The generation of Near Infrared Reflectance Spectroscopy (NIRS) equations for the prediction of chemical composition, in vivo digestibility, and degradability on fresh scanned maize silage.

Steve Shelley – Eurofins UK

1. Sample preparation and scanning details

In total there were 90 frozen samples received from Reading University. On receipt these were thawed and allowed to equilibrate to the ambient conditions of the scanning room. Samples were emptied onto a mixing tray and a representative sub-sample was transferred to a mould lined with cling film. Six cling film wrapped packings, each of dimensions 1 cm x 4.5 cm x 20 cm were prepared for each sample. Packings were scanned from 1100 to 2498 nanometres with data collected every 2 nanometres in a NIRSystems high fat/moisture cell using the FAA maize silage master instrument, a FOSS NIRSystems model 5000 scanning monochromator. The spectra were stored as log 1 over reflectance.

2. Calibration

Spectral models for the prediction of chemical composition, in vivo digestibility, and degradability characteristics were developed using the modified partial least squares technique within the WINISI II version 1.60 software. In order to extract the chemical and physical information from the spectra, which will also contain effects due to variation in sample particle size, a scatter correction and derivative math treatment was applied to the spectra. Finding the 'best' treatments to apply for each analyte is a matter of trial and error. Three scatter correction techniques were tried along with three math treatments, these were standard normal variate - detrended (SNVD), normal multiplicative scatter correction (MSC), and modified multiplicative scatter correction (MMSC), along with a first order, a second order, and no derivatisation. To determine the best correlation between spectral and reference data, calibrations were run on both the meaned (n = 90) and non meaned spectral datasets (n = 540).

3. Statistical analysis

Selection of the 'best' spectral model in each case from the total exploratory runs was done by assessment of the equation statistics, the coefficient of determination (R^2) and the standard error of calibration (SEC). Validation was carried out by sequentially removing samples from the calibration development process to act as both calibrators and validators; this was done automatically by the software on setting the number of cross validation groups. This was assessed by the standard error of cross validation (SECV) and '1 minus the variance ratio' (1 - VR), a R^2 term for the validation set. The best equation was deemed to be the equation producing the highest calibration R^2, the lowest SECV, and the closest 1- VR to the calibration R^2. The number of principal component terms used in the equation to explain the analyte variance was also taken into account before selecting the equation for use. The cross validation process used in the software should prevent over fitting of the equation to the calibration set as the optimum number of terms are selected when the SECV is at its lowest and 1 – VR is at its highest. Addition of more terms than necessary will increase the prediction error and over fit the equation to its calibration set resulting in poor predictive performance on samples outside the calibration set. Usually a medium sized model is preferred (Martens and Naes 1989).

4. Results

Principal component loadings were obtained for the dataset. The PCA scores file for the total dataset indicated that all samples collected could be regarded as a single spectral population with only three samples 3534, 3535, & 3590 giving global H values above 3.

4.1 Prediction of in vivo digestibility DOMD

Tables 1 & 2 show the statistics for the digestibility exploratory regressions. Using the above criteria the best equation was found to be the second derivative SNVD equation from the replicate scan dataset achieving a R^2 of 0.64. The SECV of this equation was selected as the lowest was achieved by a 16 term equation so was rejected. The selected equation also has the highest 1 – VR at 0.56 and an acceptable number of terms (5). There are higher R^2 equations with a similar number of terms however they have slightly inferior cross validation 1 – VRs and have higher SECV's.

4.2 Prediction of degradability and solubility characteristics

Tables 3 & 4 show poor regressions for soluble dry matter. The highest R^2 achieved was only 0.25 and is therefore of little use.

Tables 5 & 6 indicate the best equation statistics for predicting Dry matter degradability (a) was achieved by the first derivative MMSC equation from the replicate dataset. The number of terms is not the lowest however it does give the highest 1-VR (0.81) and the lowest SECV.

Tables 7 through to 10 show poor regressions for Dry matter degradability (b) and (c) achieving the best R^2s of 0.35 and 0.49 respectively. These equations also have a high number of terms and therefore would not be expected to perform well.

