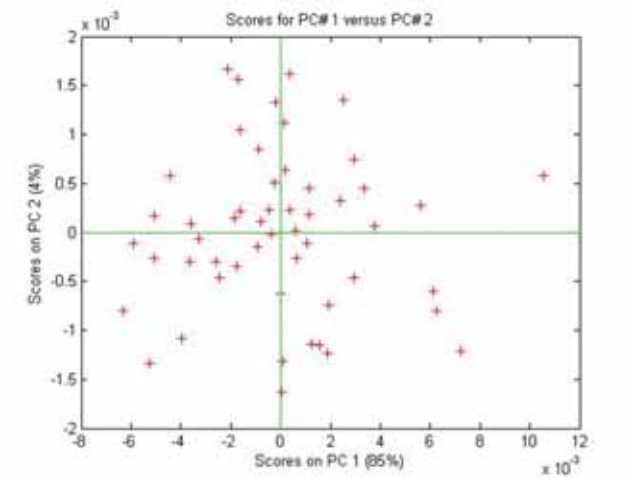


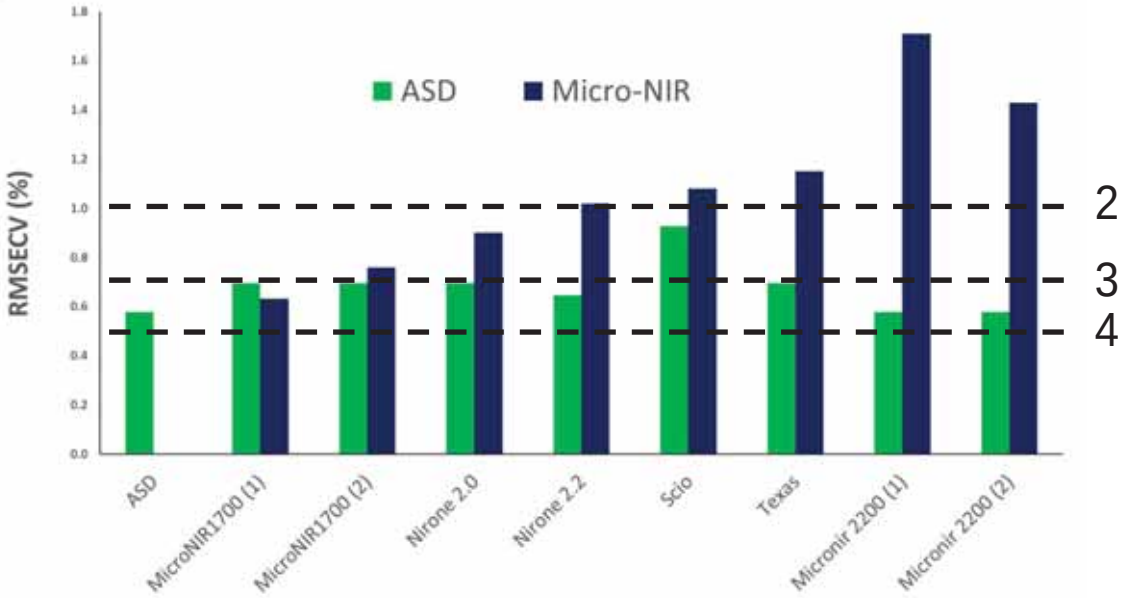


WOOD RESULTS

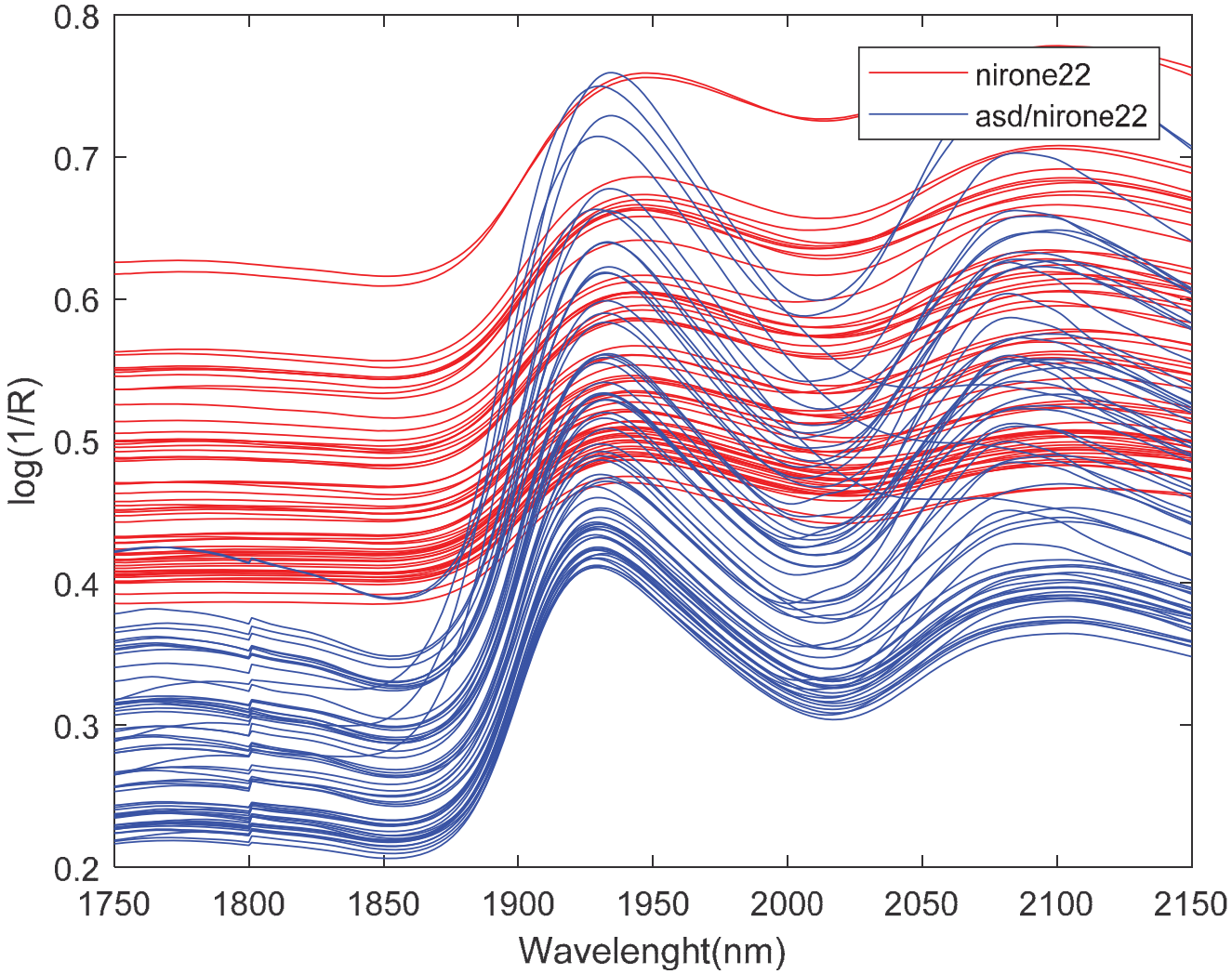
Wood powder
Extractive contents

Equipment	RMSECV	ASD RMSECV	R^2	VL
ASD Full	0.58			
MicroNIR1700 (1)	0.63	0.70	0.901	5
MicroNIR1700 (2)	0.76	0.70	0.857	5
Nirone 2.0	0.90	0.70	0.800	5
Nirone 2.2	1.02	0.65	0.729	5
Scio	1.08	0.93	0.710	6
Texas	1.15	0.70	0.675	6
Micronir 2200 (1)	1.71	0.58	0.400	5
Micronir 2200 (2)	1.43	0.58	0.494	5

