



This is an author produced version of a paper published in
Computers and Electronics in Agriculture.

This paper has been peer-reviewed but may not include the final publisher
proof-corrections or pagination.

Citation for the published paper:

Zhenjiang Zhou, Julien Morel, David Parsons, Sergey V. Kucheryavskiy,
Anne-Maj Gustavsson. (2019) Estimation of yield and quality of legume and
grass mixtures using partial least squares and support vector machine
analysis of spectral data. *Computers and Electronics in Agriculture*.

Volume: 162, Number: July 2019, pp 246-253.

<https://doi.org/10.1016/j.compag.2019.03.038>

Access to the published version may require journal subscription.

Published with permission from: Elsevier.

Standard set statement from the publisher:

© Elsevier, 2019 This manuscript version is made available under the CC-BY-NC-ND 4.0
license <http://creativecommons.org/licenses/by-nc-nd/4.0/>

Epsilon Open Archive <http://epsilon.slu.se>

1 **Estimation of yield and quality of legume and grass mixtures using partial least squares**
2 **and support vector machine analysis of spectral data**

3 *Zhenjiang Zhou^{a b#}, Julien Morel^{b#}, David Parsons^b, Sergey V. Kucheryavskiy^c, Anne-Maj*
4 *Gustavsson^{b*}*

5 *^a College of Biosystems Engineering & Food Science, Zhejiang University, 310058*
6 *Hangzhou, China*

7 *^b Department of Agricultural Research for Northern Sweden, Swedish University of*
8 *Agricultural Sciences, SE-901 83 Umeå, Sweden*

9 *^c Department of Chemistry and Bioscience, Aalborg University, DK-6700 Esbjerg, Denmark*

10 **Corresponding author: Anne-Maj Gustavsson*

11 *Email: Anne-Maj.Gustavsson@slu.se*

12 *# Shared first author*

13 *Email of authors:*

14 *Zhenjiang Zhou Email: zhenjiangz@zju.edu.cn*

15 *Julien Morel Email: julien.morel@slu.se;*

16 *David Parsons Email: david.parsons@slu.se;*

17 *Sergey V. Kucheryavskiy Email: svk@bio.aau.dk;*

18 *Anne-Maj Gustavsson Email: Anne-Maj.Gustavsson@slu.se;*

19

20

21

22 **Abstract**

23 The project aim was to estimate N uptake (N_{up}), dry matter yield (DMY) and crude protein
24 concentration (CP) of forage crops both during typical harvest times and at a very early
25 developmental stage. Canopy spectral reflectance of legume and grass mixtures was
26 measured in Sweden using a commercialized radiometer (400 – 1000 nm range). In total, 377
27 plant samples were tested in-situ in different grass and legume mixtures (6 grass species and
28 2 clover species) across two years, two locations and five N rates. Two mathematical
29 methods, namely partial least squares (PLS) and support vector machine (SVM) were used to
30 build prediction models between N_{up} , DMY and CP, and canopy spectral reflectance. Of the
31 total 377 samples, 251 were randomly selected and used for calibration, and the remaining
32 126 samples were used as an independent dataset for validation. Results showed that the
33 performance of SVM was better than PLS (based on mean absolute error (MAE) for both
34 calibration and validation datasets) for the estimation of all investigated variables. Results for
35 the validation set showed that the MAEs of PLS and SVM for N_{up} estimation were 17 and 9.2
36 kg/ha, respectively. The MAEs of PLS and SVM for DMY estimation were 587 and 283
37 kg/ha, respectively. The MAEs of PLS and SVM for CP estimation were 2.8 and 1.8 %,
38 respectively. In addition, a subsample, which corresponded to an early developmental stage,
39 was analysed separately with PLS and SVM as for the whole dataset. Results showed that
40 SVM was better than PLS for the estimation of all investigated variables. The high
41 performance of SVM to estimate legume and grass mixture N uptake and dry matter yield
42 could provide support for varying management decisions including fertilization and timing of
43 harvest.

44 **Keywords:** Dry matter yield; Forage crop; Grass; Hyperspectral reflectance; Nitrogen
45 uptake; Nutritive value; Partial least squares; Red and white clover; Support vector machine.

46

47

48 **1. Introduction**

49 Estimation of forage biomass and quality in the field is important for livestock farmers to
50 make decisions such as adjusting the stocking rate, fertilization rate and timing, and harvest
51 time. Laboratory wet chemical analysis has been used as the conventional method to
52 determine nutritive value. However, these methods are laborious and expensive, and lead to
53 time delays for decision making. Alternatively, near-infrared reflectance spectroscopy
54 (NIRS) has been applied as a faster method to estimate nutritive value (Norris et al., 1976),
55 particularly fibre, crude protein (CP), and metabolisable energy (ME). However, laboratory-
56 based NIRS still involves laborious cutting and processing of plant samples. A fast and less
57 laborious method is needed to estimate nutritive value, in order to provide rapid information
58 for supporting decision making.

59 The canopy spectral reflectance (CSR) method has been developed to estimate crop biomass
60 and physiochemical properties (e.g. N concentration), based on the principle that CSR in
61 visible and near-infrared (NIR) bands is primarily affected by physiochemical properties (e.g.
62 chlorophyll concentration) and cell structure of the canopy (Campbell, 1996). Numerous
63 studies have concluded that CSR in the red band correlates well with chlorophyll and N
64 concentration (Heath, 1969; Hatfield et al., 2008), and that CSR in the NIR range correlates
65 well with plant biomass and leaf area (Allen and Richardson 1968).

66 Field spectroscopy has been successfully used to estimate nutritive value of forage crop
67 (Starks et al., 2004; Biewer et al., 2009b; Pullanagari et al., 2012) and yield (Biewer et al.,
68 2009a). Currently, an already commercialized spectrometer named the Yara N-sensor (Yara
69 International ASA, Oslo, Norway), has been widely applied in Northern Europe to estimate N

70 status of winter wheat and assist N fertilization decisions. However, it has not been tested in
71 forage crops, even though increasing interest has been raised in this area, and forages often
72 dominate agricultural land use, such as in Sweden where the current study was undertaken.

73 In addition to the potential practical application, from a scientific perspective, there has been
74 little research conducted to estimate forage crop yield and quality using field spectroscopy.
75 The advantage of a field spectroscopy method is that it measures CSR in a broad range of
76 bands, providing an abundant supply of information. Chemometric methods, which are used
77 for the analysis of spectral data, include principal component analysis (PCA), partial least
78 squares regression (PLS), and machine learning methods such as support vector machine
79 (SVM) (Mutanga et al., 2005; Zhao et al., 2007; Karimi et al., 2008; Wang et al., 2013). For
80 estimation of crop agronomic variables using spectral reflectance data, PLS has typically
81 been used, for example to estimate winter wheat N concentration (Li et al., 2014a), and
82 winter wheat leaf area index (Li et al., 2014b). PLS has also been shown to work well to
83 estimate yield and quality in forage crops (Mutanga et al., 2005; Zhao et al., 2007; Biewer et
84 al., 2009). In contrast to PLS, which is a linear mathematical method, SVM is a non-linear
85 method and based upon statistical learning theory. The principle of SVM and its solution is
86 described in Cristianini and Shawe-Taylor (2000). Non-linear multivariate models of SVM
87 have been used for many applications, e.g. rice root density (Xu et al., 2017), weed and maize
88 classification (Zheng et al., 2017), wheat plant density estimation (Jin et al., 2017), leaf area
89 estimation (Durbha et al., 2007; Yang et al., 2008), crop N concentration (Karimi et al., 2008;
90 Wang et al., 2013; Zhai et al., 2013). We are unaware of any studies conducted to predict
91 yield or quality parameters of forage crops in the field using SVM. Therefore, the objective
92 of this study was to test the performance of spectral reflectance data analyzed using PLS and
93 SVM, for estimating forage yield and quality parameters.

