remote sensing

MDPI

Supplementary Material

Table S1 The wavelengths (nm) identified by the Cubist as important for prediction of NV parameters. Each wavelength used in prediction is listed along with the parameter it was linked to, the percent usage in the cubist model, possible biophysical reasons for this wavelength to be useful and references to studies that have also used the wavelengths. Parameters listed are (ADF), ash, dry matter (DM), crude protein (CP), in vivo dry matter digestibility (IVDMD), neutral detergent fibre (NDF) and water-soluble carbohydrates (WSC).

Λ	NV Trait	USE	Possible Association with Chemical Bonds	Reference
405	WSC	82%		
420	ash	85%	identified with SMLR for prediction of ash	[38]
430	NDF	71%	associated with bonds found in NDF	[41]
445	ADF	97%	previously identified for ADF using SMLR	[38]
450	NDF	94%	associated with bonds found in NDF	[41]
485	ADF	97%		
495	CP	24%		
505	NDF	94%		
515	NDF	94%		
520	ash	85%		
545	CP, IVDMD, NDF	24%, 45%, 94%		
550	IVDMD	100%	identified with SMLR for prediction of ADF	[38]
560	ash, IVDMD	62%, 100%	likely relate to chlorophyll	[57]
575	NDF	94%	identified with MLR equations to determine NDF	[43]
585	NDF	94%	identified by SMLR for prediction of ADF	[38]
605	IVDMD	100%		
610	IVDMD	100%		
615	IVDMD, NDF	100%, 94%		
620	ash	100%	likely relate to chlorophyll	[57]
625	ash	31%		
630	IVDMD, NDF	100%, 94%		
635	DM, NDF	77%, 71%	identified by SMLR for prediction of CP	[38]
640	ash, NDF	85%, 94%	likely relate to chlorophyll	[57]
645	NDF, DM	94%, 77%	identified with MLR equations to determine NDF	[43]
655	ash	85%	likely relate to chlorophyll	[57]
660	ash	100%	likely relate to chlorophyll	[57]
660	CP	100%	related to chlorophyll electron transition	[39,46]
665	CP, NDF	100%, 71%	related to chlorophyll electron transition	[39,46]
675	ash	100%	likely relate to chlorophyll	[57]
680	CP	75%	identified in prediction of nitrogen in forage	[49]
685	ash	62%	likely relate to chlorophyll	[57]
690	ash, NDF	62%, 71%	identified with SMLR for prediction of ash	[38]
695	CP, WSC	49%, 82%	identified in prediction of nitrogen in forage	[49]
700	CP, WSC	49%, 82%	identified in prediction of nitrogen in forage	[49]
705	ADF, WSC, CP	77%, 84%, 51%		
710	WSC, ADF, CP, IVDMD	100%, 77%, 100%, 100%	identified as important for prediction of nitrogen in forage	[49]
715	WSC	100%	related to chlorophyll electron transition	[39,46]
720	IVDMD	100%	718 nm corelates to ADF and CP prediction	[59]
725	ADF, WSC, NDF	77%, 66%, 71%	identified as important for prediction of sugars in forage	[49]
730	IVDMD, DM, NDF	100%, 73%, 71%	associated with bonds found in NDF	[41]
735	WSC	100%		
740	NDF	71%		
750	ADF	77%	important for prediction of sugars in forage	[49]
755	ADF, CP	77%, 51%	associated with bonds found in NDF	[41]
780	DM	72%		
790	IVDMD	86%	important for prediction of nitrogen in forage	[49]
810	WSC	84%		