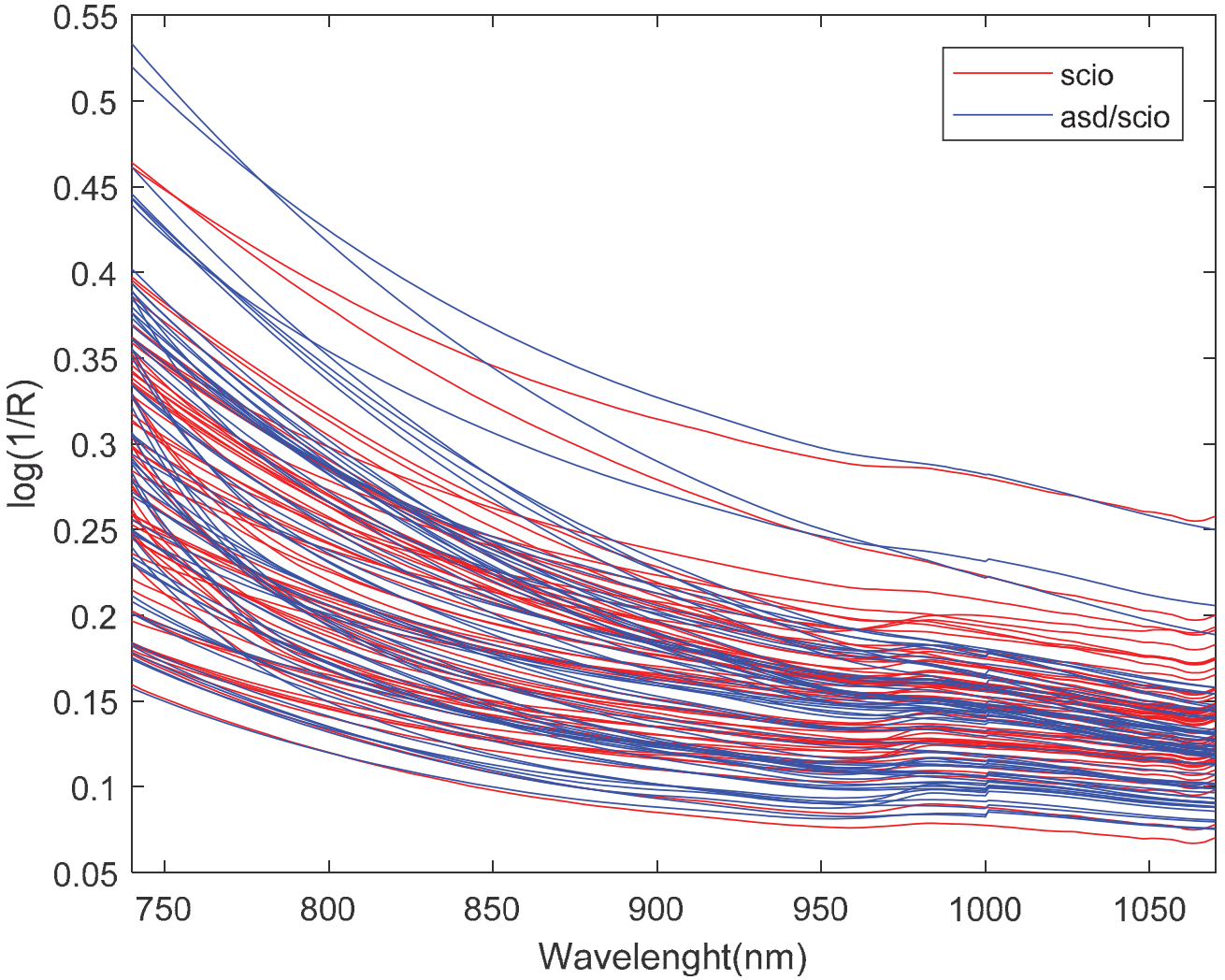




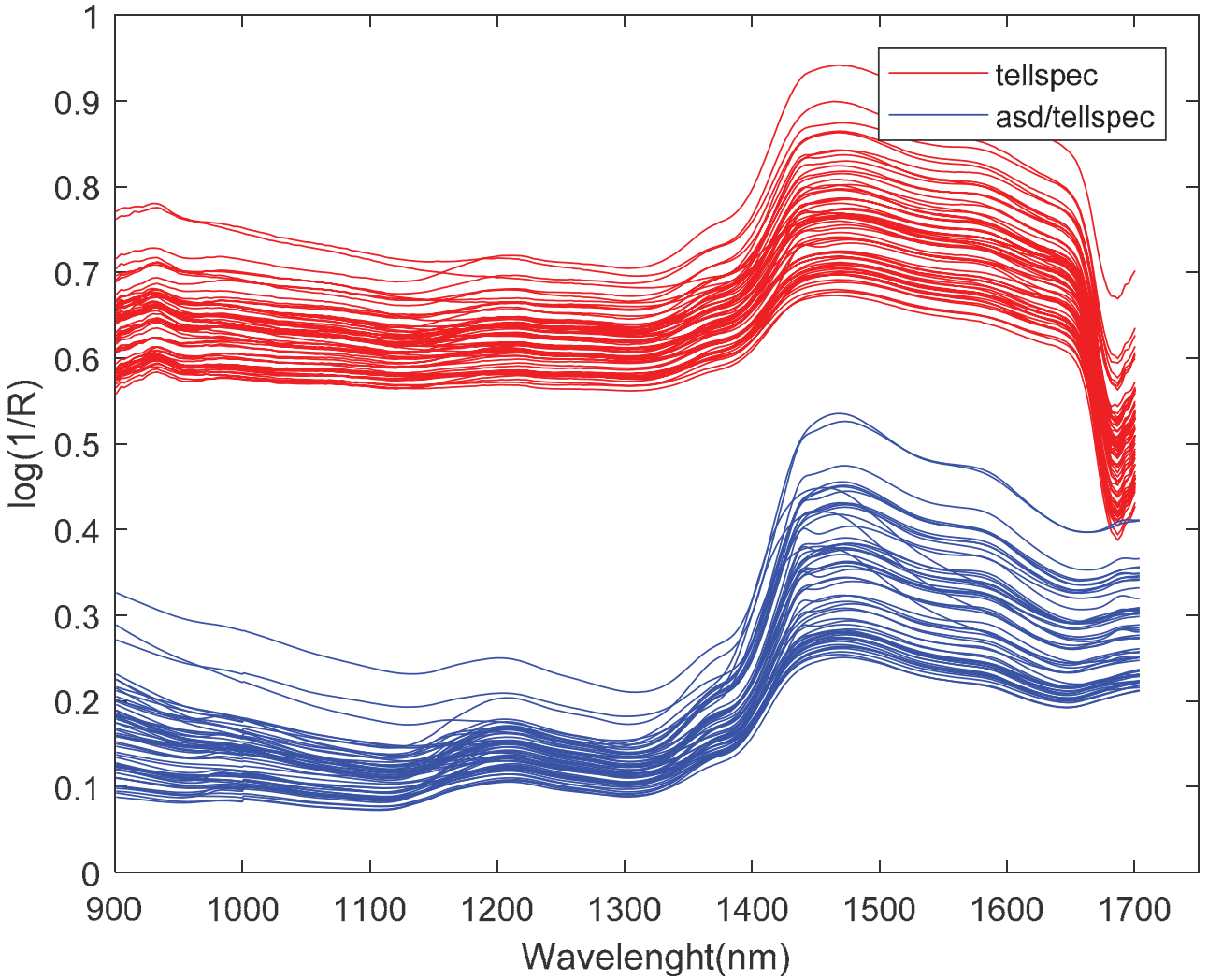
Sugarcane spectres



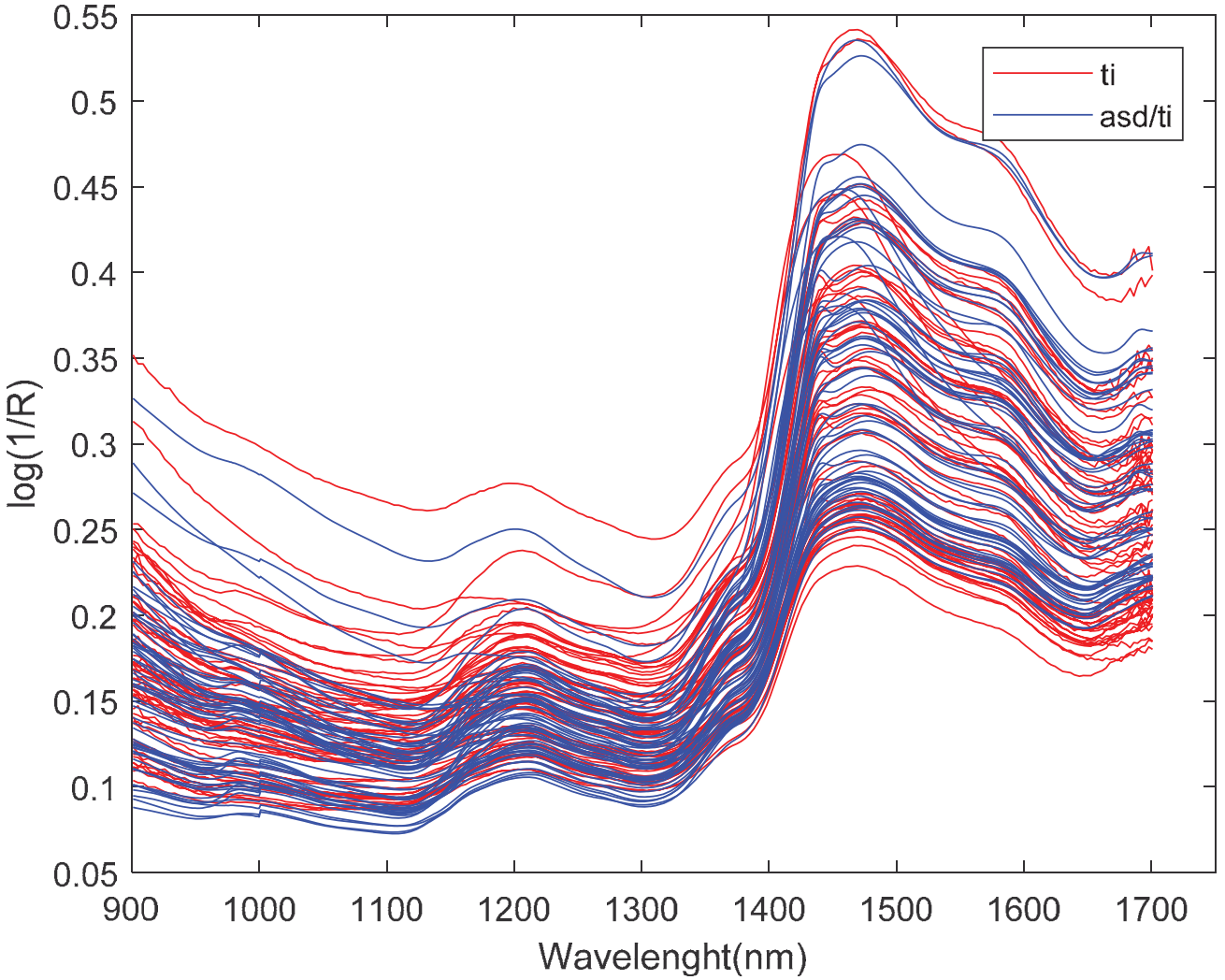
Sugarcane spectres



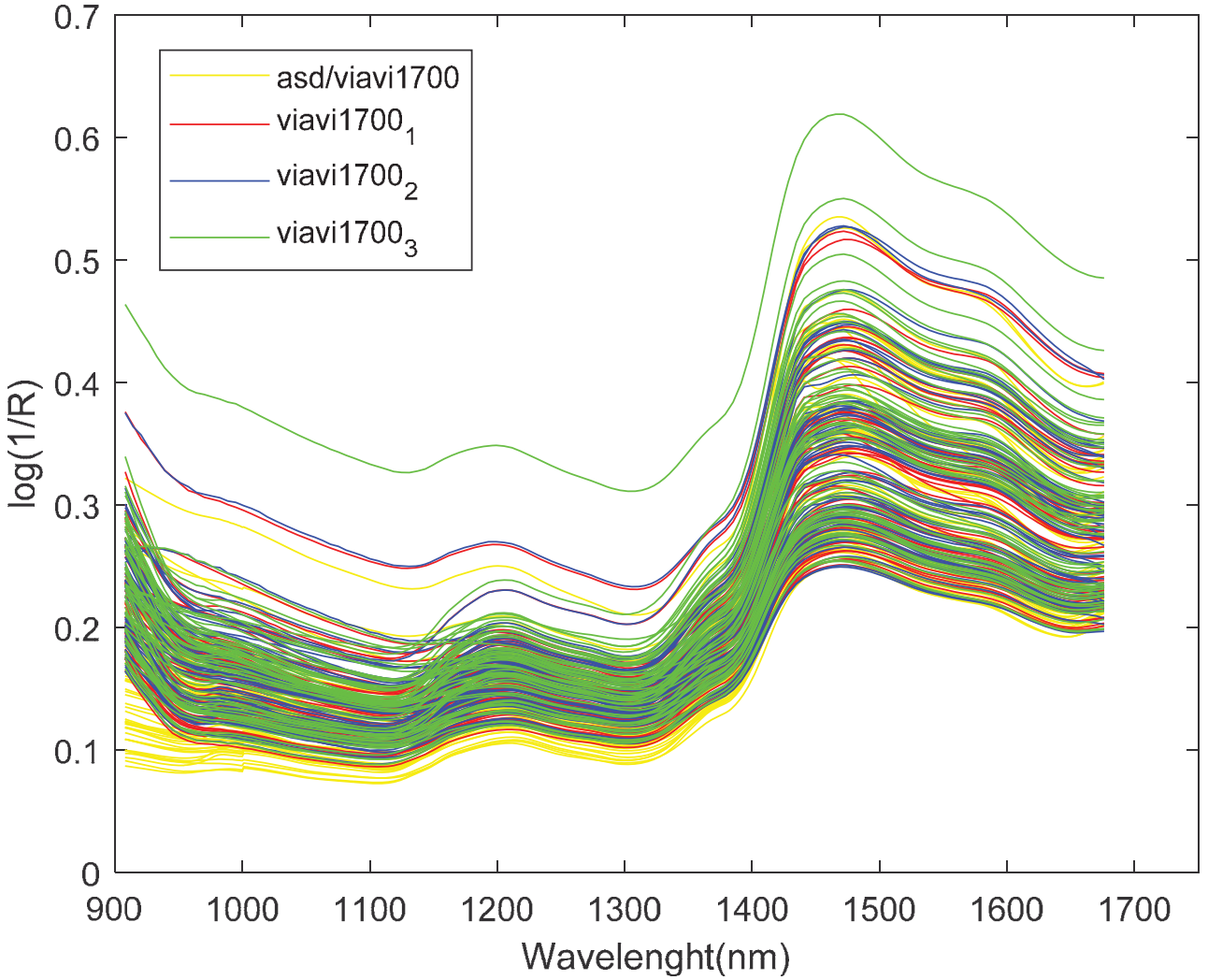
Sugarcane spectres



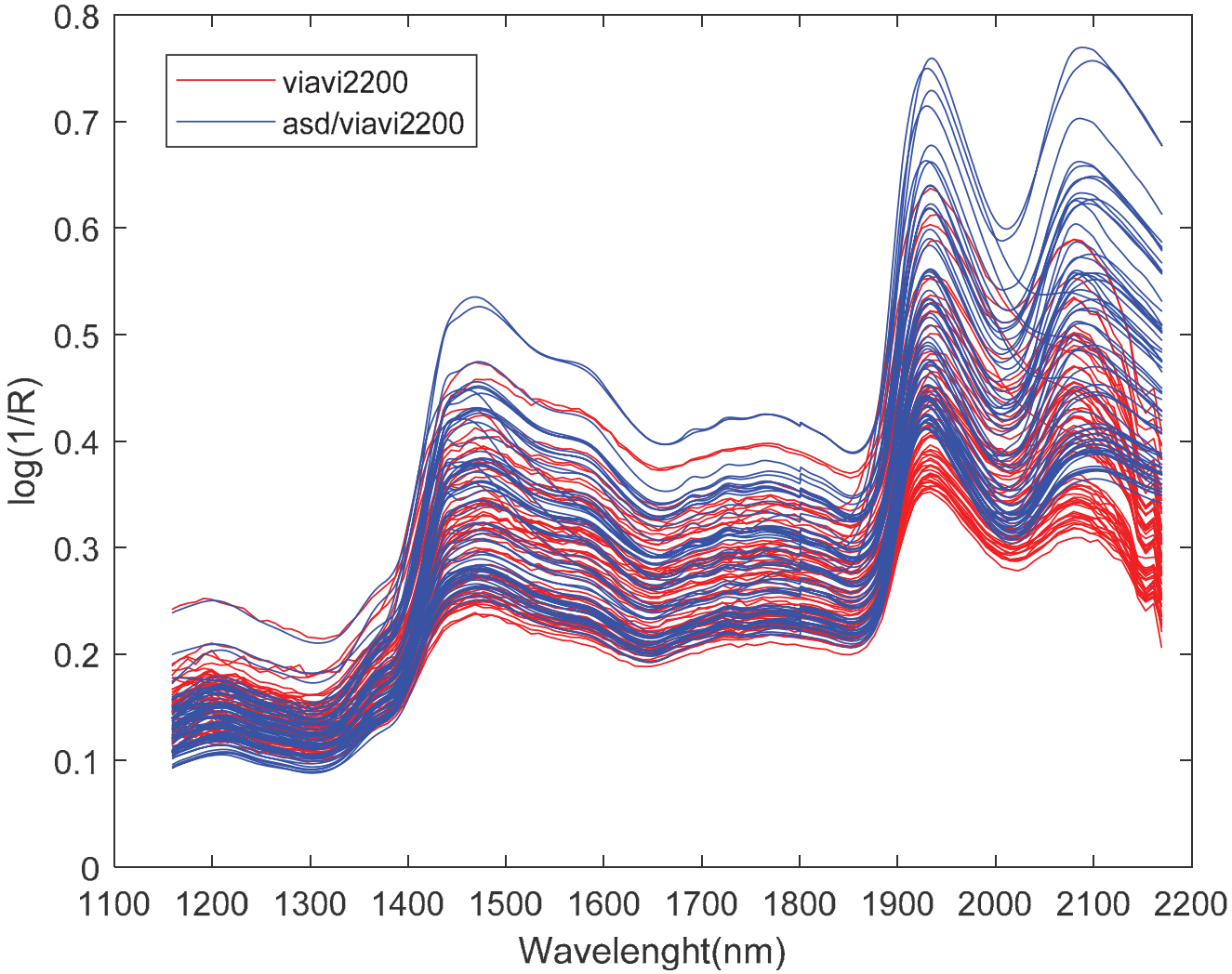