Tables 11 & 12 indicate the best equation for predicting soluble nitrogen was the first derivative MSC equation from the replicate scans dataset. This gave the lowest SECV and highest 1 – VR (0.69). R^2 is acceptable at 0.76.

Tables 25 through to 30 show poor regressions for the starch degradability (a), (b), and (c) achieving R^2s at best of 0.5 and 1 – VR only of 0.45. This equation having a reasonable number of terms would still not be expected to perform well.

4.3 Prediction of chemical composition

4.3.1 Neutral Detergent Fibre (amylase treated)

Tables 13 & 14 show the equation with the fewest terms (5), the highest R^2 (0.73) and 1 – VR (0.70) was achieved with the first derivative MSC equation from the replicate scan dataset. The SECV is not the lowest but is very close (0.9204 g/100g).

4.3.2 Dry matter

Tables 15 & 16 show the best equation statistics was achieved by the first derivative MSC equation from the meaned scan dataset with a R^2 of 0.98. The SECV at 0.93 g/100g is one of the lowest and the 1 – VR is the highest at 0.96 with only 7 terms.

4.3.3 Crude protein

Tables 17 & 18 show the best equation R^2 was achieved from the replicate dataset however there are a lot of terms selected for these. The chosen equation was the one that produced a reasonable number of terms (8) with the highest R^2 (0.86) and 1 – VR (0.81). This was the MMSC equation with no derivatisation applied to the spectra and was from the meaned scan dataset.

4.3.4 Starch

Tables 19 & 20. The equation selected, the first derivative SNVD equation from the meaned scan dataset, gave with the highest R^2 (0.87) and 1 – VR (0.75). This equation also gives the lowest SECV.

4.3.5 Ash

Tables 21 & 22. The selected equation has the highest 1 – VR (0.55) with a slightly lower R^2 (0.63) than the highest in the tables but has a good number of terms (8). This was achieved from the first derivative MMSC equation from the replicate dataset.

4.3.6 pH

Tables 23 &24 show the equation statistics for pH. The selected equation was the second derivative MMSC scatter corrected equation (R^2 0.92, 1 - VR 0.84) with 5 terms.

Table 1. MPLS statistics for in vivo DOMD (g/100gDM). All replicate scans used.

DOMD	Math	SC	n	Mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	531	68.15	0.5376	2.2130	2.3232	0.4896	13
		MSC	528	68.20	0.6090	2.0367	2.1711	0.5552	16
		MMSC	531	68.19	0.5754	2.1216	2.2397	0.5263	15
	1,4,4,1	SNVD	535	68.20	0.5979	2.1028	2.2402	0.5428	8
		MSC	534	68.20	0.6287	2.0157	2.2070	0.5540	9
		MMSC	534	68.20	0.6290	2.0147	2.2067	0.5542	9
	2,4,4,1	**SNVD**	**529**	**68.12**	**0.6354**	**1.9930**	**2.1997**	**0.5551**	**5**
		MSC	529	68.12	0.6351	1.9938	2.1995	0.5552	5
		MMSC	530	68.13	0.6297	2.0143	2.2130	0.5522	5

Table 2. PLS statistics for in vivo DOMD (g/100gDM). Averaged scans used.

DOMD	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	88	68.23	0.1407	2.8506	2.8711	0.1354	2
		MSC	90	68.21	0.3398	2.7205	2.9164	0.2469	4
		MMSC	90	68.21	0.3250	2.7508	3.0017	0.2022	4
	1,4,4,1	SNVD	90	68.21	0.4928	2.3846	2.7090	0.3502	4
		MSC	87	68.46	0.6387	1.8467	2.6135	0.2904	7
		MMSC	90	68.21	0.7462	1.6868	2.6075	0.3980	9
	2,4,4,1	SNVD	88	68.20	0.8570	1.2696	2.3070	0.5321	6
		MSC	88	68.20	0.8542	1.2821	2.2946	0.5372	6
		MMSC	90	68.21	0.8492	1.3001	2.5210	0.4373	7

Table 3. MPLS statistics for soluble dry matter (g/100gDM). All replicate scans used.

