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Visible and NIR hyperspectral imaging and chemometrics for prediction of microbial quality of beef *Longissimus dorsi m.* under simulated normal and abuse storage conditions

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CRediT authorship contribution statement

**Eva Achata:** Investigation, Data Curation, Formal analysis, Visualization, Writing - Original draft, **Marcia Oliveira:** Investigation, Data Curation **Carlos Esquerre:** Software, Writing - Review & Editing **Brijesh Tiwari:** Conceptualization, Methodology, Resources **Colm O'Donnell:** Conceptualization, Resources, Writing - Review & Editing, Supervision, Funding acquisition

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1 **Visible and NIR hyperspectral imaging and chemometrics for prediction of microbial**  
2 **quality of beef *Longissimus dorsi m.* under simulated normal and abuse storage**  
3 **conditions**

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8 **Abstract**

9 There is a need to develop a rapid technique to provide real time information on the microbial  
10 load of meat along the supply chain. Hyperspectral imaging (HSI) is a rapid, non-destructive  
11 technique well suited to food analysis applications. In this study, HSI in both the visible and  
12 near infrared spectral ranges, and chemometrics were studied for prediction of the bacterial  
13 growth on beef *Longissimus dorsi m.* (*LD*) under simulated normal (4 °C) and abuse (10 °C)  
14 storage conditions. Total viable count (TVC) prediction models were developed using partial  
15 least squares regression (PLS-R), spectral pre-treatments, band selection and data fusion  
16 methods. The best TVC prediction models developed for storage at 4 (RMSE<sub>p</sub> 0.58 log  
17 CFU/g, RPD<sub>p</sub> 4.13, R<sup>2</sup><sub>p</sub> 0.96), 10 °C (RMSE<sub>p</sub> 0.97 log CFU/g, RPD<sub>p</sub> 3.28, R<sup>2</sup><sub>p</sub> 0.94) or at  
18 either 4 or 10 °C (RMSE<sub>p</sub> 0.89 log CFU/g, RPD<sub>p</sub> 2.27, R<sup>2</sup><sub>p</sub> 0.86) were developed using high-  
19 level data fusion of both spectral regions. The use of appropriate spectral pre-treatments and  
20 band selection methods was key for robust model development. This study demonstrated the  
21 potential of HSI and chemometrics for real time monitoring to predict microbial growth on  
22 *LD* along the meat supply chain.

23 Key words: Hyperspectral imaging, chemometrics, TVC prediction, data fusion, meat.

## 24 1. Introduction

25 The *Longissimus dorsi m. (LD)* of beef is highly valued by consumers and is normally aged  
26 to increase tenderness, juiciness and flavour. Meat processors generally age *LD* for 28 days or  
27 longer to improve tenderness and flavour. However colour and microbial load are also  
28 affected which potentially impacts product safety and shelf life (Borch, Kant-Muermans, &  
29 Blixt, 1996; Vitale, Pérez-Juan, Lloret, Arnau, & Realini, 2014). The design and application  
30 of quality and safety assurance systems are based on thorough risk analysis and control of  
31 critical parameters through the entire life cycle of meat products including raw material  
32 selection and control during processing and distribution. The temperature profiles during  
33 transportation and at retail level are not within the direct control of meat processors and may  
34 exceed recommended temperatures. Lack of temperature control from retail to the time of  
35 preparation and consumption may also be an issue. In southern European countries 30% of  
36 refrigerated foods were reported to be stored above 10 °C in retail cabinets and household  
37 refrigerators (Nychas, Skandamis, Tassou, & Koutsoumanis, 2008).

38 Current microbiological methods are not suitable for real time monitoring of microbial  
39 contamination of meat. The traditional plate count technique is the most commonly used  
40 method to monitor microbial load. However, it requires time consuming sample preparation  
41 and analysis. The total viable count (TVC) method is an important microbiology indicator for  
42 quality and safety evaluation of meat (Lytou, Panagou, & Nychas, 2016). The initial  
43 microbial load of meat after processing, storage temperature, pH and relative humidity are the  
44 main factors influencing microbial load throughout the supply chain. Enzyme-linked immune  
45 absorbent assay (ELISA), gene analysis-based methods such as polymerase chain reaction  
46 (PCR) and DNA sequencing are also employed for microbial contamination detection (Si et  
47 al., 2016) but are not suited to online analysis.

48 Visible (VIS) and near-infrared (NIR) spectroscopy are rapid non-destructive techniques  
49 widely used in environmental, pharmaceutical, fuel and food analysis applications. The VIS

50 and NIR spectral regions range from 380 - 740 nm and 700 - 2500 nm respectively.

51 Spectroscopic sensors usually acquire spectra from a limited field of view which limits their

52 applicability for rapid safety analysis of large volume batches or analysis of heterogeneous

53 samples such as meat products (Millar, Moss, & Stevenson, 1996).

54 Hyperspectral imaging (HSI) is a rapid analytical tool for non-destructive measurement of

55 food quality and safety. HSI integrates traditional imaging and spectroscopy to acquire both

56 spatial and spectral information from samples. Each pixel in a hyperspectral image contains

57 the spectrum of that specific position, i.e. the light-absorbing and/or scattering properties of

58 the spatial region represented, which can be used to characterise the composition of that

59 particular pixel (Gowen, O'Donnell, Cullen, Downey, & Frias, 2007; Kamruzzaman, Makino,

60 & Oshita, 2016). HSI techniques can be employed at different points along meat distribution

61 chains. HSI has been studied to predict microbial growth on fresh beef meat using the VIS

62 range (Peng et al., 2011; Tao, Peng, Gomes, Chao, & Qin, 2015). However, no studies have

63 been reported to date on the use of HSI in the NIR spectral range to predict microbial growth

64 on fresh beef.

65 Chemometric methods are employed to develop prediction models from HSI data. Partial

66 least squares regression (PLS-R) may be used to predict unknown concentrations and

67 generate prediction maps to estimate spatial distributions of components in samples (Gowen,

68 Burger, Esquerre, Downey, & O'Donnell, 2014). Spectral pre-treatments are used to correct

69 for the effects of natural variability in the shape and size of samples, light scattering and

70 differences in the effective path length in spectral data, which can present difficulties in the

71 application of HSI for quality assessment (Esquerre, Gowen, Burger, Downey, & O'Donnell,

72 2012). Band selection methods have been demonstrated to improve the performance of

73 regression models and to reduce the processing times required to evaluate HSI data by

74 selecting the most informative bands. The variable importance projection method (VIP), the

75 selectivity ratio method (SR) and the ensemble Monte Carlo variable selection method

76 (EMCVS) have been demonstrated to be reliable band selection methods for HSI data  
77 (Achata, Inguglia, Esquerre, Tiwari, & O'Donnell, 2019; Farrés, Platikanov, Tsakovski, &  
78 Tauler, 2015).

79 Data fusion combines information from different sources to produce a more reliable and  
80 accurate model or information. Three levels of data fusion may be employed i) low level  
81 (data-level) fusion, where data from all sources are properly transformed and concatenated  
82 for model development, ii) mid-level (feature-level) fusion, where variable selection or  
83 feature extraction is applied to each data source before the extracted features are combined;  
84 iii) and high-level (decision-level) fusion where a model is constructed for each data source  
85 separately and their predictions combined thereafter (Liu & Brown, 2004). Data fusion has  
86 been studied to detect volatile basic nitrogen (TVB-N) content in chicken meat using a  
87 colorimetric sensor and a VIS system (Khulal, Zhao, Hu, & Chen, 2017).