94 **2. Materials and Methods**

95 *2.1. Site description and plant sampling*

96 Field experiments were carried out in 2015 and 2016 at two sites in Sweden: Röbbäcksdalen
97 (63° 48' N, 20° 14' E) and Rådde (57° 36' N, 13° 15' E). Each site included different
98 mixtures of grass and legume species (Table 1-2). The soil at Röbbäcksdalen is a silt loam (1%
99 clay, 76% silt, 23% sand) with 4 % organic matter. The soil at Rådde is also a silt loam (1 %
100 clay, 53 % silt 46 % sand) with 6 % organic matter. The plot size was 1.5×13.5 m at
101 Röbbäcksdalen and 2.1×12.5 m at Rådde. The harvested area was 20.3 m² at Röbbäcksdalen
102 and 18.8 m² (1.5 ×12.5 m) at Rådde, which was used for fresh yield determination. A
103 representative sub-sample was selected from the harvested material for dry matter
104 determination and chemical analysis. Sub-samples were oven-dried at 60°C for 48 hours until
105 they reached a constant weight. Dried samples were ground to pass a 1-mm sieve. Nitrogen
106 concentration of dry samples was determined using the Kjeldahl method.

107 Crops at each site were harvested three times each year. The harvest dates at Rådde were 4
108 June, 10 July and 24 August in 2015; and 27 May, 5 July and 22 August in 2016. The harvest
109 dates at Röbbäcksdalen in 2016 were 13 June, 18 July, and 2 September, however for the 1st
110 harvest the YARA N-sensor data are not available due to equipment malfunction. In addition,
111 in 2016 samples were also taken at an early developmental stage before the 1st harvest
112 (corresponding to the time window of N fertilization), in order to investigate if crop N uptake
113 can be estimated using field measured reflectance. The early cutting dates were 12 May and 3
114 June at Rådde and Röbbäcksdalen, respectively.

115 ***Table 1 and 2***

116 *2.2. Canopy spectral reflectance measurement*

117 On the same day as harvesting, canopy spectral reflectance was measured using a Yara N-
118 sensor (Yara International ASA, Oslo, Norway) spectrometer, which is a commercialized

119 instrument used for site-specific fertilization in Sweden and other European countries. It
120 measures CSR at wavelengths of 400 – 1000 nm with resolution of 10 nm, a 25° field of view
121 and a zenith view angle of 45° (Fig.1). The solar radiation was measured simultaneously for
122 calculation of CSR reflectance by dividing the radiant exitance by the solar irradiance (the
123 reader is referred to (Schaepman-Strub et al., 2006) for definitions). The sensor was held at a
124 constant height of 1.0 m above the canopy. Measurements were taken around noon when the
125 sun was not obscured by clouds. To take into consideration the effect of solar direction on
126 CSR, measurements were taken at opposite ends of each plot, corresponding to facing the sun
127 and opposite to the sun direction. The mean value of measurements in each plot was used for
128 data analysis.

129 ***Fig. 1***

130 *2.3. Data analysis*

131 Spectral reflectance data and laboratory measurements of the variables of interests were
132 analysed with two mathematical methods, namely partial least squares (PLS) and support
133 vector machine (SVM) to build regression models between CSR and variables of interest.
134 Two datasets were used to build the models. The first one consisted of 377 samples that were
135 randomly split into calibration (251 samples) and validation (126 samples) subsets. This
136 dataset included all available data across sites, years, species, harvest dates and N fertilization
137 rates. The aim was to test if a robust prediction model could be built for estimations of N_{up}
138 (the nitrogen uptake, in kg/ha), DMY (the dry matter yield, in kg/ha) and CP (the crude
139 protein concentration, in % of DM). In the second dataset, only the data acquired at an early
140 developmental stage (i.e., sampled prior to the 1st harvest) were considered. This dataset
141 consisted of 78 samples split into calibration (52 samples) and validation (26 samples)
142 subsets. The aim of only using data from an early developmental stage was to test if the

143 variables of interest (especially N uptake) can be well estimated, as accurate estimation of N
144 uptake could provide information on soil N mineralization at a very early stage and guide
145 decision support on N fertilization.

146 *2.3.1 Partial least squares*

147 PLS is a prominent method which can effectively deal with multicollinearity in data and
148 eliminate the less important or redundant variables. It is especially useful when the number of
149 predictor variables is greater than the number of observations (Wold et al., 2001). PLS is used
150 to linearly relate predictor variables (CSR in this study) and response variables (N_{up} , DMY
151 and CP) by decomposing data matrices (predictors and response variables) simultaneously
152 using a set of orthogonal latent variables (PLS-components). The orientation of latent
153 variables is selected to maximize covariance between the predictors and response values
154 represented by the components.

155 In this research we implemented PLS methods using the “mdatools” package in the R
156 programming environment (R Core Team, 2016). Models were built using a calibration set
157 and full cross-validation. The optimal number of components was identified by looking at the
158 minimum root mean square error (RMSE) for the cross-validated predictions. External
159 validation using an independent validation dataset was subsequently conducted to test the
160 performance of the calibrated model.

161 *2.3.2. Support vector machine*

162 Support vector machine (SVM) is a supervised statistical learning algorithm developed by
163 Vapnik (1982) that can be applied to both classification and regression tasks. It has gained
164 increasing popularity for various purposes such as expression recognition (Lekdioui et al.,
165 2017), water resources management (Deo et al., 2017) and medicine (Zheng et al., 2014). The
166 general idea behind SVM is to map the vectors of covariates into a higher dimensional

167 feature space using a kernel trick where a linear regression can be performed. Details of the
168 theory of SVM are described in Cristianini and Shawe-Taylor (2000). The linearity of the
169 relationship between N_{up} , CP and DMY and the spectral reflectance remains uncertain. With
170 this consideration, a SVM, capable of constructing both linear and nonlinear inversion, was
171 employed in this study. We used the *svm* function from the “e1071” package of the R
172 software (R Core Team, 2016) to estimate N_{up} , CP and DMY of the experimental plots based
173 on their spectral reflectance. Based on a radial basis kernel, we performed a grid search to set
174 the optimal values of the hyper-parameters ε , C and γ , as they influence the accuracy and
175 generalisation capabilities of the SVM (Cherkassky and Ma, 2004; Wang et al., 2003). ε is
176 the insensitive-loss function that penalizes the prediction errors that fall within the $\pm\varepsilon$ range.
177 C is the cost parameter that defines the penalty weight of deviations higher than $\pm\varepsilon$. Finally, γ
178 is a radial basis kernel-specific parameter that controls the tradeoff between error due to bias
179 and the variance in the adjusted model.