DMSol	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	534	13.75	0.2270	4.6099	4.7940	0.1625	11
		MSC	528	13.77	0.2465	4.4454	4.6118	0.1875	11
		MMSC	**529**	**13.80**	**0.2518**	**4.4583**	**4.6000**	**0.2020**	**11**
	1,4,4,1	SNVD	530	13.66	0.2154	4.5761	4.7673	0.1469	5
		MSC	530	13.64	0.2659	4.3888	4.6969	0.1578	6
		MMSC	532	13.69	0.2578	4.4703	4.7801	0.1499	6
	2,4,4,1	SNVD	532	13.71	0.1510	4.7902	4.9735	0.0831	2
		MSC	532	13.61	0.1504	4.7917	4.9728	0.0833	2
		MMSC	532	13.61	0.1513	4.7893	4.9688	0.0848	2

Table 4. MPLS statistics for soluble dry matter (g/100gDM). Average scans used.

DMSol	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	87	13.66	0.0168	5.2025	5.2659	0.0057	1
		MSC	87	13.66	0.0186	5.1977	5.2588	0.0084	1
		MMSC	86	13.72	0.0109	5.2243	5.2834	0.0017	1
	1,4,4,1	SNVD	87	13.66	0.0264	5.1771	5.2965	-0.006	1
		MSC	88	13.61	0.0313	5.1607	5.2706	-0.001	1
		MMSC	88	13.61	0.0315	5.1602	5.2716	-0.002	1
	2,4,4,1	SNVD	88	13.61	0.0626	5.0764	5.2771	-0.004	1
		MSC	88	13.61	0.0630	5.0755	5.2756	-0.003	1
		MMSC	88	13.61	0.0640	5.0729	5.2752	-0.003	1

Table 5. MPLS statistics for dry matter degradability (a). All replicate scans used.

DM a	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	520	41.72	0.7979	2.5315	2.7030	0.7695	13
		MSC	520	41.72	0.7812	2.5961	2.7425	0.7557	14
		MMSC	522	41.75	0.7788	2.5662	2.7557	0.7448	14
	1,4,4,1	SNVD	517	41.85	0.8187	2.3102	2.4810	0.7909	9
		MSC	516	41.82	0.8268	2.2778	2.4885	0.7936	10
		MMSC	**514**	**41.81**	**0.8374**	**2.2263**	**2.4197**	**0.8081**	**10**
	2,4,4,1	SNVD	519	41.72	0.8001	2.4866	2.8373	0.7396	6
		MSC	519	41.74	0.7985	2.4910	2.8546	0.7353	6
		MMSC	520	41.76	0.7910	2.5305	2.8795	0.7294	6

Table 6. MPLS statistics for dry matter degradability (a). Averaged scans used.

DM a	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	84	42.06	0.8650	1.9785	2.6149	0.7668	9
		MSC	85	41.96	0.7234	2.9218	3.2404	0.6658	5
		MMSC	84	41.93	0.8620	1.9888	2.7579	0.7376	9
	1,4,4,1	SNVD	86	41.89	0.9203	1.5435	2.6211	0.7719	9
		MSC	85	41.94	0.8159	2.3519	2.6571	0.7662	5
		MMSC	85	41.94	0.8119	2.3771	2.6672	0.7644	5
	2,4,4,1	SNVD	85	41.94	0.8624	2.0332	2.6802	0.7630	4
		MSC	85	41.94	0.8618	2.0374	2.6850	0.7621	4
		MMSC	85	41.94	0.8595	2.0546	2.6947	0.7604	4

Table 7. MPLS statistics for dry matter degradability (b). All replicate scans used.

DM b	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	**SNVD**	**527**	**46.39**	**0.3535**	**4.8991**	**5.2144**	**0.2667**	**13**
		MSC	518	46.10	0.3035	4.7762	4.9373	0.2545	10
		MMSC	521	46.19	0.2897	4.9164	5.0730	0.2430	10
	1,4,4,1	SNVD	527	46.31	0.2704	5.0461	5.3051	0.1922	5
		MSC	527	46.31	0.2563	5.0947	5.3167	0.1887	5
		MMSC	527	46.31	0.2536	5.1041	5.3283	0.1851	5
	2,4,4,1	SNVD	528	46.35	0.1623	5.4776	5.5969	0.1244	2
		MSC	528	46.35	0.1625	5.4771	5.5961	0.1246	2
		MMSC	528	46.35	0.1634	5.4740	5.5934	0.1255	2

Table 8. MPLS statistics for dry matter degradability (b). Averaged scans used.