88 The objective of this study was to investigate the potential of HSI and chemometrics for the  
89 prediction of the microbial quality of beef under simulated normal (4 °C ) and abuse (10 °C)  
90 storage conditions.

91

## 92 **2. Materials and methods**

### 93 **2.1. Sample preparation**

94 *LD* samples (n = 104) from 9 cattle (denoted S1 to S9) of ca. 25 mm thickness were obtained  
95 from local supermarkets and a meat processing facility. The samples were placed in sealed  
96 food containers and randomly assigned for storage at either 4 °C (n = 53) for 360 hours or at  
97 10 °C (n = 51) for 168 hours. Three randomly selected samples (from 3 cattle) were removed  
98 from storage and scanned using a visible short wave near infrared (VIS-SWNIR) and an NIR  
99 HSI systems. The TVC of samples was measured after scanning using the ISO 48833-1:2013  
100 methodology (ISO, 2013). Briefly 25 g of each sample was suspended in 225 ml of buffered  
101 peptone water (BPW, Oxoid, Hampshire, England) and aseptically homogenized in a

102 stomacher (Star-Blender LB 400, VWR) for 2 min. Further decimal dilutions were made with  
103 maximum recovery diluent (MRD, HyServe, Germany). Three replicates were assessed per  
104 sample at each sampling time. Reported populations represent the mean of three values.

105

## 106 **2.2. Hyperspectral images**

107 Hyperspectral images of the *LD* samples were obtained using a VIS-SWNIR HSI system  
108 (400 – 1000 nm) and an NIR HSI system (880 – 1720 nm) (DV Optics, Padova, Italy).  
109 Calibration of both HSI systems was performed as outlined by Achata, Esquerre, O'Donnell,  
110 and Gowen (2015). The acquired hypercubes were saved in ENVI formatted files and  
111 imported into MATLAB (The MathWorks Inc., Natick, MA, USA) for further spatial and  
112 spectral data pre-processing and chemometric analysis, using in-house developed functions  
113 and scripts.

114

### 115 **2.2.1. VIS-SWNIR HSI spatial and spectral pre-processing**

116 The noise present at both ends of the spectra was removed by trimming the spectral range to  
117 445 - 970 nm. The background was removed using a mask created using the ratio between  
118 bands 80 (840 nm) and 20 (540 nm) and removing pixels with a ratio value  $> 1.5$ . To improve  
119 the signal-to-noise ratio (SNR) and reduce processing times and data storage required,  $2 \times 2$   
120 binning was performed on the obtained hypercubes of 1000 x 580 pixel image with 106  
121 spectral bands, resulting in hypercubes of 500 x 290 pixel image with 106 spectral bands. The  
122 binned 3-dimensional hypercubes were unfolded into matrices of pixel spectra (14500 pixel x  
123 106 spectral bands) to facilitate algorithm development. The mean reflectance (*R*) spectra of  
124 each masked sample was calculated and smoothed using the Savitzky - Golay (SG) 5 points  
125 second order polynomial method prior to chemometric analysis (Savitzky & Golay, 1964).

126

### 127 2.2.2. NIR-HSI spatial and spectral pre-processing

128 The noise present at both ends of the spectra was removed by trimming the spectral range to  
129 957 - 1664 nm. Dead pixels and spikes were removed by replacing the affected values with  
130 the mean values of adjacent bands in the same spectrum. The background was removed using  
131 a mask which was created with the ratio between bands 90 (1580 nm) and 20 (1090 nm),  
132 removing pixels with a ratio value  $> 0.65$ . Images were segmented using the pixel ratio  
133 between bands 37 (1209 nm) and 43 (1251 nm) to remove fat and connective tissue (ratio  
134 value  $> 0.7$ ). The 3-dimensional hypercubes (500 x 320 pixel image with 102 bands) were  
135 unfolded into matrices of pixel spectra (160000 pixel x 102 bands). The mean reflectance  
136 spectra of each segmented sample was calculated and smoothed using the Savitzky - Golay  
137 (SG) 5 points second order polynomial method prior to chemometric analysis.

138

## 139 2.3. Chemometric analysis

### 140 2.3.1. PCA

141 PCA (not reported) was carried out to investigate the relationships between storage  
142 temperature over time and spectral data, and to identify potential outliers using the Hotelling  
143  $T^2$  statistic. A sample was considered as an outlier if the  $T^2$  value was  $> T^2_{crit} = A \times F_{(0.05, A, n - A)}$   
144  $\times (n-1)/(n-A)$ , where  $A$  is the number of significant components,  $n$  is the number of spectra  
145 in the dataset and  $F_{(0.05, A, n - A)}$  is the  $F$  statistic (with  $\alpha = 0.05$ ,  $A$  and  $n - A$  degrees of  
146 freedom).

147

### 148 2.3.2. PLS-R

149 PLS regression (Wold, Sjöström, & Eriksson, 2001) models were developed to predict TVC  
150 of samples using HSI data, spectral pre-treatments, band selection and data fusion methods.



151 Spectral data sets were split into calibration and validation sets to develop and validate the  
152 prediction models. Smoothed mean spectral data from 4 randomly selected samples (S1, S2,  
153 S4 and S6 (n=69)) was used for calibration and samples (S3 and S5) were used to validate the  
154 models (n=35). Predictions models were evaluated using the:

- 155 i) Smoothed mean spectral data of samples stored at 4 °C (n = 53)
- 156 ii) Smoothed mean spectral data of samples stored at 10 °C (n = 51)
- 157 iii) Smoothed mean spectral data of samples stored at either 4 or 10 °C (n = 104).

158 The number of latent variables (LV) were selected by analysis of the root mean square error  
159 of ten-fold cross-validation (RMSE<sub>CV</sub>) presented in Eq. (1) and roughness of the regression  
160 vector.

$$161 \quad RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} \quad (1)$$

162  $y_i$  and  $\hat{y}_i$  are the measured and predicted values of the microbial counts respectively.

163

### 164 2.3.3. Spectral pre-treatments

165 Standard normal variate (SNV), median scaled (MS), Savitzky-Golay 7 points second order  
166 polynomial first derivative (FD), Savitzky-Golay 7 points second order polynomial second  
167 derivative (SD), Savitzky-Golay 11 points fourth order polynomial third derivative (TD),  
168 linear detrending second-order polynomial (LD), asymmetric least squares (AsLs) (Barnes,  
169 Dhanoa, & Lister, 1989; Boelens, Eilers, & Hankemeier, 2005; Engel et al., 2013; Savitzky &  
170 Golay, 1964) and all combinations of any two spectral pre-treatments were applied. The  
171 Savitzky-Golay derivative (FD, SD or TD) window length and polynomial order were  
172 selected by preliminary tests on 10 randomly selected spectra.

173

### 174 2.3.4. Band selection

175 The VIP (Eriksson, Hermens, Johansson, Verhaar, & Wold, 1995; Wold et al., 2001), SR  
 176 (Rajalahti et al., 2009) and the EMCVS (Esquerre, Gowen, O'Gorman, Downey, &  
 177 O'Donnell, 2017) band selection methods were evaluated and compared with and without  
 178 spectral pre-treatments.