180 In order to test the performance of different models, mean absolute error (MAE), root mean
181 square error (RMSE) (Loague and Green, 1991), and R^2 were compared for the calibration
182 and validation subsets.

$$183 \quad MAE = \frac{\sum_{i=1}^n |P_i - O_i|}{n} \quad (1)$$

$$184 \quad RMSE = \sqrt{\frac{1}{n} \times \sum_{i=1}^n (P_i - O_i)^2} \quad (2)$$

185 where P_i and O_i are predicted and observed values, respectively, and n is the number of
186 samples.

187 **3. Results**

188 *3.1. Statistics of nitrogen uptake, dry matter yield and crude protein concentration*

189 At Rådde, the average N_{up} , DMY and CP were 84 kg/ha, 3131 kg/ha, and 17 %, respectively,
190 and at Röbbäcksdalen, 30 kg/ha, 1785 kg/ha, and 12 %, respectively (Fig.2). There was large
191 variation within all response variables at both sites, providing a wide range of data for the
192 calibration of the models.

193 **Fig. 2**

194 3.2. Spectral measurements

195 Examples of spectral reflectance signatures were plotted to show the typical effects of N rate
196 and mixture type (Fig.3, Fig.4). In the visible range (400 – 700 nm), the reflectance was
197 lower in the blue and red parts of the spectrum, and higher in the green part of the spectrum,
198 due to the leaf-contained chlorophyll. The spectral signature showed a sharp increase
199 between 680 and 740 nm (known as the red-edge domain) to reach a plateau in the measured
200 near infrared (NIR) domain, from 740 to 1000 nm. A concave shape was systematically
201 observed between 950 and 1000 nm, due to the leaf-contained water (Peñuelas et al., 1993).
202 “Pure grass” showed a higher reflectance in the visible range compared to “grass and clover
203 mixture”, whereas in the NIR the reflectance was higher for the “grass and clover mixture”
204 (Fig. 3). The N rate also had an influence on the spectral signature, as treatments fertilized
205 with high N levels (300 kg N/ha) showed higher reflectance in the NIR domain and lower
206 reflectance in the visible domain, when compared to the zero N treatment (Fig. 4). All spectra
207 showed an increase of reflectance during the season, which is particularly noticeable in the
208 NIR domain. This increase is more pronounced for the “grass and clover mixture” than for
209 the “pure grass” (Fig. 3). The dynamics are similar for the two contrasted nitrogen levels
210 (Fig. 4).

211 **Fig. 3**

212 **Fig. 4**

213 *3.3. Calibration of PLS and SVM models*

214 R^2 values obtained for PLS models were in the range of 0.65-0.77 for the whole dataset and
215 0.79-0.88 for the early cutting dataset (Table 3). R^2 values obtained for SVM were in the
216 range of 0.90-0.96 for the whole dataset and 0.95-0.98 for the early cutting dataset.

217 For the whole dataset, MAE for PLS were 15.4 kg/ha, 512 kg/ha and 2.4 %-units for N
218 uptake, dry matter yield and crude protein concentration, respectively (Table 3). These MAEs
219 were higher than the corresponding statistics for SVM. For the early cutting dataset, the
220 MAEs were lower than for the whole dataset, and were again lower for SVM than for PLS.
221 The RMSE results followed the same trend as MAE.

222 **Table 3**

223 *3.4. Validation of PLS and SVM model*

224 Both PLS and SVM were validated using randomly selected sub-samples from either the
225 whole dataset or early cutting dataset (Table 4). For the whole dataset, R^2 values for PLS
226 were 0.68 – 0.69 and for SVM 0.84 – 0.92. For the early cutting dataset, R^2 values for PLS
227 were 0.80 – 0.92 and for SVM 0.83 – 0.94. Typically, R^2 values for validation were lower
228 than those for calibration, with some exceptions.

229 For the whole dataset, MAE of SVM were 9.2 kg/ha, 283 kg/ha and 1.8 %-units for N uptake,
230 dry matter yield and crude protein concentration, respectively (Table 4). For the early cutting
231 dataset, MAE of SVM were 7.5 kg/ha, 123 kg/ha and 2.0 %-units for N uptake, dry matter
232 yield and crude protein concentration, respectively. Both MAE and RMSE of validation were
233 smaller for SVM than for PLS, irrespective of the dataset or variables.

234 The measured and predicted variables of the validation subsets were plotted using different
235 crop species and experimental sites as markers (Fig. 5 and Fig. 6). Across the whole dataset
236 and early cutting dataset they are distributed evenly around the 1:1 lines. No distinct groups

237 of species or site factors were detected, implying that forage species, cultivars and sites did
238 not impose substantial influence on the prediction using PLS and SVM models. A stronger
239 relationship between measured and predicted values was found in the early cutting dataset
240 than the whole dataset.

241 ***Table 4***

242 ***Fig. 5 and Fig. 6***

243 **4. Discussion**

244 *4.1. Reflectance measurements*

245 The observed effects of N fertilization on reflectance are consistent with previous studies
246 (e.g., Hinzman et al., 1986; McMurtrey et al., 1994; Yoder and Pettigrew-Crosby, 1995;
247 Daughtry, 2000). These results are mainly related to (i) an increase in chlorophyll content that
248 leads to a reduced reflectance in the visible range (especially in the green and red domains of
249 the spectrum) and (ii) an increase of the leaf biomass that leads to an increased reflectance in
250 the NIR range (Fig. 4).

251 A similar pattern is observed when clover is added in the crop mixture (Fig. 3). Clover is a
252 leguminous plant, and as such, it is less sensitive to low N fertilization, due to its ability to fix
253 atmospheric N. This can explain the differences in reflectance measured for pure grass vs
254 clover-grass mixtures, although the differences in leaf chemistry and architecture between
255 species might also impose influence on their spectral reflectance signatures.

256 An increase of the measured reflectance is observed for all samples (exemplified in Fig. 3 and
257 Fig. 4). Such an increase can be explained by the concomitant increase of temperatures
258 throughout the summer. The greater increase for the “grass and clover mixture” might
259 suggest that there is either (i) a lower nitrogen limitation for the growth when compared to

260 “pure grass” or (ii) that the canopy structure of the “grass and clover mixture” would induce a
261 stronger light reflection when compared to “pure grass”.