845	CP	75%		
855	ash, ADF, DM	85%, 97%, 72%	identified by SMLR as important for CP, C-H stretches, and aromatics found in lignin	[38,40]
880	WSC, CP	84%, 75%		
895	ADF	97%		
900	ash	31%		
905	DM	93%	previously identified to relate to ADF using SMLR	[38]
920	DM	93%	identified by SMLR as important for CP	[38]
925	ash	85%		
930	DM	99%	Oil C-H stretch, third overtone	[39,41]
935	DM	77%		
940	DM	99%	absorption by the C-H bond in oil molecules	[39]
945	ADF, DM, WSC, NDF	77%, 95%, 84%, 100%	absorption by the C-H bond in oil molecules	[39]
950	ash, IVDMD, NDF, DM	62%, 86%, 100%, 73%	associated with absorption by the C-H bond in oil molecules, may relate to the O-H deformations in starch	[39]
960	DM	73%	NDF wavelength determined with PLSR	[60]
965	ADF, DM, IVDMD	97%, 21%, 86%	may relate to the O-H deformations in starch	[39]
970	ash	85%	water, starch O-H bend first overtone	[41]
975	ash, DM	100%, 72%	O2 absorption	[57]
980	ADF, DM,	75%, 99%,	O2 absorption	[57]
985	ash, IVDMD	19%, 86%	cellulose C-H stretches and or deformations	[39]
990	DM, WSC, IVDMD	93%, 84%, 45%	Starch O-H stretch 2nd overtone	[41]
995	ash, WSC	35%, 84%		
1000	ADF, WSC, IVDMD	99%, 84%, 86%		
1005	WSC	84%		
1010	DM, IVDMD	77%, 86%		
1015	DM, WSC	77%, 84%		
1020	ash, IVDMD	85%, 86%	Protein, N-H stretch	[39]
1025	ADF, ash	75%, 31%		
1035	ash	85%		
1050	WSC, ash, IVDMD	82%, 100%, 86%	O2 absorption	[57]
1055	ADF	77%		
1060	ash, ADF	93%, 77%	Protein, N-H stretch	[39]
1065	WSC	82%		
1075	WSC	100%		
1080	ash, WSC	100%, 18%	lignin C-H stretches in starch molecules and C-H bends	[39]
1085	ash, WSC, IVDMD	93%, 100%, 100%	lignin C-H stretches in starch molecules and C-H bends	[39]
1090	IVDMD	100%		
1095	NDF	94%		
1105	ADF, IVDMD, NDF	97%, 86%, 71%		
1110	DM, CP, NDF	93%, 100%, 94%		
1115	CP, Ash	49%, 100%	lignin C-H stretches in starch molecules and C-H bends in lignin	[39]
1120	ash, IVDMD	65%, 86%	lignin C-H stretches in starch molecules and C-H bends in lignin	[41]
1125	CP, IVDMD	51%, 86%		
1130	CP	100%		
1135	ash, IVDMD	15%, 82%		
1140	WSC, ash, IVDMD	82%,100%, 100%	lignin C-H stretches in starch molecules and C-H bends	[39]
1145	DM, WSC, IVDMD	93%,100%, 100%		
1150	ADF	99%		
1150	ash	62%		
1155	WSC	82%	C-H stretches, and aromatics found in lignin	[40]
1165	ADF, ash	97%, 100%	lignin C-H stretches in starch molecules and C-H bends	[39]
1175	ADF, DM, WSC	77%, 93%, 82%	lignin C-H stretches in starch molecules and C-H bends	[39]
1180	ash	62%		
1190	ash	85%		