179 The performance of the regression models was assessed using the root mean square error  
 180 (RMSE), the ratio of standard deviation of the reference data of the calibration set and the  
 181 RMSE (RPD) and the coefficient of determination ( $R^2$ ) for calibration (C), cross-validation  
 182 (CV) and prediction (P) sets (Eq. 2-4). The best model was selected based on the number of  
 183 latent variables, selected wavebands and the geometric mean of the RPD values from  
 184 calibration, cross-validation, and prediction sets. Prediction models developed for complex  
 185 matrices can be classified as excellent (RPD > 4.1), very good (RPD 3.5 – 4.0), good (RPD 3.0 – 3.4),  
 186 fair (RPD 2.5 – 2.9) and poor (RPD 2.0 – 2.4) (Williams, 2014).

$$187 \quad RPD = \frac{S_{y_{cal}}}{SEP} \quad (2)$$

$$188 \quad SEP = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i - bias)^2}{n-1}} \quad (3)$$

$$189 \quad R^2 = \left( \frac{\sum_{i=1}^n (y_i \hat{y}_i) - n \bar{y} \bar{\hat{y}}}{\sqrt{\sum_{i=1}^n y_i^2 - n \bar{y}^2} \sqrt{\sum_{i=1}^n \hat{y}_i^2 - n \bar{\hat{y}}^2}} \right)^2 \quad (4)$$

190 Where the *bias* is the average difference between reference value and predicted value (Eq. 5).

$$191 \quad bias = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)}{n} \quad (5)$$

192

### 193 2.3.5. Data fusion

194 Prediction models for TVC of samples were developed for low level (LL), medium level  
 195 (ML) and high-level (HL) data fusion of VIS-SWNIR and NIR HSI data. For the LL data  
 196 fusion, the spectral data of both systems was concatenated before model development. For  
 197 the ML data fusion, the selected spectral bands (obtained by the band selection method that  
 198 achieved the best performance for each system) were combined. When the variance of the

199 pre-treated VIS-SWNIR and NIR HSI data was different, each data block was scaled to unit  
200 variance. The calibration, validation and prediction sets were scaled using the inverse of the  
201 standard deviation of the calibration set (Forshed, Idborg, & Jacobsson, 2007). For the HL  
202 data fusion, prediction models were developed by averaging the predictions of the best  
203 performing models identified for each system.

204

### 205 **3. Results and discussion**

#### 206 **3.1. TVC of samples**

207 The TVC of *LD* samples during storage at 4 °C and 10 °C are presented in Table 1. TVC  
208 values increased from 3.4 to 14.1 log CFU/g over 360 h storage at 4 °C and increased from  
209 3.4 to 13.1 log CFU/g over 168 h storage at 10 °C. Initial TVC values (day 0) varied  
210 according to the origin of the *LD* samples. *LD* S1 to S6 samples were purchased from local  
211 supermarkets and had initial TVC values > 6 log CFU/g. However, *LD* samples purchased  
212 directly from the meat processing facility (S7 to S9) had lower initial TVC values. *LD* S9  
213 (non aged) samples had the lowest TVC values (3.4 log CFU/g), while samples from the *LD*  
214 S7 and S8 which were both aged for 28 days had TVC values of ca. 5.3 log CFU/g.

215 Previous studies reported that *LD* samples with TVC values < 7 log CFU/g are acceptable,  
216 and samples with values > 7 log CFU/g are spoiled (Tao et al., 2015). Moreover, the presence  
217 of slime and discolouration has been reported for meat samples with TVC values > 7 log  
218 CFU/g (Bell & Garout, 1994).

219

#### 220 **3.2. Spectral characteristics of *LD* samples**

221 PCA analysis revealed the presence of one outlier in the VIS-SWNIR spectra of the *LD*  
222 samples stored at 4 °C, which was removed from the dataset. No outliers were identified in  
223 the NIR spectra. Figs. 1 and 2 show the spectral variations between samples during storage at  
224 4 and 10 °C respectively. The SD + AsLs pre-treated log (1/R) NIR spectra were used for

225 TVC prediction at 4 °C, whereas the SD+MS pre-treated reflectance VIS-SWNIR spectra  
226 were selected for TVC prediction at 10 °C. Spectral shifts are more apparent during storage  
227 due to changes in physical characteristics, chemical composition and microbial activity.  
228 Spoiled samples exhibited broader absorption bands compared to unspoiled samples.

229 Absorbance peaks observed at 1076 and 1342 nm in Fig. 1 may be related to the C-H  
230 stretching of the first and second overtone regions respectively, and the peak at 1580 nm may  
231 be related to the 1<sup>st</sup> overtone of O-H stretching (glucose) (Osborne, Fearn, & Hindle, 1993).  
232 The selected bands highlighted in Fig.1 provide complementary information on the samples  
233 and are related to the 2<sup>nd</sup> overtone of O-H stretching (978 nm) of water and the 1<sup>st</sup> overtone of  
234 N-H stretching (1496 nm) of protein. Similar spectral bands were observed by Barbin,  
235 ElMasry, Sun, Allen, and Morsy (2013) for pork samples. The observed differences between  
236 spoiled and fresh meat may relate to the presence of protein, free amino acids, amines or  
237 nitrogen bearing substances and their interactions with water. Such observations are  
238 consistent with the proteolytic changes which occur during microbial spoilage (Atanassova,  
239 Veleva, & Stoyanchev, 2018).

240 Fig. 2 shows the characteristic peaks of the of oxymyoglobin ( $\text{MbFe}^{\text{II}}\text{O}_2$ ) at 545 and 580 nm  
241 (Achata et al., 2019; Alamprese, Casale, Sinelli, Lanteri, & Casiraghi, 2013; Millar et al.,  
242 1996). These bands are prominent at the start of storage and increase in intensity after 24 h  
243 storage at 10 °C ( $\text{TVC} < 7.3 \log \text{CFU/g}$ ). The intensity of these bands decreases after 48 h  
244 corresponding to TVC values  $> 7.5 \log \text{CFU/g}$ . These changes may correspond to a decrease  
245 in the concentration of red pigments due to microbial growth during storage. The prominent  
246 peak at 765 nm may be related to the 3<sup>rd</sup> overtone C-H stretching. The selected bands  
247 highlighted in Fig. 2 provide complementary information on the samples and may be related  
248 to the 3<sup>rd</sup> overtone of C-H stretching (750 - 780 nm) (Osborne et al., 1993).

249

### 250 3.3. TVC prediction models

251 SD, SNV and the combination of SD+LD, and SNV+SD were identified as the best  
252 performing spectral pre-treatments after evaluating 50 combinations for each band selection  
253 method (Appendix 1). Models developed using the variable selection approach were  
254 compared with the best models developed using the full spectral range for both the VIS-  
255 SWNIR and NIR HSI spectral regions.

256 The best performing PLS-R model developed to predict TVC during storage at 4 °C (Table  
257 2) was developed using the NIR-HSI data and EMCVS of the SD+AsLs pre-treated log(1/R)  
258 spectra (17 selected bands, LV 7, RMSE<sub>P</sub> 0.81 log CFU/g, RPD<sub>P</sub> 3.09, R<sup>2</sup><sub>P</sub> 0.95). Lower  
259 coefficients of determination for the prediction of pork meat TVC were obtained by Barbin  
260 et al. (2013). Fig. 3a shows the predicted versus measured TVC values for *LD* samples  
261 stored at 4 °C obtained with the SD+AsLs pre-treated log(1/R) spectra. HL data fusion  
262 improved the performance of the prediction models (RMSE<sub>P</sub> 0.58 log CFU/g, RPD<sub>P</sub> 4.13,  
263 R<sup>2</sup><sub>P</sub> 0.96) compared to those obtained with LL data fusion, ML data fusion and the best  
264 models selected for the VIS-SWNIR and NIR HSI spectral data (Table 5).