262 *4.2. PLS and SVM*

263 The aim of this study was to predict N_{up} , DMY and CP using reflectance in the range of 400 –
264 1000 nm measured using a commercialized tool. In this study, SVM performed better than
265 PLS (in terms of MAE, RMSE and R^2) for estimation of all response variables. Advantages
266 of SVM lie in its robustness and insensitivity to the number of dimensions (Brown et al.,
267 2000; Wu et al., 2008; Yao et al., 2015). SVM is also better than other methods at coping
268 with potential confounding factors for different varieties, sites and developmental stages (Yao
269 et al., 2015). Our results indicate that a non-linear relationship might exist between leaf N and
270 canopy spectral reflectance (which can be seen in the top-right sub-plot in Fig. 5). This can
271 also be a reason that non-linear SVM was superior to linear PLS for estimating quality
272 variables in this study. Our results corroborate those of Yao et al. (2015) and Du et al. (2016),
273 who showed that SVM performed better than PLS to estimate wheat and rice N
274 concentrations.

275 *4.3. Application of oblique optics sensors and its limitations*

276 Many studies using spectral reflectance for N estimation have been conducted with handheld
277 sensors that measured CSR in the nadir direction. One novelty of this study is that the optical
278 lens had an oblique view of 45 degrees (Fig. 1). The design of the instrument imitates the
279 commercialised tractor-mounted version (Fig. 1), which is already widely used in northern
280 Europe. Therefore, the results from this study are highly transferable to the tractor-mounted
281 spectral sensor (e.g. by encoding SVM methodology to a portable and cheap computer that is
282 connected to the spectral sensor). The advantage of the oblique sensor is that it can be more
283 easily fitted to a tractor (Fig.1) than a nadir-directed sensor. However, oblique sensors can

284 potentially cause the problem of measurement variation depending on tractor driving
285 direction with respect to the sun position. For example, the spectral reflectance from the
286 oblique sensor facing to the sun-lit side of the plant will be different from the one facing the
287 shaded side of the plant. This problem was addressed in our study by measuring spectral
288 reflectance from each end of the experimental plots. For the application of this method on the
289 tractor-mounted sensor, the variation of reflectance caused by tractor driving direction and
290 sun position can be addressed by configuring the device in a way that fibre optics are oriented
291 in four directions (two fibre optics on each side of the tractor). Such a configuration can take
292 measurement in four directions, encompassing both the sun-lit and shaded sides of the plant.
293 As the interaction between canopy geometry, solar elevation angle, solar azimuth angle and
294 viewing angle influence observed reflectance (Jackson et al., 1979; Ranson et al., 1985),
295 further studies are needed to clarify the response of reflectance to different combinations of
296 solar position and sensor viewing angle for legume and grass mixture fields. A field bi-
297 directional reflectance distribution function method could be used to build such a
298 relationship. Despite the problems related to the oblique sensors mentioned above, it has been
299 demonstrated that oblique sensors allow a more accurate estimation of field traits compared
300 to nadir sensors. The potential of an oblique sensor for N status estimation has been
301 investigated by Mistele et al. (2004) and Mistele and Schmidhalter (2008), who measured
302 canopy reflectance from four oblique quadrilateral-views. This makes the measured
303 reflectance almost independent of the solar zenith angle since both the sun-lit and shaded
304 sides of plants can be captured by the sensor. Another disadvantage related to nadir
305 measurement is that it only measures the reflectance of the plant upper layer. Oblique sensors
306 can capture more information of plant structure by measuring reflectance deeper in the
307 canopy, thus improving the estimation accuracy of plant characteristics (Diner et al., 1999).
308 The advantages of oblique sensors are demonstrated in several studies. For example, Gianelle

309 and Guastella (2007) showed that oblique measurement is more appropriate than nadir for
310 determining grass dry matter yield. Aparicio et al. (2004) found that the wheat dry matter
311 yield can be more precisely estimated by oblique measurement when LAI is high. Perbandt et
312 al. (2011) demonstrated that oblique measurement is better than nadir for DMY and
313 metabolisable energy of maize, while CP is better estimated by nadir measurement.

314 The oblique sensor in this study showed good estimation of N uptake during the early
315 developmental stage, which is the most important period for N application. Mounting oblique
316 sensors on a tractor offers the possibility to scan the crop beside the tractor and apply N
317 fertilizer accordingly.

318 *4.4. Generalization of the models*

319 Heterogeneous sward structures, varying number of species and varieties, different locations,
320 and different atmospheric conditions may impose confounding effects on the relationship
321 between spectral reflectance and nutritive value. For example, Biewer et al. (2009b) built
322 separate prediction models for grass and legumes, resulting in enhanced prediction accuracy
323 for CP. The intention of our study was to estimate forage yield and quality by spectral
324 methods across sites, mixture types and developmental stages rather than have to develop
325 specific models for different sites, developmental stage and species mixtures. Neither the
326 performances of PLS or SVM models were strongly influenced by those factors (Fig. 5).
327 Thus, the model developed from the whole dataset in this study might be more generally
328 useful compared with those based on a given mixture type or developmental stage, with the
329 caveat that with more data collection such models can be improved and refined. One of the
330 constraints of this study is that spectral method was only tested on CP, while other forage
331 nutrition variables were not measured, nonetheless, there is a high correlation in forage crops
332 between CP, fibre content, ash, lignin, and metabolisable energy (Pullanagari et al., 2012),

333 indicating potential for extending the method from this study for estimation of other nutrition
334 variables.

335 **5. Conclusion**

336 The SVM method was better than PLS for forage yield and quality estimation. The
337 performance of SVM models for estimating forage yield and quality was consistent among
338 the calibration and validation datasets. These results imply that SVM is a promising tool to
339 analyze on-field acquired spectral data for the estimation of forage crop quality and yield,
340 especially when considering the tractor-mounted Yara-N sensor. Mounting oblique sensors in
341 the very early crop developmental stage on a tractor offers the possibility to scan the crop and
342 apply N fertilizer accordingly. The results presented in this study need to be confirmed with
343 further measurements that would provide a more comprehensive database of sun and sensor
344 interactions, including measurements during cloudy days, various row directions and solar
345 positions. Nevertheless, as the models showed a good robustness and accuracy for various
346 site and mixtures combinations, it is reasonable to assume that the models developed in this
347 study could provide farmers with real time information on-the-go during the harvest period,
348 informing the farmer about forage yield and quality.

349 **Acknowledgement**

350 The work was supported by the FORMAS, MISTRA and Lantmännen foundation. The study
351 was conducted using data and material from Röbbäcksdalen, SITES (Swedish Infrastructure
352 for Ecosystem Science), a national coordinated infrastructure, supported by the Swedish
353 Research Council.