DM b	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	87	46.38	0.0938	5.6527	5.8422	0.0466	2
		MSC	87	46.38	0.0642	5.7442	5.8908	0.0307	2
		MMSC	86	46.04	0.2061	5.0708	5.4096	0.1168	4
	1,4,4,1	SNVD	87	46.17	0.1821	5.2403	5.6041	0.0890	2
		MSC	87	46.17	0.0917	5.5223	5.7390	0.0446	2
		MMSC	87	46.17	0.1791	5.2501	5.6250	0.0821	2
	2,4,4,1	SNVD	87	46.38	0.0791	5.6981	5.9344	0.0163	1
		MSC	87	46.38	0.0795	5.6971	5.9353	0.0160	1
		MMSC	87	46.38	0.0797	5.6963	5.9351	0.0161	1

Table 9. MPLS statistics for dry matter degradability (c). All replicate scans used.

DM c	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	525	0.0210	0.4626	0.0046	0.0048	0.4241	11
		MSC	529	0.0210	0.4631	0.0046	0.0048	0.4230	12
		MMSC	**528**	**0.0210**	**0.4936**	**0.0045**	**0.0047**	**0.4439**	**14**
	1,4,4,1	SNVD	528	0.0211	0.4658	0.0047	0.0049	0.4137	6
		MSC	530	0.0210	0.4524	0.0047	0.0049	0.3993	6
		MMSC	529	0.0210	0.4471	0.0047	0.0049	0.3930	6
	2,4,4,1	SNVD	530	0.0211	0.4688	0.0047	0.0051	0.3773	3
		MSC	529	0.0211	0.4671	0.0047	0.0050	0.3780	3
		MMSC	530	0.0210	0.4663	0.0047	0.0050	0.3762	3

Table 10. MPLS statistics for dry matter degradability (c). Averaged scans used.

DM c	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	90	0.0214	0.4329	0.0051	0.0057	0.3101	7
		MSC	90	0.0214	0.4053	0.0052	0.0059	0.2569	6
		MMSC	90	0.0214	0.4002	0.0053	0.0059	0.2612	6
	1,4,4,1	SNVD	89	0.0211	0.5331	0.0045	0.0055	0.3131	5
		MSC	89	0.0211	0.4395	0.0049	0.0056	0.3045	3
		MMSC	89	0.0211	0.4319	0.0049	0.0056	0.2942	3
	2,4,4,1	SNVD	89	0.0211	0.4262	0.0050	0.0060	0.1949	2
		MSC	89	0.0211	0.4300	0.0049	0.0059	0.2014	2
		MMSC	89	0.0211	0.4303	0.0049	0.0059	0.2037	2

Table 11.MPLS statistics for soluble nitrogen (g/100gN). Replicate scans.

NSol	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	536	54.21	0.6888	5.5317	5.8169	0.6553	13
		MSC	533	54.12	0.6997	5.4063	5.6384	0.6729	14
		MMSC	537	54.24	0.7031	5.4061	5.7026	0.6691	15
	1,4,4,1	SNVD	534	54.37	0.7416	5.0187	5.6036	0.6773	10
		MSC	**532**	**54.41**	**0.7572**	**4.8497**	**5.4832**	**0.6891**	**11**
		MMSC	534	54.40	0.7406	5.0053	5.6053	0.6742	10
	2,4,4,1	SNVD	536	54.35	0.6569	5.7875	6.2259	0.6023	4
		MSC	536	54.35	0.6582	5.7764	6.2117	0.6041	4
		MMSC	536	54.35	0.6590	5.7693	6.2126	0.6040	4

Table 12. MPLS statistics for soluble nitrogen (g/100gN). Average scans.