265 The best performing PLS-R model developed to predict TVC during storage at 10 °C (Table  
266 3) was developed using the VIS-SWNIR - HSI data and EMCVS of the SD+MS pre-treated  
267 reflectance spectra (46 selected bands, LV 6, RMSE<sub>P</sub> 0.96 log CFU/g, RPD<sub>P</sub> 3.32, R<sup>2</sup><sub>P</sub> 0.94).  
268 Fig.3b. shows the predicted versus measured TVC values for *LD* samples stored at 10 °C  
269 obtained with the SD+MS pre-treated reflectance spectra. The use of derivative pre-  
270 treatments of VIS-SWNIR spectra has been reported to accentuate the differences in  
271 myoglobin spectra (Millar et al., 1996) by removing baseline offsets and decreasing  
272 scattering effects (Esquerre et al., 2012) as observed in Fig. 2. LL and HL data fusion  
273 yielded good prediction models, comparable to those obtained with the VIS-SWNIR data  
274 and better than the models developed using ML data fusion (Table 5).

275 The best performing PLS-R models developed to predict TVC for samples stored at either 4  
276 or 10 °C (Table 4) were developed using the VIS-SWNIR data and EMCVS of the SNV+SD  
277 pre-treated reflectance spectra (8 selected bands, LV 4, RMSEP 0.95 log CFU/g, RPD<sub>P</sub> 2.10,  
278 R<sup>2</sup><sub>P</sub> 0.85). Improved data fusion PLS-R models were developed using the LL and HL data  
279 fusion showed in Table 5 (RMSEP 0.87 log CFU/g, RPD<sub>P</sub> 2.27, R<sup>2</sup><sub>P</sub> 0.88, and RMSEP 0.89  
280 log CFU/g, RPD<sub>P</sub> 2.27, R<sup>2</sup><sub>P</sub> 0.86 respectively). Fig. 3c shows the predicted versus measured  
281 TVC values of *LD* stored at either 4 or 10 °C obtained using HL data fusion of both spectral  
282 regions.

283 Selected TVC prediction maps built using the best prediction model developed for storage at  
284 10 °C (SD+MS on the reflectance VIS-SWNIR spectra) are shown in Fig. 4.

285 Good and excellent TVC prediction models were obtained for beef *LD* samples stored at 4  
286 °C for both the NIR spectral range and HL data fusion of the VIS-SWNIR and NIR spectral  
287 regions respectively based on the RPD prediction model performance classifications reported  
288 by Williams (2014) for complex matrices. Good TVC prediction models were also obtained  
289 for samples stored at 10 °C using the VIS-SWNIR spectral range and HL data fusion of both  
290 spectral regions. However poor TVC prediction models were obtained for samples stored at  
291 either 4 °C or 10 °C using the VIS-SWNIR spectral range and HL data fusion of both  
292 spectral regions. In all cases EMCVS outperformed the other band selection methods  
293 evaluated. Combinations of SD, SNV and LD spectral pre-treatments also improved  
294 regression model development. Data fusion approaches improved prediction model  
295 performance in all cases. This is in agreement with the study reported by (Li, Chen, Zhao,  
296 and Wu (2015)) who reported that superior regression models can be obtained using data  
297 fusion and appropriate band selection methods.

298

299

#### 300 4. Conclusions

301 Excellent ( $RMSE_p$  0.58 log CFU/g,  $RPD_p$  4.13,  $R^2_p$  0.96) and good ( $RMSE_p$  0.97 log CFU/g,  
302  $RPD_p$  3.28,  $R^2_p$  0.94) TVC prediction models were developed for beef *LD* samples stored at 4  
303 °C and 10 °C respectively, using the HL data fusion of the two spectral regions. Prediction  
304 models were successfully developed using spectral pre-treatments, the full spectral range,  
305 selected bands and data fusion of both VIS-SWNIR and NIR spectral regions to predict the  
306 TVC of *LD* samples with low prediction errors.

307 The application of SD and SNV spectral pre-treatments improved the performance of the  
308 developed models using both spectral ranges and on selected bands. EMCVS improved the  
309 performance of the TVC prediction models developed compared with the full spectral range  
310 and outperformed VIP and SR methods. Data fusion approaches improved prediction model  
311 performance in all cases, HL data fusion yielded the best TVC prediction models ( $RMSE_p$   
312 0.89 log CFU/g,  $RPD_p$  2.27,  $R^2_p$  0.86) for beef samples stored at both 4 °C and 10 °C.  
313 Appropriate band selection was key for robust model development. This study demonstrated  
314 the potential of HSI and chemometrics as a rapid analytical tool for monitoring meat  
315 microbial quality along the supply chain.

316

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320

321



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Appendix 1. Performance of the TVC PLS-R models developed using VIS-SWNIR (445 - 970 nm ) data from beef *LD* samples stored at 4 °C. PLS full spectral range on reflectance (R) and logarithmic transformed ( $\log(1/R)$ ) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands | # LV | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |      |
|--------------------|------------------------|---------|------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|------|
|                    |                        |         |      | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |      |
| PLS                | R                      | None    | 106  | 7                 | 0.91             | 2.73                        | 0.87               | 1.48              | 1.69                         | 0.68              | 1.72             | 1.20                        | 0.72 |
|                    |                        | SNV     | 106  | 7                 | 0.84             | 2.97                        | 0.89               | 1.20              | 2.08                         | 0.78              | 1.62             | 1.37                        | 0.78 |
|                    |                        | SD      | 100  | 8                 | 0.61             | 4.09                        | 0.94               | 1.08              | 2.30                         | 0.82              | 2.16             | 1.21                        | 0.71 |
|                    |                        | SD+LD   | 100  | 8                 | 0.61             | 4.10                        | 0.94               | 1.09              | 2.30                         | 0.82              | 2.05             | 1.23                        | 0.71 |
|                    |                        | SNV+SD  | 100  | 6                 | 0.79             | 3.15                        | 0.90               | 1.34              | 1.86                         | 0.74              | 1.35             | 1.61                        | 0.81 |
|                    | Log(1/R)               | None    | 106  | 3                 | 1.27             | 1.96                        | 0.74               | 1.59              | 1.56                         | 0.60              | 1.79             | 1.20                        | 0.58 |
|                    |                        | SNV     | 106  | 5                 | 0.89             | 2.79                        | 0.87               | 1.16              | 2.16                         | 0.78              | 1.45             | 1.45                        | 0.75 |
|                    |                        | SD      | 100  | 6                 | 0.63             | 3.94                        | 0.94               | 1.06              | 2.37                         | 0.82              | 1.93             | 1.22                        | 0.67 |
|                    |                        | SD+LD   | 100  | 6                 | 0.64             | 3.87                        | 0.93               | 1.05              | 2.39                         | 0.82              | 1.83             | 1.25                        | 0.67 |
|                    |                        | SNV+SD  | 100  | 4                 | 0.82             | 3.06                        | 0.89               | 1.24              | 2.04                         | 0.76              | 1.45             | 1.44                        | 0.75 |
| VIP                | R                      | None    | 7    | 2                 | 1.27             | 1.97                        | 0.74               | 1.41              | 1.77                         | 0.68              | 1.79             | 1.33                        | 0.66 |
|                    |                        | SNV     | 27   | 6                 | 0.97             | 2.58                        | 0.85               | 1.20              | 2.07                         | 0.77              | 1.80             | 1.25                        | 0.75 |
|                    |                        | SD      | 28   | 7                 | 0.94             | 2.65                        | 0.86               | 1.38              | 1.81                         | 0.70              | 1.78             | 1.25                        | 0.70 |
|                    |                        | SD+LD   | 33   | 10                | 0.51             | 4.89                        | 0.96               | 0.90              | 2.79                         | 0.87              | 2.50             | 1.40                        | 0.74 |
|                    |                        | SNV+SD  | 18   | 11                | 0.46             | 5.47                        | 0.97               | 0.79              | 3.18                         | 0.90              | 1.31             | 1.92                        | 0.81 |
|                    | Log(1/R)               | None    | 4    | 3                 | 1.21             | 2.06                        | 0.76               | 1.39              | 1.79                         | 0.70              | 1.77             | 1.25                        | 0.60 |
|                    |                        | SNV     | 17   | 11                | 0.84             | 2.98                        | 0.89               | 1.21              | 2.07                         | 0.77              | 1.65             | 1.33                        | 0.71 |
|                    |                        | SD      | 18   | 6                 | 0.79             | 3.16                        | 0.90               | 1.13              | 2.21                         | 0.80              | 1.72             | 1.30                        | 0.68 |
|                    |                        | SD+LD   | 15   | 3                 | 1.10             | 2.27                        | 0.81               | 1.28              | 1.95                         | 0.74              | 1.34             | 1.66                        | 0.76 |
|                    | SNV+SD                 | 13      | 8    | 0.55              | 4.51             | 0.95                        | 0.70               | 3.56              | 0.92                         | 1.38              | 1.86             | 0.80                        |      |