Sugarcane spectres



Sugarcane spectres

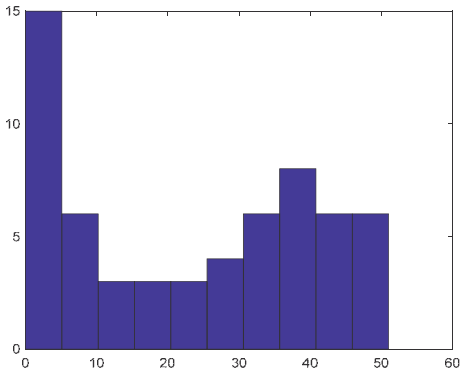


Sugarcane spectres

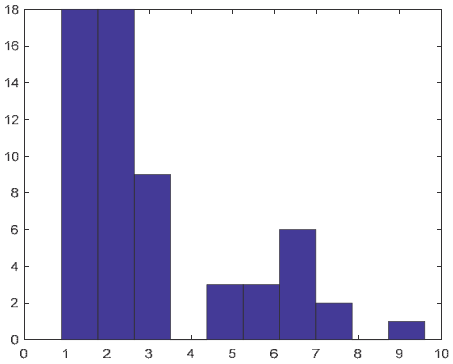


REFERENCES ON THE 60 SUGARCANE SAMPLES

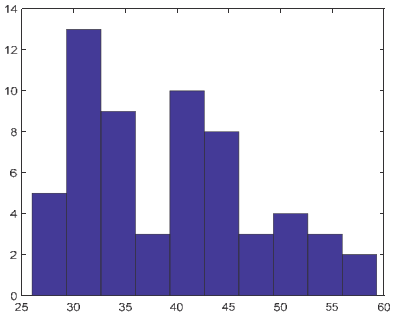
SUGARS



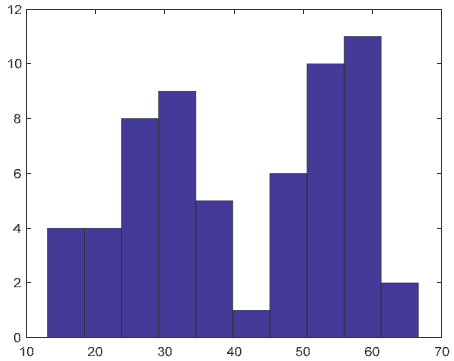