Nsol	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	90	54.26	0.6223	6.1309	6.6844	0.5503	5
		MSC	90	54.26	0.6231	6.1242	6.6521	0.5546	6
		MMSC	89	54.21	0.6660	5.7924	6.5652	0.5701	6
	1,4,4,1	SNVD	90	54.26	0.7617	4.8696	6.4888	0.5762	7
		MSC	90	54.26	0.6956	5.5037	6.5793	0.5643	5
		MMSC	90	54.26	0.6949	5.5096	6.5585	0.5670	5
	2,4,4,1	SNVD	90	54.26	0.5669	6.5646	6.9421	0.5149	2
		MSC	90	54.26	0.5674	6.5612	6.9165	0.5185	2
		MMSC	90	54.26	0.5680	6.5563	6.9208	0.5179	2

Table 13. MPLS statistics for NDFa (g/100g fresh). Replicate scans.

NDFa	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	514	14.63	0.6907	0.9344	0.9351	0.6896	3
		MSC	516	14.62	0.6952	0.9279	0.9340	0.6906	5
		MMSC	514	14.63	0.7040	0.9140	0.9204	0.6993	5
	1,4,4,1	SNVD	514	14.61	0.7133	0.8997	0.9444	0.6836	6
		MSC	**514**	**14.65**	**0.7261**	**0.9114**	**0.9503**	**0.7018**	**5**
		MMSC	514	14.65	0.7247	0.9137	0.9514	0.7010	5
	2,4,4,1	SNVD	514	14.61	0.6694	0.9626	0.9967	0.6449	2
		MSC	514	14.61	0.6697	0.9621	0.9961	0.6453	2
		MMSC	513	14.60	0.6683	0.9616	0.9965	0.6432	2

Table 14. MPLS statistics for NDFa (g/100g fresh). Average scans.

NDFa	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	85	14.64	0.7206	0.8969	0.9583	0.6799	3
		MSC	87	14.61	0.6685	0.9755	0.9896	0.6569	2
		MMSC	87	14.61	0.6646	0.9812	0.9964	0.6522	2
	1,4,4,1	SNVD	87	14.61	0.6563	0.9932	1.0823	0.5896	2
		MSC	86	14.63	0.7090	0.9124	0.9884	0.6571	3
		MMSC	86	14.63	0.7065	0.9163	0.9877	0.6575	3
	2,4,4,1	SNVD	87	14.61	0.6704	0.9726	1.0785	0.5925	2
		MSC	87	14.61	0.6717	0.9706	1.0776	0.5932	2
		MMSC	87	14.61	0.6704	0.9726	1.0794	0.5918	2

Table 15. MPLS statistics for Oven Dry Matter (g/100g). Replicate scans.

ODM	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	528	31.32	0.9368	1.0774	1.1264	0.9308	12
		MSC	529	31.30	0.9402	1.0546	1.1100	0.9336	13
		MMSC	526	31.31	0.9426	1.0323	1.0952	0.9353	14
	1,4,4,1	SNVD	528	31.31	0.9378	1.0668	1.1235	0.9309	7
		MSC	529	31.31	0.9382	1.0623	1.1189	0.9313	8
		MMSC	529	31.31	0.9385	1.0601	1.1153	0.9318	8
	2,4,4,1	SNVD	536	31.29	0.9271	1.1591	1.2533	0.9146	4
		MSC	536	31.29	0.9269	1.1606	1.2551	0.9143	4
		MMSC	536	31.29	0.9266	1.1624	1.2555	0.9143	4

Table 16. MPLS statistics for Oven Dry Matter (g/100g). Average scans.

ODM	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	88	31.41	0.9528	0.9145	1.0782	0.9346	8
		MSC	88	31.37	0.9475	0.9558	1.0680	0.9355	6
		MMSC	88	31.38	0.9558	0.8984	1.0602	0.9394	7
	1,4,4,1	SNVD	87	31.42	0.9687	0.7487	0.9249	0.9525	6
		MSC	**87**	**31.35**	**0.9765**	**0.6660**	**0.9273**	**0.9550**	**7**
		MMSC	87	31.35	0.9763	0.6683	0.9314	0.9546	7
	2,4,4,1	SNVD	89	31.26	0.9532	0.9292	1.0975	0.9353	3
		MSC	89	31.26	0.9531	0.9309	1.1009	0.9349	3
		MMSC	89	31.26	0.9534	0.9275	1.0979	0.9353	3

Table 17. MPLS statistics for Crude Protein (g/100g fresh). Replicate scans.