1200	ash	62%	identified by SMLR as important for ash. water, cellulose, lignin, starch, O-H bend 1st overtone	[38,39,41]
1210	ADF	97%		
1215	ADF	1%		
1220	ADF	97%	C-H stretches, and aromatics found in lignin	[40]
1230	WSC	16%		
1245	ash	93%	previously identified to relate to ADF using SMLR	[38]
1250	DM	99%		
1255	DM, ADF, CP	99%, 22%, 51%	cellulose C-H stretches and deformations, (within 5nm) of wavelengths used to predict ADF	[39,43]
1260	WSC	100%	cellulose C-H stretches and or deformations	[39]
1270	ADF, CP	9%, 51%		
1275	ADF	23%	Similar to MLR wavelengths equations to predict ADF, cellulose C-H stretch 2nd overtone	[39,43]
1280	WSC	66%		
1295	WSC	100%	Similar to MLR wavelengths equations to predict ADF	[43]
1305	DM	76%		
1310	ADF, DM, NDF	97%, 72%, 23%		[59]
1315	IVDMD, DM	100%, 77%	used in SRTVI for NDF	[61]
1325	ash, WSC, CP	85%, 100%, 75%		
1330	DM	99%		
1335	IVDMD	100%		
1340	CP	75%	cellulose C-H stretches and or deformations	[39]
1345	DM	99%		
1350	ash	31%		
1355	CP	75%	cellulose C-H stretches and or deformations	[39]
1365	ash, CP	13%, 51%	possibly cellulose O-H stretch/deformation	[39]
1390	WSC, ash	16%, 31%	identified as important for prediction of nitrogen in forage	[49]
1395	DM	99%	identified by stepwise multiple linear regression (SMLR) as important for prediction of ash	[38]
1400	IVDMD, WSC, CP, NDF	100%, 82%, 49%, 94%	identified as important for prediction of sugars in forage, water O-H bend, NDF wavelength determined with PLSR	[39,40,49]
1410	IVDMD, DM, NDF	100%, 99%, 94%	Water band	[40]
1415	ash	35%		
1425	IVDMD	100%	N, lignin, N-H symmetrical stretch 1st overtone	[39]
1430	DM	76%	identified by SMLR as important for prediction of ash	[38]
1445	WSC, IVDMD	100%, 100%	lignin O-H stretches aliphatic, 1st overtone/2x C- H stretch, combination band,	[40]
1450	IVDMD	100%	identified as important for prediction of sugars in forage, starch O–H stretch, 1st overtone, C–H stretch, C– H deformation, combination band	[40,41,49]
1455	DM	77%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
1460	ash	100%	N–H stretch, 1st overtone	[39]
1465	ash	93%	lignin C-H stretches in starch molecules and C-H bends in lignin	[39]
1470	ash	100%	lignin C-H stretches in starch molecules and C-H bends in lignin	[39]
1475	ash, WSC	62%, 82%		
1490	ADF	97%	cellulose, sugar, O–H stretch, 1st overtone	[39]
1495	ADF, WSC, IVDMD	97%, 100%, 86%		
1500	ash	85%	associated with O-H stretches in sugar and starch molecules	[39]
1510	IVDMD	100%	protein, N–H stretch, 1st overtone	[39,41]
1525	DM	77%		
1545	CP	51%	lignin, C=O stretch, 3rd overtone. O–H stretch, aromatic, 1st overtone	[39]
1550	CP	100%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
1555	ADF, NDF, ash	75%, 29%, 85%	amide I and Amide II region of the spectrum, identified by stepwise multiple linear regression (SMLR) as important for prediction of ash	[38,48]
1570	ADF	97%	Similar to MLR wavelengths equations to predict ADF	[43]
1575	WSC	100%		

1585	ash	100%	may relate to the O=H stretch in cellulose and was very similar to ADF related wavelength 1578 nm, previously identified with MPLS	[42]
1595	CP	75%	associated with O-H stretches in sugar and starch molecules	[39]
1600	DM, CP	21%, 49%		
1610	DM	93%		
1615	ADF, WSC, NDF	97%, 82%, 29%	identified as important for prediction of nitrogen in forage	[49]
1660	IVDMD	100%	identified as important for prediction of sugars in forage	[49]
1675	NDF	100%	lignin, C-H stretch, aromatic, 1st overtone, identified as important for metabolizable energy (ME) with MSLR	[39,39]
1700	DM	93%	linked to digestibility previously	[39]
1705	CP	75%	related to the O-H stretch in lignin	[39]
1715	CP, IVDMD	75%, 100%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
1785	CP	51%	lignin, C—H stretch, aliphatic, 1st overtone	[39]
1795	WSC	100%	identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
1800	IVDMD	100%		
1805	CP	49%		
1810	CP	49%	identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
1820	ADF	97%	cellulose, O—H stretch/C—O stretch, 2nd overtone	[39]
1825	DM	96%		
1830	DM	21%	related to cellulose aromatic or aliphatic C-H stretches, or possibly starch and lignin O-H and C-H stretches and deformations	[39,40]
1835	ADF	99%		
1850	DM	93%		
1860	DM	97%		
1875	ADF, NDF	99%, 94%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
1880	ADF, IVDMD	30%, 100%		
1885	ADF	77%		
1890	ADF, CP	75%, 75%		
1895	ADF, IVDMD, NDF	97%, 86%, 94%		
1900	ADF, CP	99%, 75%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
1910	CP, IVDMD	75%, 100%		
1935	CP	24%		
1940	ADF, WSC	77%	water, lignin, protein, starch, cellulose, O–H stretch, O–H deformation	[39]
1950	WSC	16%	O-H stretches, and deformations found in starch, water, lignin, protein and cellulose	[41]
1955	IVDMD	100%		
1965	ADF	97%		
1970	CP	75%	N—H asymmetrical stretch	[39]
1980	CP, WSC	100%, 16%	N–H asymmetry	[39]
1985	ADF, CP	75%, 75%	may be due to N-H asymmetry in protein	[46,47]
1990	ash, CP	85%, 75%		
1995	CP	100%		
2005	DM, NDF	77%, 100%		
2020	CP	49%		
2025	NDF	23%	may relate to the O-H deformations in starch	[39]
2030	DM	77%		
2035	WSC, CP	100%, 51%		
2040	ash	85%		
2045	CP	49%		
2050	CP	51%	O-H stretches, and deformation found in protein, nitrogen, starch, water, and cellulose	[41]
2055	ash, ADF, WSC	93%, 77%, 100%	protein, N—H asymmetrical stretch	[39]
2060	CP, NDF	94%, 100%	protein, N=H bend, second overtone/ N=H bend/N– H stretch	[39,41]