CP



ADF

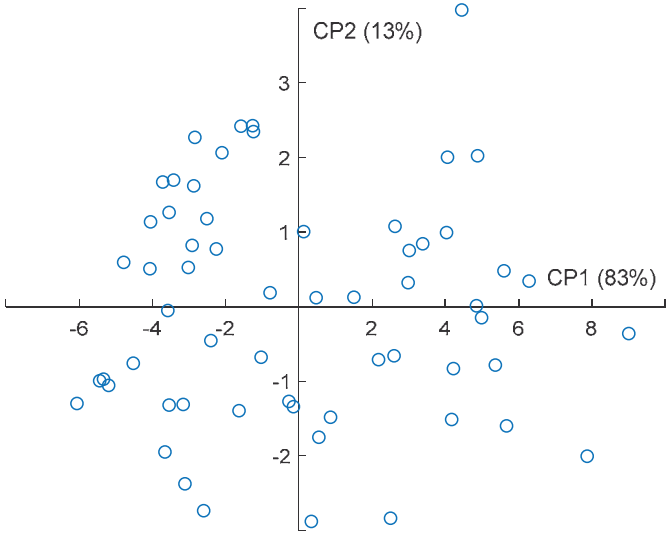


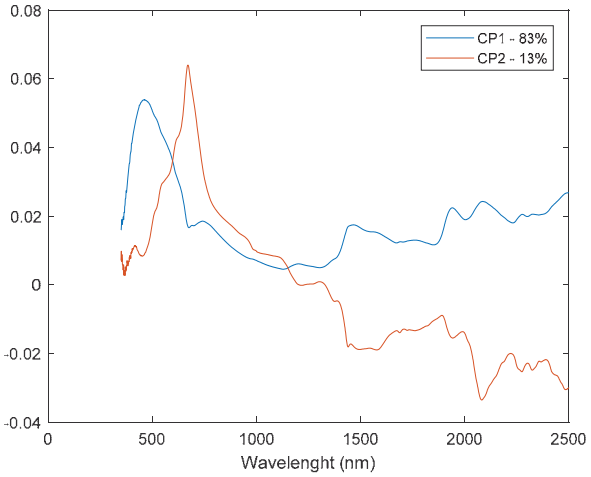
IVDMO



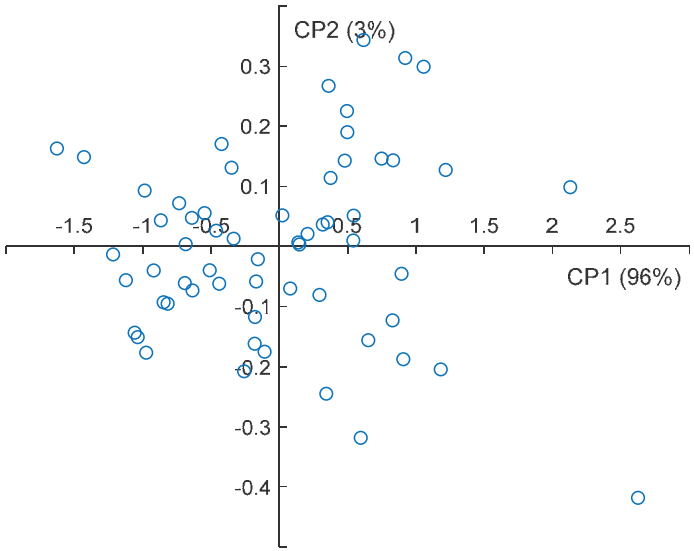
	Unité	Min	Max	Mean	SD
Sugars	%	1.1	51.0	23.4	17.3
CP	%	0.9	9.6	3.1	2.1
ADF	%	26.0	59.3	39.2	8.7
IVDMO	%	13.0	66.6	41.0	15.1