CP	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	525	2.61	0.8760	0.1494	0.1588	0.8597	15
		MSC	527	2.61	0.8621	0.1573	0.1652	0.8476	14
		MMSC	530	2.61	0.8685	0.1539	0.1627	0.8527	15
	1,4,4,1	SNVD	528	2.61	0.9047	0.1316	0.1560	0.8657	14
		MSC	526	2.61	0.9077	0.1295	0.1520	0.8725	14
		MMSC	527	2.61	0.9071	0.1299	0.1529	0.8710	14
	2,4,4,1	SNVD	528	2.61	0.8793	0.1445	0.1967	0.7758	12
		MSC	528	2.61	0.8788	0.1448	0.1970	0.7752	12
		MMSC	528	2.61	0.8797	0.1442	0.1964	0.7765	12

Table 18. MPLS statistics for Crude Protein (g/100g fresh). Average scans.

CP	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	87	2.61	0.8375	0.1690	0.1885	0.7971	6
		MSC	89	2.60	0.7830	0.1954	0.2180	0.7285	5
		MMSC	**86**	**2.60**	**0.8602**	**0.1518**	**0.1752**	**0.8128**	**8**
	1,4,4,1	SNVD	86	2.60	0.8400	0.1682	0.1853	0.8056	3
		MSC	88	2.62	0.8396	0.1713	0.1971	0.7877	4
		MMSC	88	2.62	0.8373	0.1725	0.1974	0.7869	4
	2,4,4,1	SNVD	87	2.61	0.8883	0.1408	0.1989	0.7762	4
		MSC	87	2.61	0.8879	0.1410	0.1986	0.7768	4
		MMSC	87	2.61	0.8846	0.1431	0.2003	0.7729	4

Table 19. MPLS statistics for Starch (g/100g fresh). Replicate scans.

starch	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	525	7.37	0.7033	1.2811	1.3397	0.6753	12
		MSC	521	7.35	0.7354	1.2074	1.2799	0.7024	13
		MMSC	525	7.39	0.7125	1.2700	1.3396	0.6800	11
	1,4,4,1	SNVD	523	7.34	0.7425	1.1757	1.3033	0.6835	9
		MSC	523	7.36	0.7565	1.1541	1.2890	0.6960	10
		MMSC	523	7.36	0.7626	1.1363	1.2871	0.6951	11
	2,4,4,1	SNVD	527	7.40	0.6907	1.3208	1.3629	0.6703	3
		MSC	527	7.40	0.6906	1.3211	1.3631	0.6702	3
		MMSC	527	7.40	0.6906	1.3211	1.3635	0.6700	3

Table 20. MPLS statistics for Starch (g/100g fresh). Average scans.

starch	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	87	7.37	0.7167	1.2644	1.3742	0.6689	6
		MSC	87	7.37	0.7309	1.2322	1.3769	0.6676	7
		MMSC	89	7.44	0.6874	1.3461	1.4823	0.6267	7
	1,4,4,1	**SNVD**	**86**	**7.39**	**0.8718**	**0.8513**	**1.2016**	**0.7469**	**8**
		MSC	86	7.39	0.8662	0.8697	1.2468	0.7275	8
		MMSC	86	7.39	0.8845	0.8080	1.2229	0.7278	9
	2,4,4,1	SNVD	87	7.37	0.7728	1.1324	1.2875	0.7093	3
		MSC	87	7.37	0.7726	1.1327	1.2874	0.7094	3
		MMSC	87	7.37	0.7731	1.1314	1.2865	0.7098	3

Table 21. MPLS statistics for Ash (g/100g fresh). Replicate scans.

ASH	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	532	1.23	0.5264	0.1471	0.1499	0.5075	9
		MSC	528	1.22	0.5994	0.1349	0.1410	0.5618	14
		MMSC	529	1.22	0.5671	0.1395	0.1449	0.5319	13
	1,4,4,1	SNVD	529	1.23	0.5784	0.1381	0.1478	0.5167	7
		MSC	527	1.22	0.6288	0.1299	0.1427	0.5514	8
		MMSC	**526**	**1.22**	**0.6286**	**0.1294**	**0.1419**	**0.5530**	**8**
	2,4,4,1	SNVD	532	1.23	0.5149	0.1493	0.1619	0.4292	3
		MSC	531	1.23	0.4202	0.1622	0.1641	0.4063	2
		MMSC	532	1.23	0.5155	0.1492	0.1621	0.4278	3

Table 22. MPLS statistics for Ash (g/100g fresh). Average scans.