|       |          |               |          |          |             |             |             |             |             |             |             |             |             |
|-------|----------|---------------|----------|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| SR    | R        | None          | 14       | 8        | 0.96        | 2.59        | 0.85        | 1.39        | 1.79        | 0.71        | 1.66        | 1.35        | 0.76        |
|       |          | SNV           | 1        | 1        | 1.78        | 1.40        | 0.49        | 1.86        | 1.34        | 0.44        | 2.21        | 1.31        | 0.60        |
|       |          | SD            | 7        | 4        | 1.01        | 2.47        | 0.84        | 1.27        | 1.96        | 0.74        | 1.64        | 1.35        | 0.67        |
|       |          | SD+LD         | 3        | 3        | 1.08        | 2.30        | 0.81        | 1.27        | 1.97        | 0.74        | 1.55        | 1.42        | 0.73        |
|       |          | SNV+SD        | 1        | 1        | 1.34        | 1.87        | 0.71        | 1.43        | 1.74        | 0.67        | 1.84        | 1.28        | 0.66        |
|       | Log(1/R) | None          | 11       | 8        | 0.95        | 2.64        | 0.86        | 1.29        | 1.94        | 0.74        | 1.44        | 1.59        | 0.75        |
|       |          | SNV           | 15       | 6        | 1.15        | 2.16        | 0.79        | 1.50        | 1.67        | 0.64        | 1.36        | 1.63        | 0.74        |
|       |          | SD            | 1        | 1        | 1.26        | 1.97        | 0.74        | 1.34        | 1.87        | 0.71        | 2.00        | 1.10        | 0.48        |
|       |          | SD+LD         | 5        | 3        | 1.09        | 2.28        | 0.81        | 1.26        | 1.98        | 0.75        | 1.96        | 1.23        | 0.56        |
|       |          | SNV+SD        | 7        | 5        | 1.00        | 2.48        | 0.84        | 1.30        | 1.92        | 0.73        | 1.95        | 1.64        | 0.76        |
| EMCVS | R        | None          | 6        | 3        | 1.05        | 1.94        | 0.73        | 1.18        | 1.72        | 0.67        | 2.07        | 1.10        | 0.57        |
|       |          | SNV           | 8        | 6        | 0.93        | 2.69        | 0.86        | 1.16        | 2.16        | 0.79        | 1.72        | 1.30        | 0.79        |
|       |          | SD            | 5        | 3        | 0.82        | 3.06        | 0.89        | 0.94        | 2.66        | 0.86        | 1.84        | 1.33        | 0.70        |
|       |          | SD+LD         | 10       | 5        | 0.74        | 3.38        | 0.91        | 0.89        | 2.81        | 0.87        | 2.11        | 1.25        | 0.68        |
|       |          | SNV+SD        | 7        | 3        | 0.90        | 2.77        | 0.87        | 1.02        | 2.44        | 0.83        | 1.52        | 1.47        | 0.72        |
|       | Log(1/R) | None          | 43       | 8        | 0.85        | 2.93        | 0.88        | 1.18        | 2.12        | 0.79        | 1.54        | 1.43        | 0.71        |
|       |          | SNV           | 9        | 3        | 1.02        | 2.45        | 0.83        | 1.13        | 2.20        | 0.79        | 1.64        | 1.44        | 0.71        |
|       |          | SD            | 10       | 7        | 0.69        | 3.63        | 0.92        | 0.89        | 2.82        | 0.87        | 1.42        | 1.58        | 0.73        |
|       |          | SD+LD         | 8        | 5        | 0.70        | 3.54        | 0.92        | 0.83        | 3.01        | 0.89        | 1.56        | 1.48        | 0.72        |
|       |          | <b>SNV+SD</b> | <b>6</b> | <b>5</b> | <b>0.88</b> | <b>2.83</b> | <b>0.88</b> | <b>1.03</b> | <b>2.42</b> | <b>0.83</b> | <b>1.17</b> | <b>1.88</b> | <b>0.83</b> |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for 4 °C is highlighted in bold.