354 **References**

355 Allen, W.A., Richardson, A.J., 1968. Interaction of light with a plant canopy. *J. Opt. Soc. Am.* 58, 1023-1028.

- 356 Aparicio, N., Villegas, D., Royo, C., Casadesus, J., & Araus, J. L., 2004. Effect of sensor view angle on the
357 assessment of agronomic traits by groundlevel hyperspectral reflectance measurements in durum wheat
358 under contrasting Mediterranean conditions. *International Journal of Remote Sensing*, 25, 1131-1152.
- 359 Biewer, S., Erasmi, S., Fricke, T., Wachendorf, M., 2009a. Prediction of yield and the contribution of legumes
360 in legume-grass mixtures using field spectrometry. *Precision Agriculture* 10, 128-144.
- 361 Biewer, S., Fricke, T., Wachendorf, M., 2009b. Development of canopy reflectance models to predict forage
362 quality of legume-grass mixtures. *Crop Science* 49, 1917-1926.
- 363 Brown, M.P., Grundy, W.N., Lin, D., Cristianini, N., Sugnet, C.W., Furey, T.S., Ares, M., Haussler, D., 2000.
364 Knowledge-based analysis of microarray gene expression data by using support vector machines. *Proc.*
365 *Natl. Acad. Sci. USA*, 97, 262-267.
- 366 Campbell, J.B., 1996. *Introduction of remote sensing*. 2nd ed. The Guilford Press, London.
- 367 Cherkassky, V., Ma, Y., 2004. Practical selection of SVM parameters and noise estimation for SVM regression.
368 *Neural Netw.* 17, 113-126. [https://doi.org/10.1016/S0893-6080\(03\)00169-2](https://doi.org/10.1016/S0893-6080(03)00169-2)
- 369 Cristianini, N., Shawe-Taylor, J., 2000. *An Introduction to Support Vector Machines and Other Kernel-based*
370 *Learning Methods*. Cambridge University Press, Cambridge.
371 <https://doi.org/10.1017/CBO9780511801389>
- 372 Daughtry, C., 2000. Estimating Corn Leaf Chlorophyll Concentration from Leaf and Canopy Reflectance.
373 *Remote Sens. Environ.* 74, 229-239. [https://doi.org/10.1016/S0034-4257\(00\)00113-9](https://doi.org/10.1016/S0034-4257(00)00113-9)
- 374 Deo, R.C., Kisi, O., Singh, V.P., 2017. Drought forecasting in eastern Australia using multivariate adaptive
375 regression spline, least square support vector machine and M5Tree model. *Atmospheric Res.* 184, 149-
376 175. <https://doi.org/10.1016/j.atmosres.2016.10.004>
- 377 Diner, D.J., Asner, G.P., Davies, R., Knyazikhin, Y., Muller, J.-P., Nolin, A.W., Pinty, B., Schaaf, C.B.,
378 Stroeve, J., 1999. New directions in earth observing: Scientific applications of Multiangle remote sensing.
379 *Bulletin of the American Meteorological Society* 80, 2209-2228.
- 380 Du, L., Shi, S., Yang, J., Sun, J., Gong, W., 2016. Using Different Regression Methods to Estimate Leaf
381 Nitrogen Content in Rice by Fusing Hyperspectral LiDAR Data and Laser-Induced Chlorophyll
382 Fluorescence Data. *Remote Sens.* 8, 526.
- 383 Durbha, S.S., King, R.L., Younan, N.H., 2007. Support vector machines regression for retrieval of leaf area
384 index from multiangle imaging spectroradiometer. *Remote Sensing of Environment* 107, 348-361.
- 385 Gianelle, D., Guastella, F., 2007. Nadir and off-nadir hyperspectral field data: Strengths and limitations in
386 estimating grassland biophysical characteristics. *International Journal of Remote Sensing*, 28, 1547-1560.
- 387 Hatfield, J., Gitelson, A.A., Schepers, J.S., Walthall, C., 2008. Application of spectral remote sensing for
388 agronomic decisions. *Agron. J.* 100, 117-131.
- 389 Heath, O.V.S., 1969. Physiological aspects of photosynthesis. <http://agris.fao.org/agris>
390 [search/search.do?recordID=US201300595563](http://agris.fao.org/agris/search/search.do?recordID=US201300595563)
- 391 Hinzman, L., Bauer, M., Daughtry, C., 1986. Effects of nitrogen fertilization on growth and reflectance
392 characteristics of winter wheat. *Remote Sens. Environ.* 19, 47-61. [https://doi.org/10.1016/0034-](https://doi.org/10.1016/0034-4257(86)90040-4)
393 [4257\(86\)90040-4](https://doi.org/10.1016/0034-4257(86)90040-4)
- 394 Jackson, R.D., Pinter, P.J., Idso, S.B., Reginato, R.J., 1979. Wheat spectral reflectance: Interactions between
395 crop configuration, sun elevation, and azimuth angle. *Appl. Opt.* 18, 3730-3733.
- 396 Jin, X., Liu, S., Baret, F., Hemerlé, M., Comar, A., 2017. Estimates of plant density of wheat crops at emergence
397 from very low altitude UAV imagery. *Remote Sensing of Environment* 198, 105-114.

398 Karimi, Y., Prasher, S., Madani, A., Kim, S., 2008. Application of support vector machine technology for the
399 estimation of crop biophysical parameters using aerial hyperspectral observations. *Canadian Biosystems*
400 *Engineering* 50, 13-20.

401 Lekdioui, K., Messoussi, R., Ruichek, Y., Chaabi, Y., Touahni, R., 2017. Facial decomposition for expression
402 recognition using texture/shape descriptors and SVM classifier. *Signal Process. Image Commun.* 58,
403 300–312. <https://doi.org/10.1016/j.image.2017.08.001>

404 Li, F., Mistele, B., Hu, Y., Chen, X., and Schmidhalter, U., 2014a. Reflectance estimation of canopy nitrogen
405 content in winter wheat using optimised hyperspectral spectral indices and partial least squares
406 regression. *European Journal of Agronomy* 52, 198-209.

407 Li, X., Zhang, Y., Bao, Y., Luo, J., Jin, X., Xu, X., Song, X., and Yang, G., 2014b. Exploring the best
408 hyperspectral features for LAI estimation using partial least squares regression. *Remote Sensing* 6, 6221-
409 6241.

410 Loague, K., and Green, R., E., 1991. Statistical and graphical methods for evaluating solute transport models:
411 overview and application. *Journal of contaminant hydrology* 7, 51-73.

412 McMurtrey, J., Chappelle, E., Kim, M., Meisinger, J., Corp, L., 1994. Distinguishing nitrogen fertilization levels
413 in field corn (*Zea mays* L.) with actively induced fluorescence and passive reflectance measurements.
414 *Remote Sens. Environ.* 47, 36–44. [https://doi.org/10.1016/0034-4257\(94\)90125-2](https://doi.org/10.1016/0034-4257(94)90125-2)

415 Mistele, B., Gutser, R., Schmidhalter, U., 2004. Validation of field-scaled spectral measurements of the nitrogen
416 status in winter wheat. In: Mulla, D.J. (Ed.), *Proceedings of the 7th International Conference on Precision*
417 *Agriculture and other precision resources management*. Minneapolis, Minnesota, USA, (CD ROM), pp.
418 1187-1195.

419 Mistele, B., Schmidhalter, U., 2008. Spectral measurements of the total aerial N and biomass dry weight in
420 maize using a quadrilateral-view optic. *Field Crops Research*, 106, 94-103.

421 Mutanga, O., Skidmore, A., K., Kumar, L., & Ferwerda, J., 2005. Estimating tropical pasture quality at canopy
422 level using band depth analysis with continuum removal in the visible domain. *International Journal of*
423 *Remote Sensing*, 26 (6), 1093-1108.