ASH	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	87	1.24	0.6121	0.1273	0.1492	0.4720	8
		MSC	87	1.24	0.6411	0.1204	0.1444	0.4845	9
		MMSC	88	1.23	0.6247	0.1287	0.1515	0.4819	8
	1,4,4,1	SNVD	87	1.23	0.3454	0.1671	0.1701	0.3299	1
		MSC	87	1.23	0.3402	0.1678	0.1710	0.3299	1
		MMSC	87	1.23	0.3405	0.1678	0.1710	0.3225	1
	2,4,4,1	SNVD	87	1.23	0.3915	0.1611	0.1646	0.3723	1
		MSC	87	1.23	0.3913	0.1612	0.1647	0.3718	1
		MMSC	87	1.23	0.3920	0.1611	0.1646	0.3722	1

Table 23. MPLS statistics for pH. Replicate scans.

pH	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	529	3.70	0.7816	0.0866	0.0931	0.7474	16
		MSC	524	3.70	0.7721	0.0872	0.0918	0.7476	15
		MMSC	520	3.70	0.7829	0.0854	0.0891	0.7635	15
	1,4,4,1	SNVD	524	3.70	0.8395	0.0737	0.0834	0.7942	12
		MSC	528	3.70	0.8195	0.0785	0.0870	0.7782	11
		MMSC	528	3.70	0.8327	0.0757	0.0866	0.7806	12
	2,4,4,1	SNVD	517	3.70	0.8198	0.0782	0.0860	0.7820	5
		MSC	516	3.70	0.8200	0.0779	0.0856	0.7825	5
		MMSC	516	3.70	0.8205	0.0778	0.0854	0.7838	5

Table 24. MPLS statistics for pH. Average scans.

pH	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	85	3.69	0.7916	0.0839	0.1043	0.6783	9
		MSC	85	3.69	0.7361	0.0944	0.1115	0.6321	8
		MMSC	86	3.69	0.7882	0.0841	0.1110	0.6312	9
	1,4,4,1	SNVD	85	3.70	0.9280	0.0503	0.0747	0.8407	9
		MSC	86	3.70	0.9027	0.0590	0.0805	0.8183	8
		MMSC	86	3.70	0.8946	0.0614	0.0816	0.8130	8
	2,4,4,1	SNVD	83	3.70	0.9029	0.0561	0.0753	0.8262	4
		MSC	83	3.70	0.9027	0.0562	0.0755	0.8254	4
		MMSC	**83**	**3.70**	**0.9206**	**0.0507**	**0.0733**	**0.8352**	**5**

Table 25. MPLS statistics for starch degradability (a). All replicate scans used.

ST a	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	532	66.50	0.4585	11.4235	11.9414	0.4075	13
		MSC	533	66.46	0.4444	11.5841	11.9198	0.4107	13
		MMSC	533	66.39	0.4672	11.3981	12.0703	0.4015	14
	1,4,4,1	SNVD	535	66.33	0.4835	11.2484	11.9591	0.4155	7
		MSC	533	66.35	0.5138	10.8668	11.7988	0.4263	8
		MMSC	**536**	**66.28**	**0.5205**	**10.8539**	**11.8384**	**0.4289**	**9**
	2,4,4,1	SNVD	532	66.30	0.5209	10.7821	12.3275	0.3727	5
		MSC	532	66.30	0.5215	10.7748	12.3181	0.3737	5
		MMSC	532	66.30	0.5185	10.8089	12.3259	0.3729	5

Table 26. MPLS statistics for starch degradability (a). Averaged scans used.