Appendix 2. Performance of the TVC PLS-R models developed using VIS-SWNIR (445 - 970 nm ) data from beef *LD* samples stored at 10 °C. PLS full spectral range on reflectance (R) and logarithmic transformed (log(1/R)) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands    | # LV      | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |
|--------------------|------------------------|------------|-----------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|
|                    |                        |            |           | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |
| PLS                | R                      | None       | 106       | 8                 | 0.37             | 5.84                        | 0.97               | 0.64              | 3.38                         | 0.92              | 1.38             | 1.66                        | 0.75        |
|                    |                        | SNV        | 106       | 7                 | 0.39             | 5.59                        | 0.97               | 0.63              | 3.45                         | 0.92              | 1.39             | 1.56                        | 0.74        |
|                    |                        | SD         | 100       | 6                 | 0.66             | 3.27                        | 0.91               | 1.00              | 2.17                         | 0.79              | 1.18             | 1.67                        | 0.75        |
|                    |                        | SD+LD      | 100       | 5                 | 0.69             | 3.13                        | 0.90               | 1.02              | 2.12                         | 0.78              | 1.15             | 1.72                        | 0.76        |
|                    |                        | SNV+SD     | 100       | 4                 | 0.60             | 3.59                        | 0.92               | 0.81              | 2.68                         | 0.86              | 0.80             | 2.63                        | 0.89        |
|                    | Log(1/R)               | None       | 106       | 8                 | 0.42             | 5.14                        | 0.96               | 0.71              | 3.05                         | 0.89              | 1.14             | 2.48                        | 0.88        |
|                    |                        | SNV        | 106       | 7                 | 0.42             | 5.13                        | 0.96               | 0.69              | 3.15                         | 0.90              | 1.02             | 2.32                        | 0.86        |
|                    |                        | SD         | 100       | 4                 | 0.64             | 3.41                        | 0.91               | 0.84              | 2.58                         | 0.85              | 1.21             | 1.84                        | 0.80        |
|                    |                        | SD+LD      | 100       | 5                 | 0.53             | 4.11                        | 0.94               | 0.74              | 2.92                         | 0.88              | 1.16             | 2.02                        | 0.82        |
|                    |                        | SNV+SD     | 100       | 5                 | 0.54             | 4.05                        | 0.94               | 0.73              | 2.98                         | 0.89              | 1.01             | 2.31                        | 0.87        |
| VIP                | R                      | None       | 20        | 8                 | 0.48             | 4.49                        | 0.95               | 0.73              | 2.97                         | 0.89              | 1.06             | 1.99                        | 0.84        |
|                    |                        | SNV        | 37        | 8                 | 0.41             | 5.29                        | 0.96               | 0.63              | 3.42                         | 0.91              | 1.58             | 1.27                        | 0.72        |
|                    |                        | SD         | 33        | 5                 | 0.76             | 2.86                        | 0.88               | 1.03              | 2.10                         | 0.78              | 1.09             | 1.77                        | 0.81        |
|                    |                        | SD+LD      | 27        | 6                 | 0.72             | 3.03                        | 0.89               | 1.05              | 2.06                         | 0.76              | 0.91             | 1.97                        | 0.82        |
|                    |                        | SNV+SD     | 9         | 4                 | 0.65             | 3.34                        | 0.91               | 0.80              | 2.72                         | 0.87              | 0.92             | 2.27                        | 0.87        |
|                    | Log(1/R)               | None       | 15        | 6                 | 0.52             | 4.13                        | 0.94               | 0.72              | 3.03                         | 0.89              | 1.10             | 2.42                        | 0.88        |
|                    |                        | <b>SNV</b> | <b>33</b> | <b>7</b>          | <b>0.53</b>      | <b>4.11</b>                 | <b>0.94</b>        | <b>0.79</b>       | <b>2.75</b>                  | <b>0.87</b>       | <b>0.83</b>      | <b>3.10</b>                 | <b>0.93</b> |
|                    |                        | SD         | 10        | 5                 | 0.63             | 3.44                        | 0.92               | 0.80              | 2.70                         | 0.86              | 1.12             | 1.94                        | 0.83        |
|                    |                        | SD+LD      | 13        | 4                 | 0.66             | 3.29                        | 0.91               | 0.80              | 2.71                         | 0.86              | 1.34             | 1.59                        | 0.78        |
|                    |                        | SNV+SD     | 10        | 5                 | 0.60             | 3.59                        | 0.92               | 0.78              | 2.78                         | 0.87              | 1.04             | 2.16                        | 0.87        |
| SR                 | R                      | None       | 8         | 5                 | 1.07             | 2.02                        | 0.75               | 1.30              | 1.66                         | 0.65              | 0.82             | 2.67                        | 0.93        |

|                 |                 |        |    |      |      |      |      |      |      |      |             |             |      |
|-----------------|-----------------|--------|----|------|------|------|------|------|------|------|-------------|-------------|------|
|                 | SNV             | 21     | 9  | 0.55 | 3.97 | 0.94 | 0.87 | 2.50 | 0.84 | 0.95 | <b>2.20</b> | 0.86        |      |
|                 | SD              | 13     | 6  | 0.67 | 3.25 | 0.91 | 0.92 | 2.35 | 0.82 | 1.00 | <b>2.07</b> | 0.87        |      |
|                 | SD+LD           | 17     | 6  | 0.74 | 2.94 | 0.88 | 1.04 | 2.08 | 0.77 | 0.88 | <b>2.37</b> | 0.89        |      |
|                 | SNV+SD          | 20     | 7  | 0.60 | 3.59 | 0.92 | 0.88 | 2.46 | 0.84 | 0.91 | <b>2.09</b> | 0.86        |      |
|                 | None            | 8      | 5  | 0.90 | 2.39 | 0.83 | 1.12 | 1.93 | 0.73 | 1.07 | <b>2.12</b> | 0.86        |      |
| <b>Log(1/R)</b> | SNV             | 16     | 7  | 0.52 | 4.16 | 0.94 | 0.82 | 2.64 | 0.86 | 0.81 | <b>3.16</b> | 0.93        |      |
|                 | SD              | 9      | 7  | 0.54 | 4.05 | 0.94 | 0.73 | 2.96 | 0.89 | 1.38 | <b>1.81</b> | 0.79        |      |
|                 | SD+LD           | 17     | 4  | 0.67 | 3.25 | 0.91 | 0.85 | 2.55 | 0.85 | 1.34 | <b>1.64</b> | 0.79        |      |
|                 | SNV+SD          | 17     | 4  | 0.65 | 3.32 | 0.91 | 0.86 | 2.51 | 0.84 | 1.15 | <b>1.98</b> | 0.85        |      |
| <b>EMCVS</b>    | None            | 24     | 5  | 0.44 | 4.94 | 0.96 | 0.55 | 3.91 | 0.93 | 1.51 | <b>1.47</b> | 0.77        |      |
|                 | <b>R</b>        | SNV    | 18 | 4    | 0.45 | 4.85 | 0.96 | 0.56 | 3.85 | 0.93 | 1.73        | <b>1.19</b> | 0.73 |
|                 |                 | SD     | 13 | 3    | 0.75 | 2.90 | 0.88 | 0.87 | 2.49 | 0.84 | 1.00        | <b>1.78</b> | 0.80 |
|                 |                 | SD+LD  | 7  | 5    | 0.63 | 3.43 | 0.91 | 0.77 | 2.80 | 0.87 | 1.15        | <b>1.60</b> | 0.75 |
|                 |                 | SNV+SD | 6  | 3    | 0.63 | 3.44 | 0.92 | 0.72 | 3.01 | 0.89 | 1.02        | <b>1.84</b> | 0.79 |
|                 | None            | 9      | 5  | 0.44 | 4.93 | 0.96 | 0.55 | 3.93 | 0.94 | 1.03 | <b>2.30</b> | 0.87        |      |
|                 | <b>Log(1/R)</b> | SNV    | 7  | 6    | 0.48 | 4.51 | 0.95 | 0.65 | 3.34 | 0.91 | 1.00        | <b>2.40</b> | 0.88 |
|                 |                 | SD     | 10 | 3    | 0.66 | 3.29 | 0.91 | 0.75 | 2.89 | 0.88 | 1.04        | <b>1.96</b> | 0.83 |
|                 |                 | SD+LD  | 11 | 3    | 0.67 | 3.23 | 0.90 | 0.77 | 2.83 | 0.88 | 1.12        | <b>1.87</b> | 0.82 |
|                 |                 | SNV+SD | 9  | 4    | 0.53 | 4.08 | 0.94 | 0.65 | 3.36 | 0.91 | 0.84        | <b>2.50</b> | 0.89 |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for 10 °C is highlighted in bold.