2065	ADF, DM, WSC	97%, 73%, 82%	related to the second overtone N=H bend in protein, relates to protein and nitrogen with a N=H bend, associated with hemicellulose, a component of ADF	[39,46,47]
2070	IVDMD	100%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
2075	IVDMD, ADF	45%, 99%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2085	ADF, ash, IVDMD	97%, 93%, 89%		
2090	ADF	97%	identified by SMLR as important for prediction of ash	[38]
2095	DM, NDF	77%, 94%		
2100	ADF, DM, WSC, IVDMD, NDF	97%, 21%, 44%, 100%, 100%	associated with bonds found in NDF, related to cellulose aromatic or aliphatic C-H stretches, starch and lignin O-H and C-H stretches and deformations, linked to the organic bonds found in cellulose, protein and starch in grass silage	[39,40,41,45]
2105	ADF, DM, IVDMD	97%, 73%, 86%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage, related to cellulose aromatic or aliphatic C-H stretches, or possibly starch and lignin O-H and C-H stretches and deformations	[39,40,44,45]
2110	DM, IVDMD	76%, 86%	linked to the organic bonds found in cellulose, protein and starch in grass silage, wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2115	ash	62%		
2120	ADF, ash, DM	99%, 62%, 77%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2125	WSC, CP, IVDMD	44%, 24%, 100%		
2130	ash, NDF	62%, 94%	identified by SMLR as important for prediction of CP	[38]
2135	IVDMD	86%		
2140	CP, ADF	49%, 97%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2145	DM, IVDMD	93%, 100%	related to cellulose aromatic or aliphatic C-H stretches, or possibly starch and lignin O-H and C-H stretches and deformations	[39,40]
2180	CP	100%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
2200	DM	77%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2215	DM	77%	N-H bends, C-H stretches and C=O stretches in protein	[39]
2250	WSC	82%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
2255	DM, ash, WSC	21%, 62%, 82%	link to starch O-H stretches and deformations	[46]
2260	WSC, IVDMD	100%, 37%	digestibility	[39]
2265	WSC, ADF, DM	82%, 97%, 77%	related to cellulose aromatic or aliphatic C-H stretches, or possibly starch and lignin O-H and C-H stretches and deformations, linked to digestibility previously	[39,40]
2270	ash, DM, IVDMD	62%, 99%, 100%	C–H stretch/O–H stretch/CH2 bend/CH2 stretches found in cellulose and lignin	[39,41]
2275	IVDMD	86%	cellulose, sugar and starch C-H or O-H stretches and CH2 bends	[39]
2280	CP, DM	75%, 76%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage, C─H stretch/CH2 deformation found in starch and cellulose	[41,44,45]
2295	DM	96%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[45]
2300	IVDMD	86%	cellulose C═C stretch	[39]
2315	WSC, ADF	22%, 22%	wavelengths identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2320	IVDMD	86%	O-H stretch found in cellulose and has been previously associated with ADF	[41]

2325	DM,	93%,	O-H stretch found in cellulose and has been previously associated with ADF	[41]
2345	IVDMD	86%	protein, N–H bend, 2nd overtone	[39]
2365	ADF	47%	linked to the organic bonds found in cellulose, protein and starch in grass silage	[44]
2370	IVDMD	37%		
2380	ash	19%	O-H stretches and aromatic deformations	[41]
2385	WSC	84%	identified by PCA and SMLR analysis of IVDMD in grass silage	[44,45]
2405	IVDMD	86%		
2425	DM	73%		
2435	ash	65%		