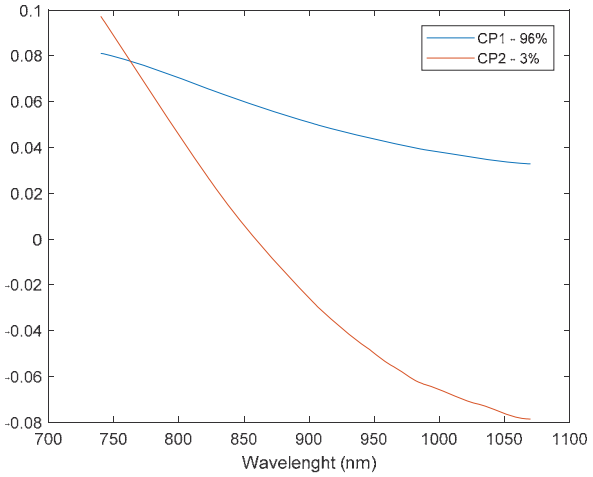
PCA - ASD full

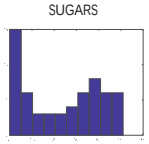


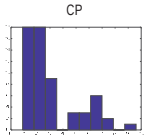


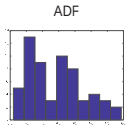
PCA - SCIO

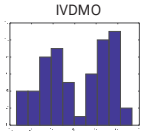




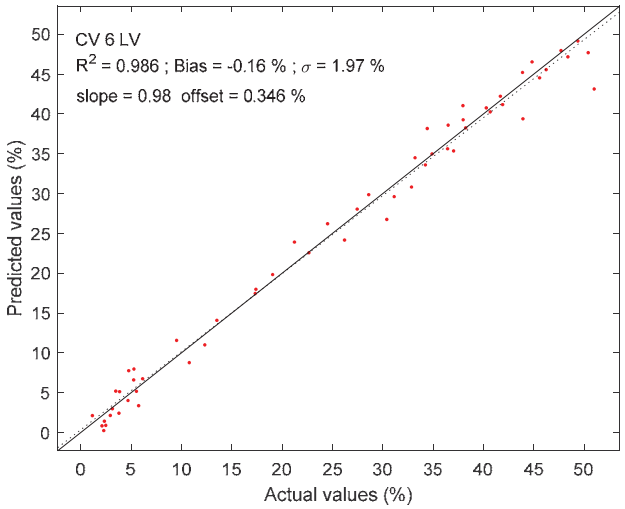




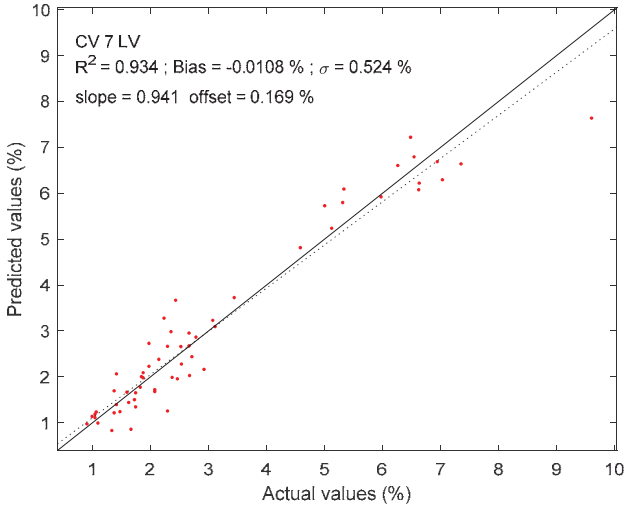




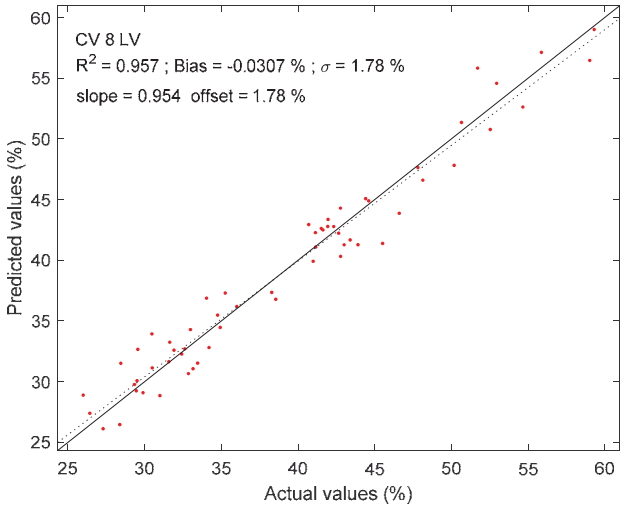
asd sugars snvd1



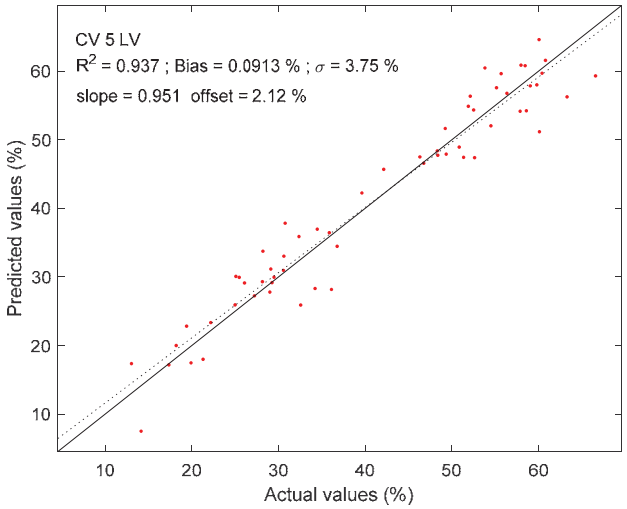
asd cp snvd1



asd adf snvd2



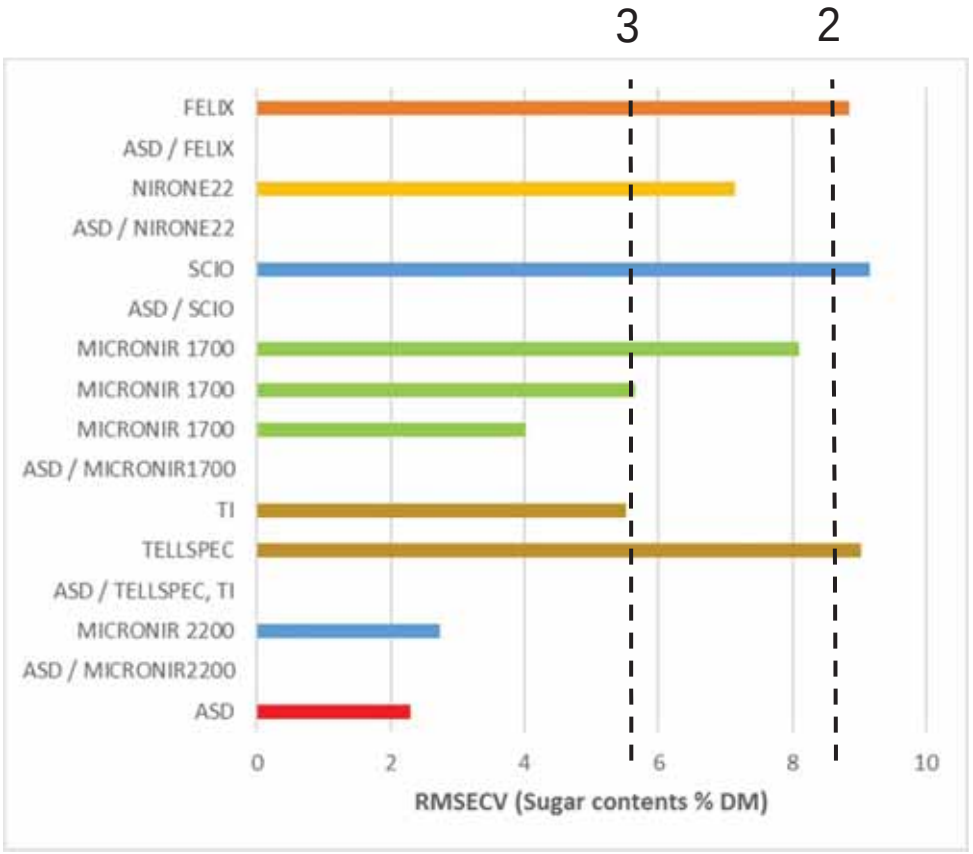
asd ivdmo snvd2



SUGAR CANE RESULTS – Sugar contents

Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	SNVD1	6	3.53	0.958
ASD (1100-2500)	SNVD1	6	2.30	0.982
ASD (1150-2150)	SNVD1	6	1.77	0.989
MICRONIR 2200	SNVD1	7	2.25	0.982
ASD (900-1700)	SNVD1	6	2.90	0.970
TELLSPEC	D1	4	9.03	0.711
TI	D2	4	5.51	0.912
ASD (900-1700)	SNVD1	6	3.03	0.967
MICRONIR 1700	SNVD1	5	4.02	0.943
MICRONIR 1700	SNVD2	8	5.65	0.886
MICRONIR 1700	D2	5	8.10	0.767
ASD (750-1050)	D1	5	7.31	0.810
SCIO	D1	4	9.15	0.702
ASD (1750-2150)	SNVD1	3	3.70	0.951
NIRONE22	SNVD2	6	7.15	0.819
ASD (450-1140)	D2	8	6.23	0.862
FELIX	NORM	4	8.85	0.722

Mettre les scores



	Unité	Min	Max	Mean	SD
Sugars	% DM	1.1	51.0	23.4	17.3

SUGAR CANE RESULTS – Sugar contents

Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	SNVD1	6	3.53	0.958
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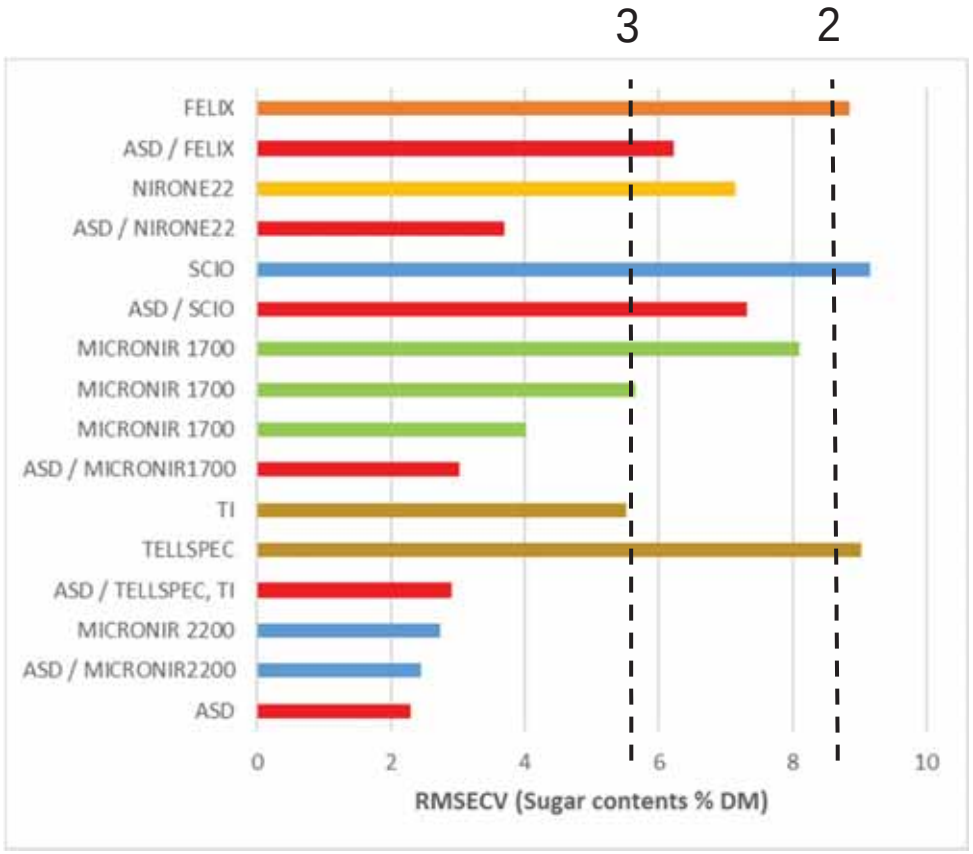
ASD (1750-2150)	SNVD1	3	3.70	0.951
NIRONE22	SNVD2	6	7.15	0.819
ASD (450-1140)	D2	8	6.23	0.862
FELIX	NORM	4	8.85	0.722