Appendix 3. Performance of the TVC PLS-R models developed using VIS-SWNIR (445 - 970 nm ) data from beef *LD* samples stored at 4 °C or 10 °C. PLS full spectral range on reflectance (R) and logarithmic transformed ( $\log(1/R)$ ) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands | # LV | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |      |
|--------------------|------------------------|---------|------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|------|
|                    |                        |         |      | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |      |
| PLS                | R                      | None    | 106  | 6                 | 0.95             | 2.46                        | 0.83               | 1.11              | 2.11                         | 0.78              | 1.40             | 1.52                        | 0.75 |
|                    |                        | SNV     | 106  | 6                 | 0.85             | 2.76                        | 0.87               | 1.01              | 2.32                         | 0.81              | 1.33             | 1.47                        | 0.78 |
|                    |                        | SD      | 100  | 5                 | 0.96             | 2.43                        | 0.83               | 1.19              | 1.96                         | 0.74              | 1.11             | 1.76                        | 0.79 |
|                    |                        | SNV+SD  | 100  | 7                 | 0.86             | 2.72                        | 0.87               | 1.09              | 2.15                         | 0.78              | 0.98             | 1.99                        | 0.84 |
|                    |                        | SD+LD   | 100  | 6                 | 0.92             | 2.53                        | 0.84               | 1.15              | 2.04                         | 0.76              | 1.22             | 1.61                        | 0.76 |
|                    | Log(1/R)               | None    | 106  | 6                 | 0.92             | 2.54                        | 0.85               | 1.17              | 2.00                         | 0.76              | 1.23             | 1.71                        | 0.77 |
|                    |                        | SNV     | 106  | 6                 | 0.83             | 2.83                        | 0.87               | 0.98              | 2.39                         | 0.83              | 1.36             | 1.44                        | 0.73 |
|                    |                        | SD      | 100  | 5                 | 0.90             | 2.59                        | 0.85               | 1.11              | 2.11                         | 0.78              | 1.11             | 1.80                        | 0.79 |
|                    |                        | SNV+SD  | 100  | 4                 | 0.94             | 2.50                        | 0.84               | 1.09              | 2.14                         | 0.78              | 1.11             | 1.76                        | 0.79 |
|                    |                        | SD+LD   | 100  | 4                 | 0.94             | 2.49                        | 0.84               | 1.13              | 2.07                         | 0.77              | 1.16             | 1.71                        | 0.77 |
| VIP                | R                      | None    | 8    | 5                 | 1.03             | 2.28                        | 0.81               | 1.13              | 2.06                         | 0.77              | 1.51             | 1.42                        | 0.69 |
|                    |                        | SNV     | 22   | 7                 | 0.86             | 2.73                        | 0.87               | 0.96              | 2.43                         | 0.83              | 1.55             | 1.28                        | 0.74 |
|                    |                        | SD      | 7    | 4                 | 1.19             | 1.96                        | 0.74               | 1.29              | 1.82                         | 0.70              | 1.08             | 1.85                        | 0.80 |
|                    |                        | SNV+SD  | 8    | 3                 | 1.21             | 1.93                        | 0.73               | 1.32              | 1.77                         | 0.68              | 1.31             | 1.63                        | 0.74 |
|                    |                        | SD+LD   | 19   | 6                 | 1.12             | 2.09                        | 0.77               | 1.26              | 1.85                         | 0.71              | 1.32             | 1.51                        | 0.72 |
|                    | Log(1/R)               | None    | 8    | 3                 | 1.04             | 2.26                        | 0.80               | 1.09              | 2.14                         | 0.78              | 1.51             | 1.37                        | 0.65 |
|                    |                        | SNV     | 10   | 6                 | 0.92             | 2.55                        | 0.85               | 1.03              | 2.28                         | 0.81              | 1.24             | 1.68                        | 0.77 |
|                    |                        | SD      | 30   | 4                 | 0.99             | 2.37                        | 0.82               | 1.12              | 2.08                         | 0.77              | 1.15             | 1.76                        | 0.78 |
|                    |                        | SNV+SD  | 24   | 5                 | 0.95             | 2.46                        | 0.83               | 1.10              | 2.12                         | 0.78              | 1.06             | 1.88                        | 0.80 |
|                    |                        | SD+LD   | 15   | 5                 | 1.03             | 2.27                        | 0.81               | 1.15              | 2.03                         | 0.76              | 1.28             | 1.57                        | 0.72 |
| SR                 | R                      | None    | 7    | 5                 | 1.41             | 1.66                        | 0.64               | 1.59              | 1.47                         | 0.54              | 1.44             | 1.60                        | 0.74 |
|                    |                        | SNV     | 14   | 8                 | 1.11             | 2.11                        | 0.78               | 1.24              | 1.89                         | 0.72              | 1.27             | 1.74                        | 0.81 |

|                 |               |          |          |             |             |             |             |             |             |             |             |             |
|-----------------|---------------|----------|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|                 | SD            | 16       | 6        | 1.08        | 2.16        | 0.79        | 1.24        | 1.89        | 0.72        | 1.17        | 1.70        | 0.78        |
|                 | SNV+SD        | 11       | 6        | 1.10        | 2.13        | 0.78        | 1.25        | 1.87        | 0.72        | 1.25        | 1.58        | 0.74        |
|                 | SD+LD         | 17       | 6        | 1.02        | 2.29        | 0.81        | 1.20        | 1.96        | 0.74        | 1.24        | 1.60        | 0.75        |
|                 | None          | 14       | 7        | 1.02        | 2.30        | 0.81        | 1.23        | 1.90        | 0.73        | 1.27        | 1.63        | 0.74        |
|                 | SNV           | 17       | 5        | 1.02        | 2.29        | 0.81        | 1.22        | 1.92        | 0.73        | 1.24        | 1.61        | 0.75        |
| <b>Log(1/R)</b> | SD            | 13       | 7        | 0.97        | 2.40        | 0.83        | 1.15        | 2.03        | 0.76        | 1.23        | 1.70        | 0.76        |
|                 | SNV+SD        | 17       | 5        | 1.07        | 2.18        | 0.79        | 1.24        | 1.89        | 0.72        | 1.41        | 1.43        | 0.68        |
|                 | SD+LD         | 14       | 6        | 0.99        | 2.37        | 0.82        | 1.16        | 2.02        | 0.76        | 1.11        | 1.81        | 0.79        |
|                 | None          | 3        | 2        | 1.02        | 1.65        | 0.63        | 1.07        | 1.57        | 0.59        | 1.66        | 1.29        | 0.60        |
|                 | SNV           | 9        | 6        | 0.81        | 2.90        | 0.88        | 0.90        | 2.61        | 0.85        | 1.56        | 1.27        | 0.74        |
| <b>R</b>        | SD            | 3        | 3        | 1.10        | 2.13        | 0.78        | 1.17        | 2.01        | 0.75        | 1.01        | 1.97        | 0.83        |
|                 | <b>SNV+SD</b> | <b>8</b> | <b>4</b> | <b>0.94</b> | <b>2.48</b> | <b>0.84</b> | <b>1.05</b> | <b>2.22</b> | <b>0.80</b> | <b>0.95</b> | <b>2.10</b> | <b>0.85</b> |
| <b>EMCVS</b>    | SD+LD         | 4        | 3        | 0.92        | 2.55        | 0.85        | 0.96        | 2.43        | 0.83        | 1.24        | 1.61        | 0.76        |
|                 | None          | 23       | 13       | 0.61        | 3.82        | 0.93        | 0.77        | 3.04        | 0.89        | 0.88        | 2.25        | 0.86        |
|                 | SNV           | 15       | 6        | 0.91        | 2.57        | 0.85        | 1.01        | 2.32        | 0.81        | 1.20        | 1.71        | 0.78        |
| <b>Log(1/R)</b> | SD            | 8        | 6        | 0.93        | 2.50        | 0.84        | 1.05        | 2.22        | 0.80        | 1.21        | 1.69        | 0.76        |
|                 | SNV+SD        | 8        | 3        | 0.95        | 2.45        | 0.83        | 1.01        | 2.31        | 0.81        | 0.96        | 2.10        | 0.84        |
|                 | SD+LD         | 9        | 3        | 0.95        | 2.45        | 0.83        | 1.03        | 2.27        | 0.81        | 1.04        | 1.92        | 0.81        |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for 10 °C is highlighted in bold.