424 Norris, K.H., Barnes, R.,F., Moore, J.,E., and Shenk, J.,S., 1976. Predicting forage quality by infrared
425 reflectance spectroscopy. *J. Anim. Sci.* 43: 889–897.

426 Peñuelas, J., Filella, I., Biel, C., Serrano, L., Savé, R., 1993. The reflectance at the 950-970 nm region as an
427 indicator of plant water status. *Int. J. Remote Sens.* 14, 1887–1905.
428 <https://doi.org/10.1080/01431169308954010>

429 Perbandt, D., Fricke, T., Wachendorf, M., 2011. Off-nadir hyperspectral measurements in maize to predict dry
430 matter yield, protein content and metabolisable energy in total biomass. *Precision Agriculture* 12, 249-
431 265.

432 Pullanagari, R., Yule, I., Tuohy, M., Hedley, M., Dynes, R., King, W., 2012. In-field hyperspectral proximal
433 sensing for estimating quality parameters of mixed pasture. *Precision Agriculture* 13, 351-369.

434 R Core Team, (2016), R: A language and environment for statistical computing. R Foundation for Statistical
435 Computing, Vienna, Austria. URL. <https://www.R-project.org/>.

436 Ranson, K.J., Daughtry, C.S.T., Biehl, L.L., Bauer, M.E., 1985. Sun-view angle effects on reflectance factors of
437 corn canopies. *Remote Sens. Environ.* 18,147-161.

438 Schaepman-Strub, G., Schaepman, M., Painter, T.H., Dangel, S., Martonchik, J.V., 2006. Reflectance quantities
439 in optical remote sensing-Definitions and case studies. *Remote sensing of environment* 103, 27-42.

440 Starks, P.J., Coleman, S.W., Phillips, W.A., 2004. Determination of forage chemical composition using remote
441 sensing. *Journal of range management* 57, 635-640.

442 Starks, P.J., Zhao, D., Phillips, W.A., Coleman, S.W., 2006. Herbage mass, nutritive value and canopy spectral
443 reflectance of bermudagrass pastures. *Grass Forage Sci.* 61, 101–111.

444 Vapnik, V., 1982. *Estimation of Dependences Based on Empirical Data: Springer Series in Statistics (Springer*
445 *Series in Statistics)*. Springer-Verlag New York, Inc.

446 Wang, W., Xu, Z., Lu, W., Zhang, X., 2003. Determination of the spread parameter in the Gaussian kernel for
447 classification and regression. *Neurocomputing* 55, 643–663. [https://doi.org/10.1016/S0925-](https://doi.org/10.1016/S0925-2312(02)00632-X)
448 [2312\(02\)00632-X](https://doi.org/10.1016/S0925-2312(02)00632-X)

449 Wang, F., Huang, J., Wang, Y., Liu, Z., Zhang, F., 2013. Estimating nitrogen concentration in rape from
450 hyperspectral data at canopy level using support vector machines. *Precision Agriculture* 14, 172-183.

451 Wold, S., Sjostrom, M., Eriksson, L., 2001. PLS-regression: A basic tool of chemometrics. *Chemometrics and*
452 *Intelligent Laboratory Systems*, 58(2), 109–130.

453 Wu, X., Kumar, V., Quinlan, J.R., Ghosh, J., Yang, Q., Motoda, H., McLachlan, G.J., Ng, A., Liu, B., Philip,
454 S.Y., 2008. Top 10 algorithms in data mining. *Knowledge and information systems* 14, 1-37.

455 Xu, S.X., Zhao, Y.C., Wang, M.Y., Shi, X.Z., 2017. Determination of rice root density from Vis-NIR
456 spectroscopy by support vector machine regression and spectral variable selection techniques. *Catena*
457 157, 12-23.

458 Yang, X.-H., Huang, J.F., Wang, X.Z., Wang, F.M., 2008. The estimation model of rice leaf area index using
459 hyperspectral data based on support vector machine. *Spectroscopy and Spectral Analysis* 28, 1837-1841.

460 Yao, X., Huang, Y., Shang, G., Zhou, C., Cheng, T., Tian, Y., Cao, W., Zhu, Y., 2015. Evaluation of six
461 algorithms to monitor wheat leaf nitrogen concentration. *Remote Sens.* 7, 14939-14966.

462 Yoder, B.J., Pettigrew-Crosby, R.E., 1995. Predicting nitrogen and chlorophyll content and concentrations from
463 reflectance spectra (400–2500 nm) at leaf and canopy scales. *Remote Sens. Environ.* 53, 199–211.
464 [https://doi.org/10.1016/0034-4257\(95\)00135-N](https://doi.org/10.1016/0034-4257(95)00135-N)

465 Zhai, Y., Cui, L., Zhou, X., Gao, Y., Fei, T., Gao, W., 2013. Estimation of nitrogen, phosphorus, and potassium
466 contents in the leaves of different plants using laboratory-based visible and near-infrared reflectance
467 spectroscopy: comparison of partial least-square regression and support vector machine regression
468 methods. *Int. J. Remote Sens.* 34, 2502-2518.

469 Zhao, D., Starks, P. J., Brown, M. A., Phillips, W. A., & Coleman, S. W., 2007. Assessment of forage biomass
470 and quality parameters of Bermuda grass using proximal sensing of pasture canopy reflectance.
471 *Grassland Science*, 53(1), 39-49.

472 Zheng, B., Yoon, S.W., Lam, S.S., 2014. Breast cancer diagnosis based on feature extraction using a hybrid of
473 K-means and support vector machine algorithms. *Expert Syst. Appl.* 41, 1476–1482.
474 <https://doi.org/10.1016/j.eswa.2013.08.044>

475 Zheng, Y., Zhu, Q.B., Huang, M., Guo, Y., Qin, J.W., 2017. Maize and weed classification using color indices
476 with support vector data description in outdoor fields. *Computers and Electronics in Agriculture* 141,
477 215-222.

478

479

480

481

482

483

484

485
486

Table 1
Species, cultivars (cv), and seed rates used in the R b cksdalen field experiment.

Mixture treatment	Seed rate of different species and varieties (kg ha ⁻¹)						
	Timothy cv. Grindstad	Meadow fescue cv. Revansch	Tall fescue cv. Swaj	Festulolium cv. Hykor	Perennial ryegrass mixture of cvs.	Red clover cv. Torun	White clover cv. Undrom
TiMF	12.0	10.0					
TiTall	12.0		10.0				
TiHyk	12.0			10.0			
TiPerHyk	10.4			9.1	2.5		
TiTall-clover	9.7		7.9			3.3	1.1

487
488
489

Table 2
Species, cultivars (cv), and seed rates used in the R dde field experiment.