ST a	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	88	66.14	0.4115	11.9774	13.5458	0.2600	8
		MSC	90	66.11	0.2193	13.9784	14.8323	0.1429	2
		MMSC	90	66.11	0.2095	14.0654	14.5135	0.1794	2
	1,4,4,1	SNVD	88	66.64	0.5861	10.0314	12.6518	0.3529	6
		MSC	89	66.38	0.4877	11.2298	13.3937	0.2842	5
		MMSC	89	66.38	0.4790	11.3250	13.2996	0.2942	5
	2,4,4,1	SNVD	90	66.11	0.3308	12.9410	14.4326	0.1885	2
		MSC	90	66.11	0.3285	12.9636	14.4516	0.1864	2
		MMSC	90	66.11	0.3269	12.9796	14.4174	0.1902	2

Table 27. MPLS statistics for starch degradability (b). All replicate scans used.

ST b	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	530	32.93	0.4986	10.8495	11.3971	0.4458	15
		MSC	530	32.91	0.4724	11.1047	11.4900	0.4343	13
		MMSC	532	32.98	0.4696	11.1608	11.6578	0.4204	14
	1,4,4,1	SNVD	531	32.95	0.5080	10.7545	11.5082	0.4360	7
		MSC	**532**	**33.08**	**0.5261**	**10.5741**	**11.3850**	**0.4498**	**8**
		MMSC	532	32.96	0.5203	10.5954	11.5117	0.4332	8
	2,4,4,1	SNVD	533	33.13	0.5234	10.6259	12.1313	0.3780	5
		MSC	533	33.13	0.5240	10.6197	12.1234	0.3788	5
		MMSC	530	33.07	0.5290	10.5061	11.9271	0.3921	5

Table 28. MPLS statistics for starch degradability (b). Averaged scans used.

ST b	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	88	33.25	0.4254	11.6192	13.1015	0.2809	8
		MSC	90	33.27	0.2072	13.8820	14.5931	0.1445	2
		MMSC	89	33.53	0.1667	14.1223	14.3277	0.1620	2
	1,4,4,1	SNVD	88	32.73	0.5952	9.7609	12.3091	0.3664	6
		MSC	90	33.27	0.3672	12.4022	14.3439	0.1735	4
		MMSC	88	33.25	0.4947	10.8963	13.0902	0.2822	5
	2,4,4,1	SNVD	89	33.52	0.5080	10.8697	13.4834	0.2633	3
		MSC	89	33.52	0.5047	10.9063	13.5101	0.2603	3
		MMSC	89	33.52	0.5017	10.9384	13.4968	0.2618	3

Table 29. MPLS statistics for starch degradability (c). All replicate scans used.

ST c	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	517	0.0906	0.2568	0.0358	0.0362	0.2405	4
		MSC	518	0.0908	0.2461	0.0362	0.0364	0.2353	4
		MMSC	526	0.0923	0.1963	0.0387	0.0389	0.1864	3
	1,4,4,1	SNVD	514	0.0901	0.3622	0.0329	0.0347	0.2893	6
		MSC	514	0.0900	0.3571	0.0327	0.0347	0.2767	6
		MMSC	**514**	**0.0901**	**0.3842**	**0.0323**	**0.0344**	**0.3012**	**7**
	2,4,4,1	SNVD	514	0.0901	0.2703	0.0350	0.0359	0.2343	2
		MSC	514	0.0901	0.2697	0.0350	0.0359	0.2338	2
		MMSC	514	0.0901	0.2708	0.0350	0.0359	0.2342	2

Table 30. MPLS statistics for starch degradability (c). Averaged scans used.

ST c	Math	SC	n	mean	r^2	SEC	SECV	1 - VR	terms
	0,0,1,1	SNVD	88	0.0927	0.2384	0.0382	0.0400	0.1629	3
		MSC	87	0.0916	0.2402	0.0372	0.0390	0.1720	3
		MMSC	86	0.0909	0.1918	0.0382	0.0392	0.1581	2
	1,4,4,1	SNVD	89	0.0938	0.0901	0.0426	0.0429	0.0753	1
		MSC	89	0.0938	0.0894	0.0426	0.0429	0.0748	1
		MMSC	89	0.0938	0.0889	0.0426	0.0429	0.0744	1
	2,4,4,1	SNVD	87	0.0931	0.1175	0.0411	0.0421	0.0789	1
		MSC	87	0.0931	0.1176	0.0411	0.0421	0.0787	1
		MMSC	88	0.0942	0.0974	0.0425	0.0434	0.0564	1