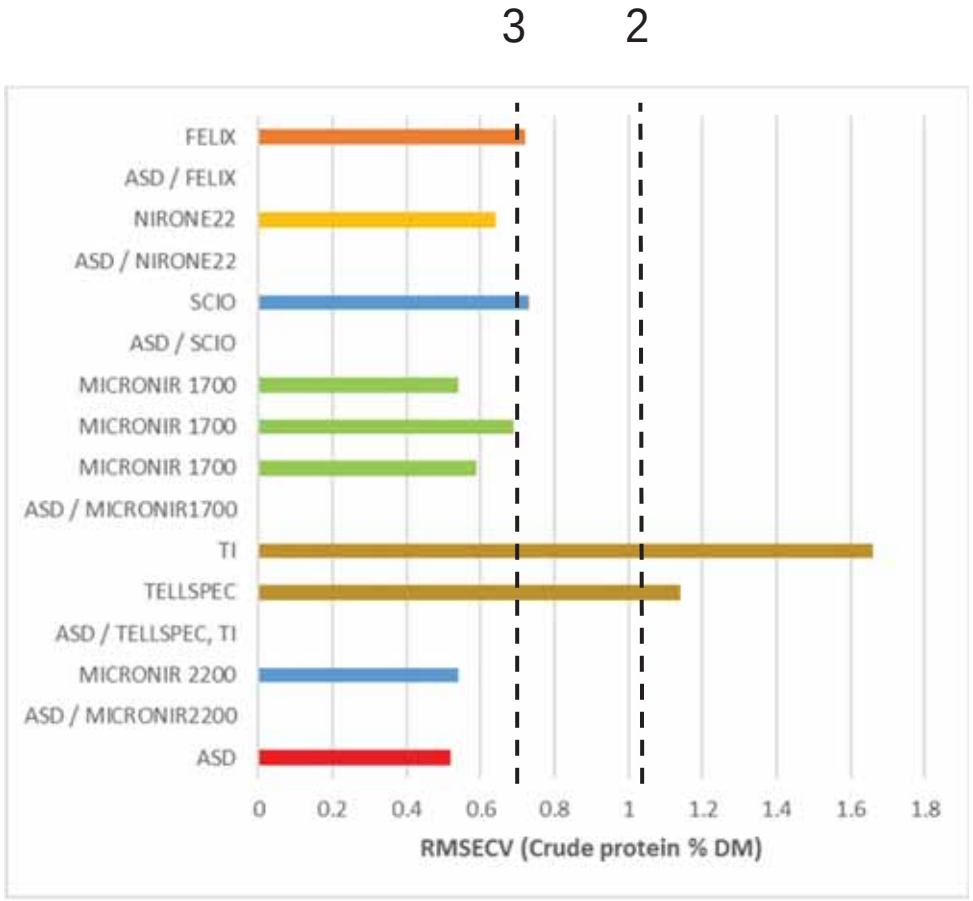
Mettre les scores



	Unité	Min	Max	Mean	SD
Sugars	% DM	1.1	51.0	23.4	17.3

SUGAR CANE RESULTS - Crude protein

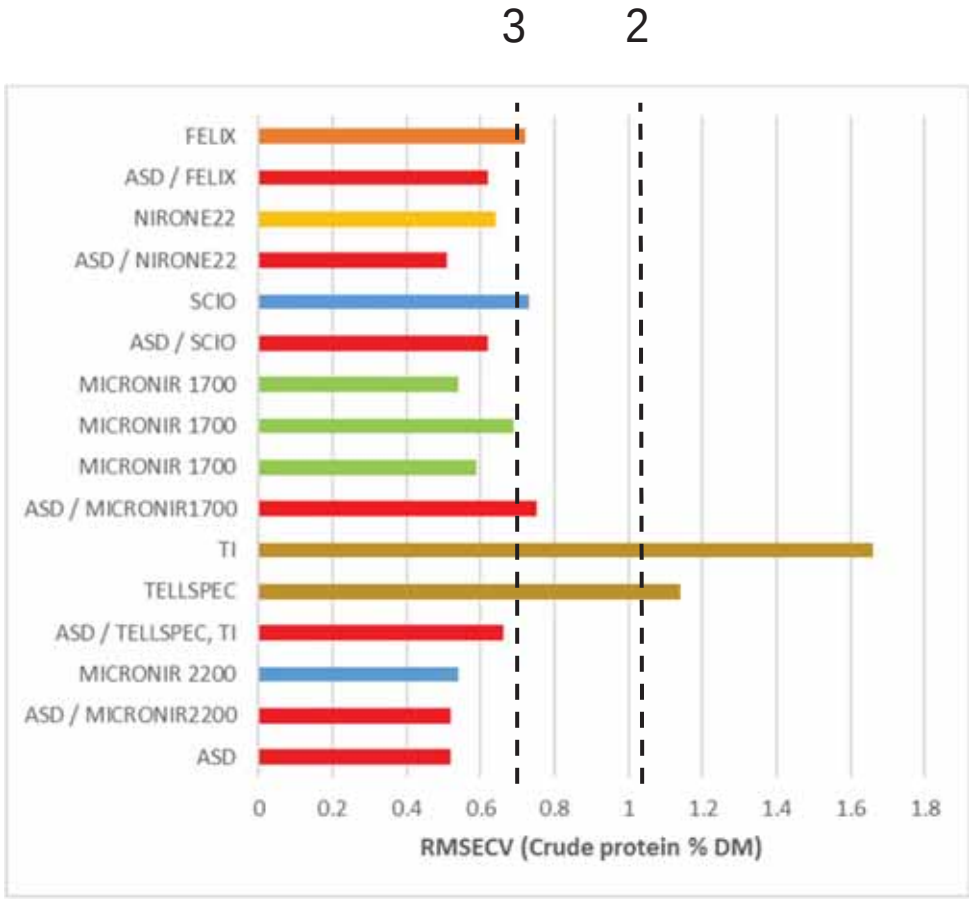
Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	NORM	3	0.64	0.901
ASD (1100-2500)	SNVD1	7	0.52	0.934
ASD (1150-2150)	D1	6	0.52	0.935
MICRONIR 2200	SNVD1	7	0.54	0.929
ASD (900-1700)	SNVD1	6	0.66	0.896
TELLSPEC	-	6	1.14	0.687
TI	SNVD1	2	1.66	0.347
ASD (900-1700)	SNVD2	7	0.75	0.865
MICRONIR 1700	SNVD2	9	0.59	0.917
MICRONIR 1700	SNVD1	9	0.69	0.886
MICRONIR 1700	SNVD2	10	0.54	0.929
ASD (750-1050)	-	5	0.62	0.908
SCIO	-	4	0.73	0.871
ASD (1750-2150)	SNVD1	6	0.51	0.937
NIRONE22	SNVD1	8	0.64	0.902
ASD (450-1140)	LOG	3	0.62	0.907
FELIX	NORM	3	0.72	0.874



	Unité	Min	Max	Mean	SD
CP	% DM	0.9	9.6	3.1	2.1

SUGAR CANE RESULTS - Crude protein

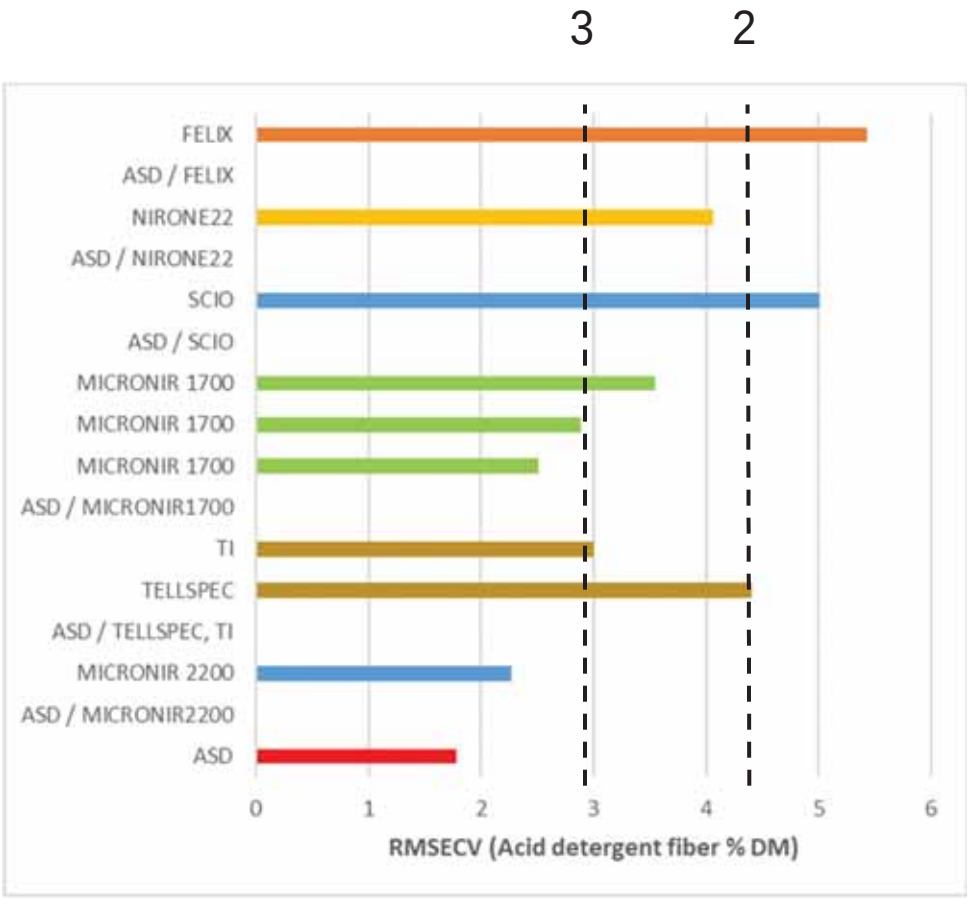
Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	NORM	3	0.64	0.901
ASD (1100-2500)	SNVD1	7	0.52	0.934
ASD (1150-2150)	D1	6	0.52	0.935
MICRONIR 2200	SNVD1	7	0.54	0.929
ASD (900-1700)	SNVD1	6	0.66	0.896
TELLSPEC	-	6	1.14	0.687
TI	SNVD1	2	1.66	0.347
ASD (900-1700)	SNVD2	7	0.75	0.865
MICRONIR 1700	SNVD2	9	0.59	0.917
MICRONIR 1700	SNVD1	9	0.69	0.886
MICRONIR 1700	SNVD2	10	0.54	0.929
ASD (750-1050)	-	5	0.62	0.908
SCIO	-	4	0.73	0.871
ASD (1750-2150)	SNVD1	6	0.51	0.937
NIRONE22	SNVD1	8	0.64	0.902
ASD (450-1140)	LOG	3	0.62	0.907
FELIX	NORM	3	0.72	0.874