Mixture treatment	Seed rate of different species and varieties (kg ha ⁻¹)							
	Timothy cv. Switch	Perennial ryegrass cv. Foxtrot	Perennial ryegrass cv. Kentaur	Festulolium cv. Hykor	Red clover cv. Vicky	White clover cv. Klondike	Festulolium cv. Felopa	Meadow fescue cv. Minto
TiPerHyk	10.4	1.25	1.25	9.1				
TiPerHyk-clover	8.4	1.0	1.0	7.3	3.3	1.1		
TiPerHyk-Fel	10.4	1.25	1.25	4.6			4.5	
TiMF	12.1							9.9

490
491
492

Table 3

493 Calibration statistics of the prediction of N uptake, crude protein concentration and dry matter yield by partial
494 least squares regression (PLS) and support vector machine (SVM).

Dataset	Variables	n	Mean	PLS model			SVM model		
				MAE	RMSE	R ²	MAE	RMSE	R ²
All harvests	N uptake (kg/ha)	251	65	15.4	19	0.75	6.8	11	0.92
	Dry matter yield (kg/ha)	251	2696	512	667	0.77	200	284	0.96
	Crude protein (% of DM)	251	15	2.4	3.1	0.65	1.2	1.7	0.90
Early cutting	N uptake (kg/ha)	52	30	8.7	10	0.86	3.1	4	0.98
	Dry matter yield (kg/ha)	52	822	176	209	0.88	114	141	0.95
	Crude protein (% of DM)	52	19	2.1	2.8	0.79	1.2	1.3	0.95

495 n indicates the number of measurements, Mean is the average of measurements. MAE is mean absolute error.
496 RMSE is root mean square error.

497
498
499

Table 4

500 Validation statistics of the prediction of N uptake, crude protein concentration and dry matter yield by partial
 501 least squares regression (PLS) and support vector machine (SVM).

Dataset	Variables	n	Mean	PLS model			SVM model		
				MAE	RMSE	R ²	MAE	RMSE	R ²
All harvests	N uptake (kg/ha)	126	67	17	21	0.69	9.2	12.6	0.89
	Dry matter yield (kg/ha)	126	2660	587	732	0.68	283	374	0.92
	Crude protein (% of DM)	126	16	2.8	3.5	0.69	1.8	2.5	0.84
Early cutting	N uptake (kg/ha)	26	39	7.9	9.7	0.90	7.5	9.9	0.89
	Dry matter yield (kg/ha)	26	972	153	182	0.92	123	156	0.94
	Crude protein (% of DM)	26	22	2.5	3.2	0.80	2.0	2.7	0.83

502 n indicates the number of measurements, Mean is the average of measurements. MAE is mean absolute error.
 503 RMSE is root mean square error

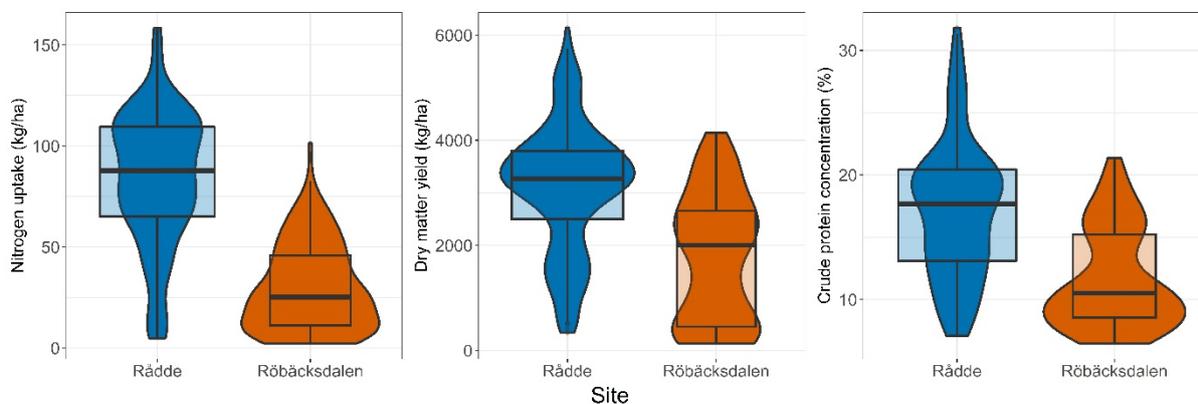
504



505
 506 **Fig. 1.** The photo on the left shows the hand-held sensor used in this project. The photo on the right shows the
 507 tractor-mounted Yara-N sensor and is from the Yara company homepage. The white instrument on the roof of the
 508 tractor is the N sensor, which has an oblique view angle, enabling the estimation of N status on the crop on both
 509 sides of the tractor. The yellow triangle in both photos is a depiction of the field of view of the reflectance
 510 measurement.

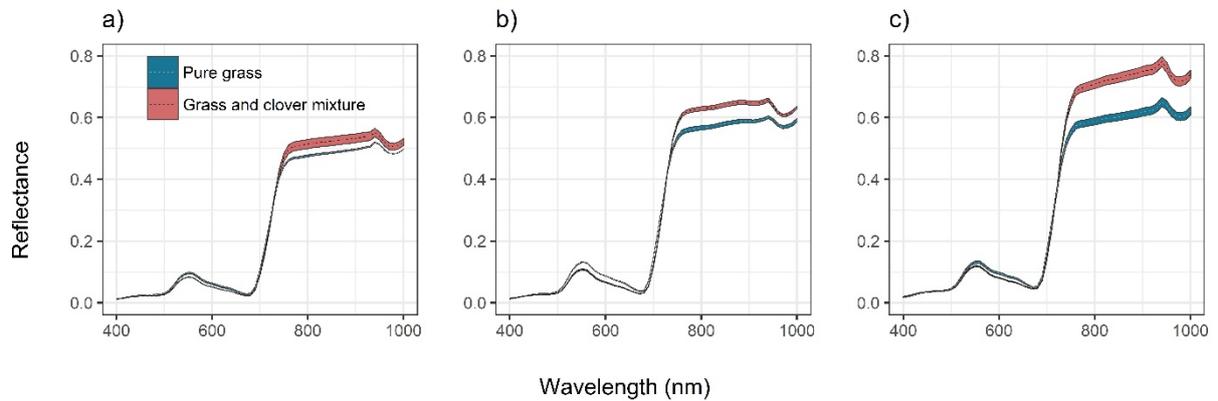
511

512



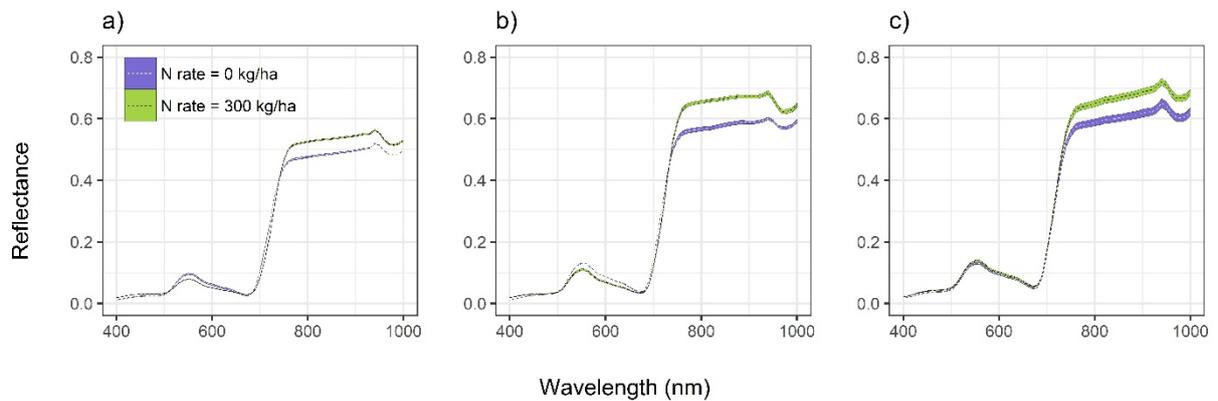
513
 514 **Fig. 2.** Variation of agronomy variables of the whole dataset (377 samples) at two sites in 2015 and in 2016 for
 515 nitrogen uptake, dry matter yield and crude protein concentration. The horizontal lines indicate the minimum,

516 first quartile, median, third quartile, and maximum of the dataset. Sample distribution is indicated by the width
517 of the colored area.
518



519

520 **Fig. 3.** Comparison of the spectral signatures of pure grass (TiTall) and grass and clover mixture (TiTall-clover)
521 for three dates: a) 03/06/2016, b) 18/07/2016, c) 02/09/2016 at R b cksdalen. Only the zero N treatment was
522 used for plotting the spectral signature.

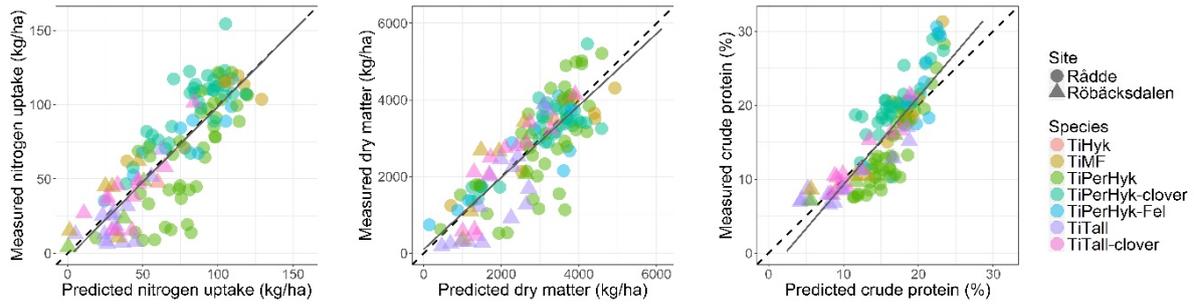


523

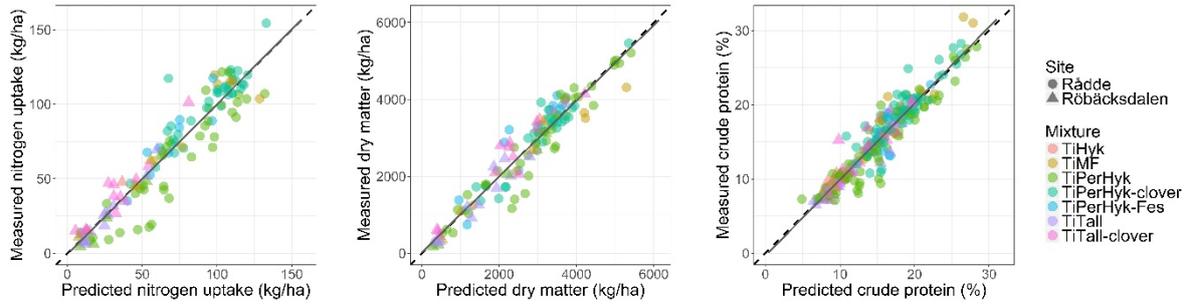
524 **Fig. 4.** Comparison of the spectral signatures of two contrasting nitrogen treatments for three dates: a)
525 03/06/2016, b) 18/07/2016, c) 02/09/2016 at R b cksdalen. Only the pure grass (TiTall) treatment was used for
526 plotting the spectral signature.

527

528



529

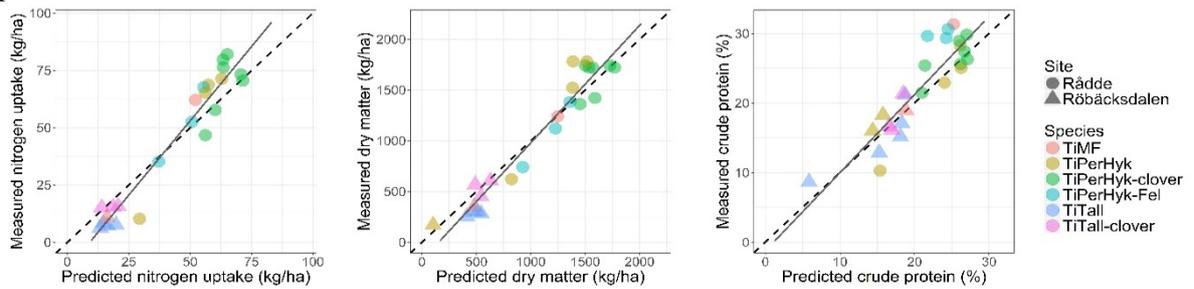


530

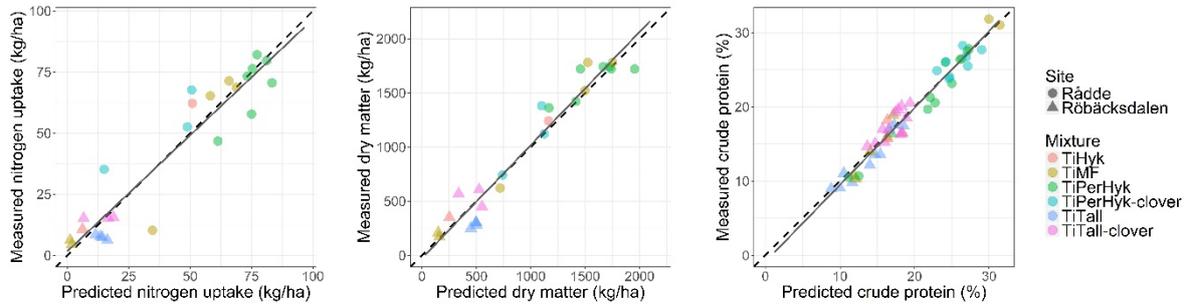
Fig. 5. Validation of partial least squares (upper graphs) and support vector machine (lower graphs) models for nitrogen uptake, dry matter yield and crude protein concentration using data from all harvests. Abbreviations for species mixtures are described in Tables 1 and 2.

531
532

533



534



535

Fig. 6. Validation of partial least squares (upper graphs) and support vector machine (lower graphs) models for nitrogen uptake, dry matter yield and crude protein concentration using data from the early cutting only. Abbreviations for species mixtures are described in Tables 1 and 2.

536
537

538

539