	Unité	Min	Max	Mean	SD
CP	% DM	0.9	9.6	3.1	2.1

SUGAR CANE RESULTS - Acid detergent fiber

Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	SNV	7	2.92	0.885
ASD (1100-2500)	SNVD2	8	1.78	0.957
ASD (1150-2150)	SNVD1	6	2.01	0.946
MICRONIR 2200	SNVD2	6	2.27	0.930
ASD (900-1700)	SNVD2	5	2.32	0.928
TELLSEPC	SNVD1	6	4.40	0.739
TI	SNVD2	6	3.00	0.879
ASD (900-1700)	SNVD1	7	1.91	0.951
MICRONIR 1700	SNVD2	5	2.51	0.915
MICRONIR 1700	SNVD2	6	2.89	0.888
MICRONIR 1700	D2	6	3.55	0.831
ASD (750-1050)	D2	6	4.43	0.736
SCIO	SNVD1	4	5.01	0.662
ASD (1750-2150)	SNVD2	5	2.78	0.897
NIRONE22	SNVD1	7	4.06	0.779
ASD (450-1140)	D2	9	3.63	0.822
FELIX	NORM	4	5.43	0.607



	Unité	Min	Max	Mean	SD
ADF	% DM	26.0	59.3	39.2	8.7

SUGAR CANE RESULTS - Acid detergent fiber

Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	SNV	7	2.92	0.885
ASD (1100-2500)	SNVD2	8	1.78	0.957
ASD (1150-2150)	SNVD1	6	2.01	0.946
MICRONIR 2200	SNVD2	6	2.27	0.930
ASD (900-1700)	SNVD2	5	2.32	0.928
TELLSEPC	SNVD1	6	4.40	0.739
TI	SNVD2	6	3.00	0.879
ASD (900-1700)	SNVD1	7	1.91	0.951
MICRONIR 1700	SNVD2	5	2.51	0.915
MICRONIR 1700	SNVD2	6	2.89	0.888
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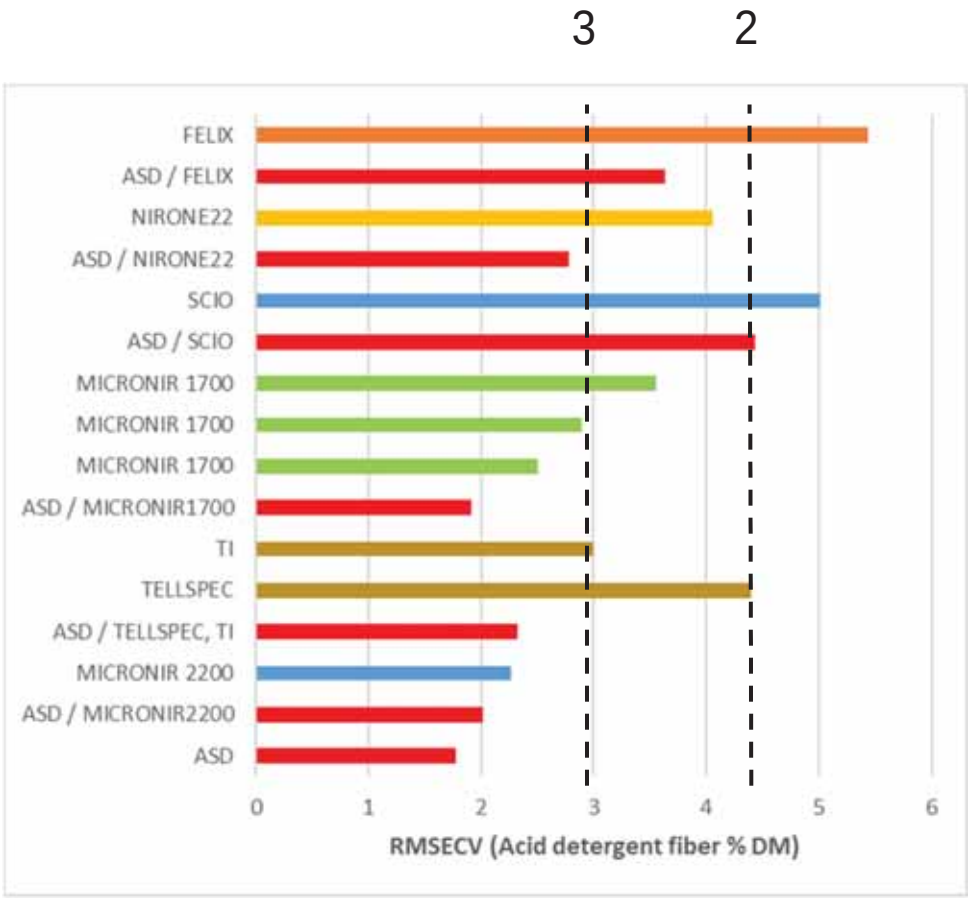
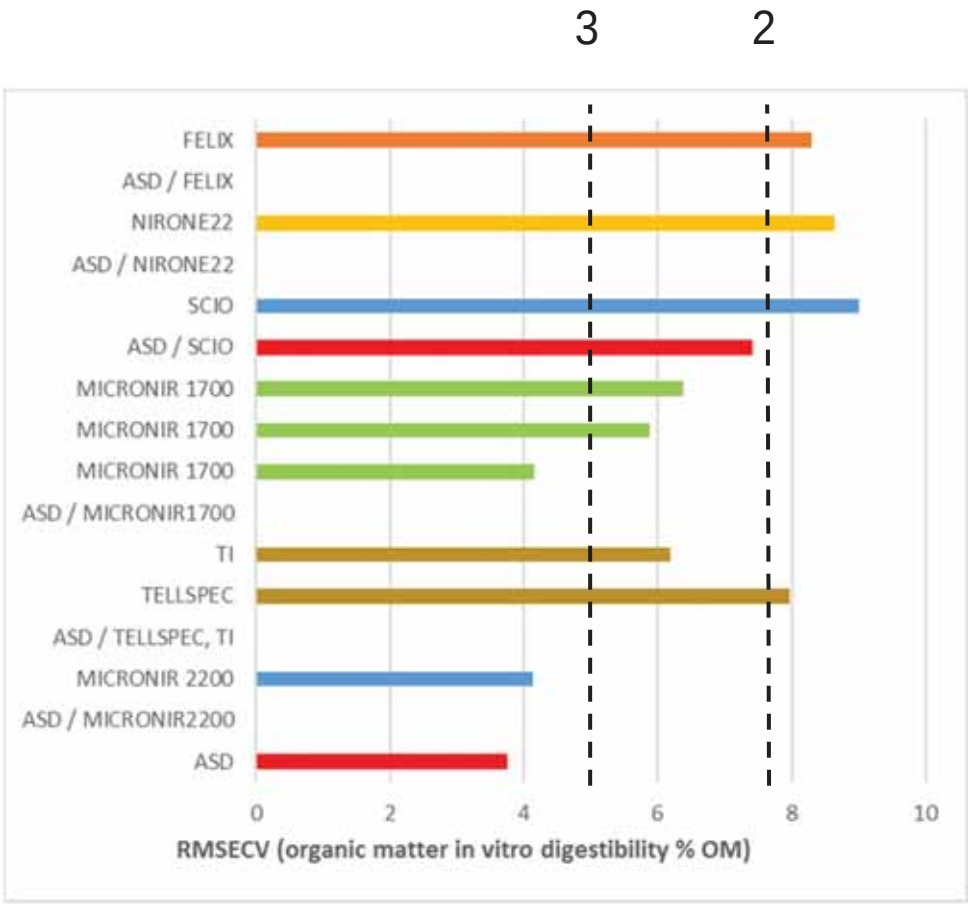


	Unité	Min	Max	Mean	SD
ADF	% DM	26.0	59.3	39.2	8.7

SUGAR CANE RESULTS - Organic matter in vitro digestibility

Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	NORM	7	4.96	0.890
ASD (1100-2500)	SNVD2	5	3.75	0.937
ASD (1150-2150)	SNV	7	3.60	0.942
MICRONIR 2200	SNV+D1	6	4.14	0.924
ASD (900-1700)	SNVD1	5	4.07	0.927
TELLSPEC	SNVD2	5	7.98	0.721
TI	SNVD2	4	6.18	0.830
ASD (900-1700)	SNVD2	5	4.01	0.928
MICRONIR 1700	SNVD2	7	4.16	0.925
MICRONIR 1700	D2	5	5.88	0.846
MICRONIR 1700	SNVD2	5	6.38	0.819
ASD (750-1050)	D1	5	7.42	0.756
SCIO	SNVD2	3	9.01	0.644
ASD (1750-2150)	SNV	3	4.67	0.903
NIRONE22	SNV	2	8.65	0.668
ASD (450-1140)	D2	7	6.45	0.815
FELIX	NORM	4	8.30	0.694



	Unité	Min	Max	Mean	SD
IVDMO	% DM	13.0	66.6	41.0	15.1

SUGAR CANE RESULTS - Organic matter in vitro digestibility

Equipment	Prétraitement	LV	RMSECV %	R^2_{cv}
ASD (350-2500)	NORM	7	4.96	0.890
ASD (1100-2500)	SNVD2	5	3.75	0.937
ASD (1150-2150)	SNV	7	3.60	0.942
MICRONIR 2200	SNV+D1	6	4.14	0.924
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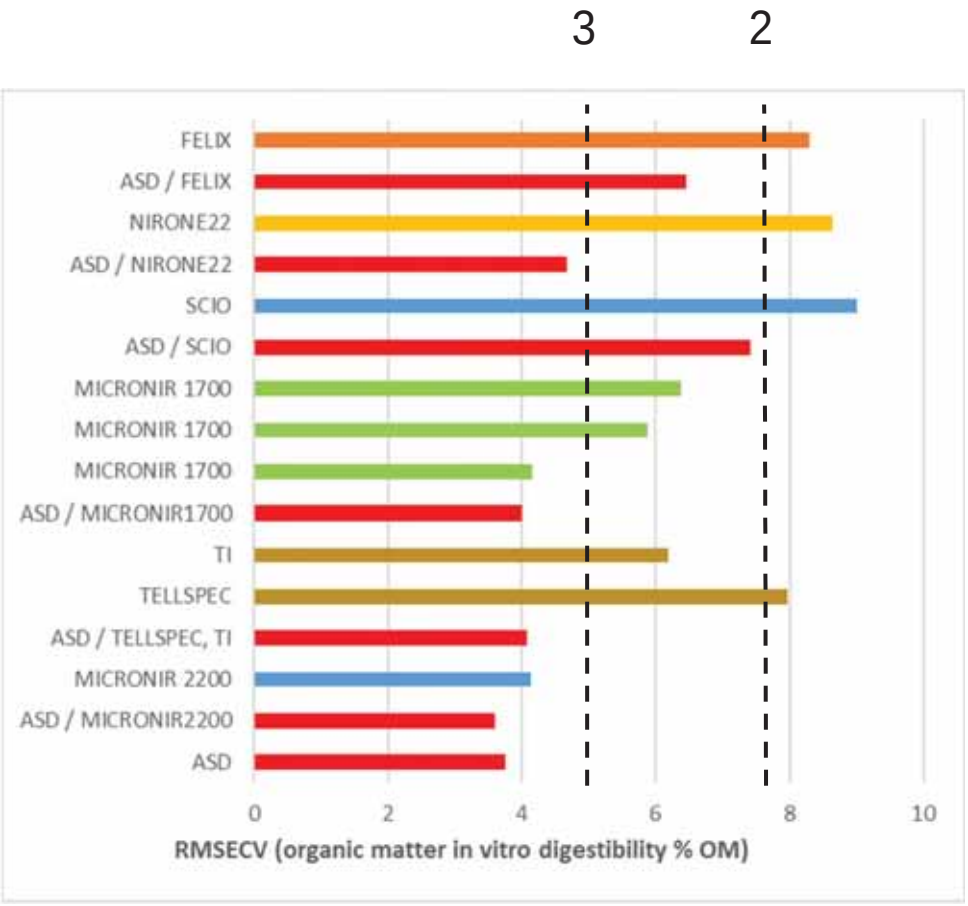
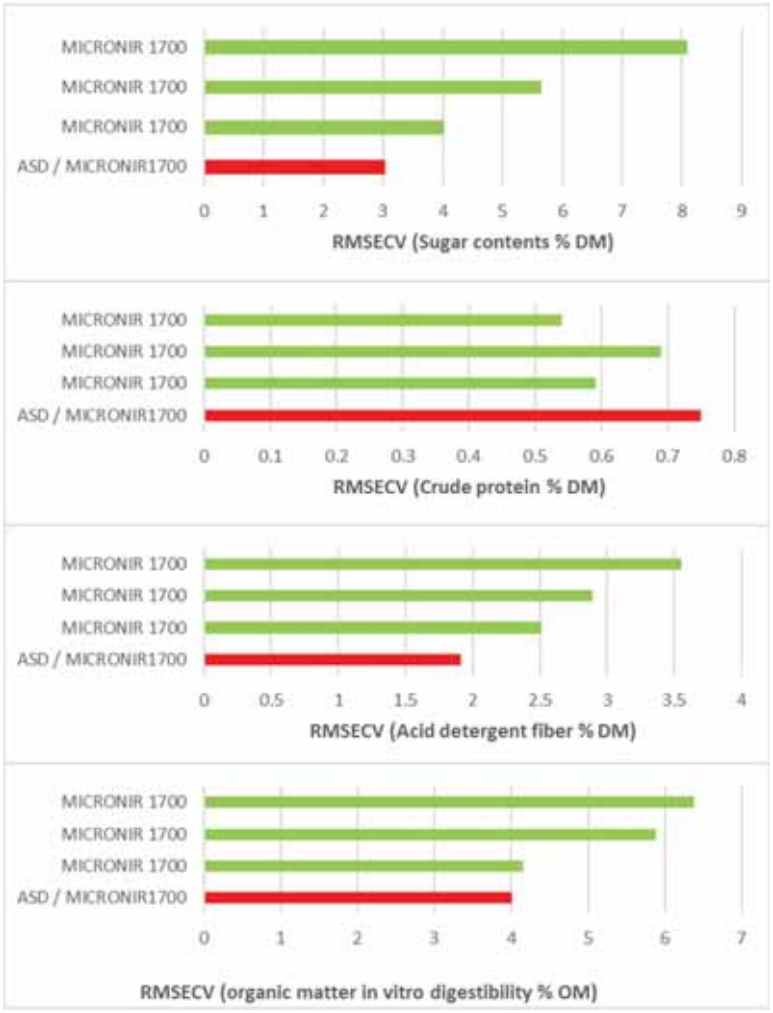


	Unité	Min	Max	Mean	SD
IVDMO	% DM	13.0	66.6	41.0	15.1

SUGAR CANE RESULTS – Repeatability MicroNir1700

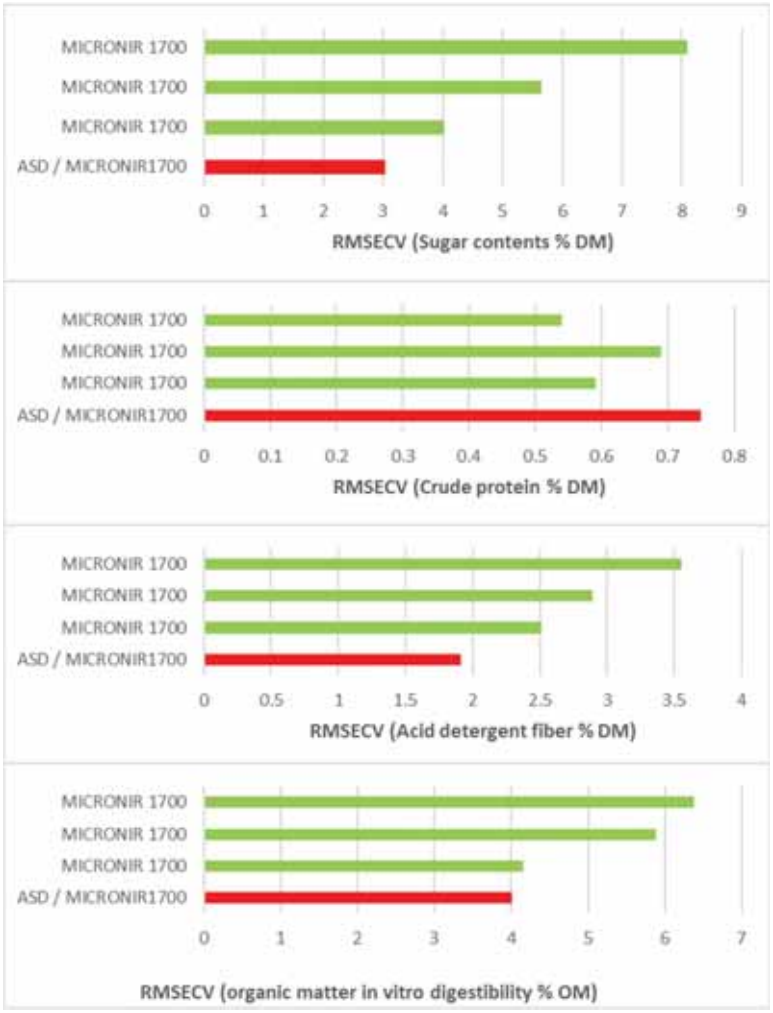
Same equipment, 3 repeated measures 23/07, 26/07, 30/07/2018



Avec optimisation prétraitement, LV

SUGAR CANE RESULTS – Repeatability MicroNir1700

Same equipment, 3 repeated measures 23/07, 26/07, 30/07/2018



Avec optimisation prétraitement, LV

SNVD2 pretreatment, LV (5-7 depending with the Y)

CONCLUSIONS

Les performances dépendent de la matrice et de la propriété considérée

Résultats portent sur le choix de tirer le mieux de chaque spectromètre en optimisant (bande spectrale complète, traitement, LV, ajustement du nom de)

Du spectro de laboratoire au microspectro : tendance plus de variables latentes, plus de traitement des spectres

PERSPECTIVES

Reste à faire (beaucoup)

- Déterminer et retirer les zones bruités notament en fin début et fin de gamme spectrale
- Comparaisons sans prétraitement, fixer les prétraitements, fixer le nombre de variables latentes, ajuster la dérivée aux résolutions spectrales
- Comparer statistiquement des SECV
- Exploiter les mesures spectrales des échantillons de standardisation
- Publier

Pistes et idées

- Présenter et discuter des résultats, des méthodes à ChemHouse (en cours)
- Proposer des groupes de travail sur quelques points cruciaux / méthodes
- Comparer les spectres de chaque spectromètre aux spectres du spectro de référence
- Analyse de variance sur les rmsecv en intégrant les différents paramètres (spectro / prétraitement / plage spectrale etc).

Dans le futur

Organiser au niveau HelioSPIR une étude / veille associant les équipementiers, les experts en analyse de données (ChemHouse, Ondalys) : une bonne idée de Bernard