Appendix 4. Performance of the TVC PLS-R models developed using NIR (957 - 1664 nm ) data from beef *LD* samples stored at 4 °C, PLS full spectral range on reflectance (R) and logarithmic transformed (log(1/R)) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands | # LV | Calibration |      |                  | Cross validation |       |                   | Prediction |      |                  |      |
|--------------------|------------------------|---------|------|-------------|------|------------------|------------------|-------|-------------------|------------|------|------------------|------|
|                    |                        |         |      | RMSEc       | RPDc | R <sup>2</sup> c | RMSEcv           | RPDcv | R <sup>2</sup> cv | RMSEp      | RPDp | R <sup>2</sup> p |      |
| PLS                | R                      | None    | 102  | 8           | 0.66 | 3.58             | 0.92             | 1.14  | 2.07              | 0.78       | 2.75 | 0.94             | 0.45 |
|                    |                        | SD      | 96   | 5           | 0.84 | 2.79             | 0.87             | 1.17  | 2.00              | 0.75       | 1.97 | 1.68             | 0.84 |
|                    |                        | SD+LD   | 96   | 5           | 0.84 | 2.79             | 0.87             | 1.15  | 2.04              | 0.76       | 1.91 | 1.72             | 0.84 |
|                    |                        | SNV+SD  | 96   | 5           | 0.87 | 2.70             | 0.86             | 1.19  | 1.97              | 0.74       | 1.66 | 1.69             | 0.83 |
|                    | Log(1/R)               | None    | 102  | 6           | 0.82 | 2.87             | 0.88             | 1.21  | 1.94              | 0.75       | 3.50 | 0.69             | 0.08 |
|                    |                        | SD      | 96   | 5           | 0.92 | 2.55             | 0.85             | 1.45  | 1.62              | 0.63       | 0.87 | 2.23             | 0.91 |
|                    |                        | SD+LD   | 96   | 5           | 0.93 | 2.52             | 0.84             | 1.43  | 1.64              | 0.64       | 0.83 | 2.33             | 0.91 |
|                    |                        | SNV+SD  | 96   | 4           | 0.72 | 3.28             | 0.91             | 0.97  | 2.42              | 0.83       | 1.19 | 1.63             | 0.82 |
| VIP                | R                      | None    | 12   | 7           | 0.66 | 3.55             | 0.92             | 1.03  | 2.28              | 0.82       | 2.89 | 1.33             | 0.61 |
|                    |                        | SD      | 17   | 5           | 0.85 | 2.76             | 0.87             | 1.14  | 2.06              | 0.77       | 2.74 | 1.23             | 0.57 |
|                    |                        | SD+LD   | 17   | 5           | 0.93 | 2.52             | 0.84             | 1.20  | 1.95              | 0.74       | 1.91 | 1.59             | 0.72 |
|                    |                        | SNV+SD  | 12   | 7           | 0.83 | 2.82             | 0.87             | 1.08  | 2.17              | 0.79       | 1.94 | 1.45             | 0.68 |
|                    | Log(1/R)               | None    | 14   | 7           | 0.60 | 3.93             | 0.94             | 0.86  | 2.72              | 0.87       | 2.88 | 0.96             | 0.27 |
|                    |                        | SD      | 11   | 6           | 0.86 | 2.72             | 0.86             | 1.11  | 2.11              | 0.78       | 1.58 | 2.25             | 0.86 |
|                    |                        | SD+LD   | 8    | 6           | 0.88 | 2.68             | 0.86             | 1.08  | 2.17              | 0.79       | 1.22 | 2.07             | 0.86 |
|                    |                        | SNV+SD  | 7    | 4           | 0.76 | 3.07             | 0.89             | 0.94  | 2.50              | 0.84       | 1.24 | 1.87             | 0.80 |
| SR                 | R                      | None    | 42   | 6           | 1.02 | 2.29             | 0.81             | 1.32  | 1.78              | 0.69       | 1.57 | 1.78             | 0.86 |
|                    |                        | SD      | 4    | 3           | 1.21 | 1.94             | 0.73             | 1.38  | 1.70              | 0.66       | 1.22 | 1.91             | 0.82 |
|                    |                        | SD+LD   | 2    | 1           | 1.57 | 1.49             | 0.55             | 1.64  | 1.43              | 0.51       | 1.73 | 1.37             | 0.64 |
|                    |                        | SNV+SD  | 1    | 1           | 1.51 | 1.55             | 0.58             | 1.59  | 1.48              | 0.54       | 2.28 | 1.01             | 0.32 |
|                    | Log(1/R)               | None    | 29   | 6           | 1.04 | 2.26             | 0.80             | 1.40  | 1.68              | 0.66       | 1.12 | 2.26             | 0.87 |
|                    |                        | SD      | 6    | 2           | 1.44 | 1.63             | 0.62             | 1.58  | 1.49              | 0.55       | 1.23 | 2.00             | 0.90 |

|       |          |              |           |          |             |             |             |             |             |             |             |             |             |
|-------|----------|--------------|-----------|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|       |          | SD+LD        | 4         | 4        | 1.35        | 1.74        | 0.67        | 1.60        | 1.47        | 0.54        | 1.13        | 2.12        | 0.91        |
|       |          | SNV+SD       | 1         | 1        | 1.67        | 1.40        | 0.49        | 1.75        | 1.34        | 0.44        | 2.56        | 0.90        | 0.15        |
| EMCVS | R        | None         | 8         | 5        | 0.72        | 3.24        | 0.90        | 1.00        | 2.34        | 0.82        | 3.91        | 0.82        | 0.07        |
|       |          | SD           | 16        | 4        | 0.94        | 2.50        | 0.84        | 1.14        | 2.06        | 0.76        | 2.83        | 1.30        | 0.63        |
|       |          | SD+LD        | 6         | 4        | 0.93        | 2.52        | 0.84        | 1.10        | 2.14        | 0.78        | 1.98        | 1.59        | 0.73        |
|       |          | SNV+SD       | 8         | 6        | 0.65        | 3.63        | 0.92        | 0.79        | 2.95        | 0.89        | 1.15        | 2.18        | 0.85        |
|       |          | None         | 19        | 5        | 0.86        | 2.69        | 0.86        | 1.06        | 2.20        | 0.79        | 3.85        | 0.75        | 0.01        |
|       | Log(1/R) | SD           | 10        | 4        | 0.80        | 2.93        | 0.88        | 1.01        | 2.32        | 0.82        | 0.93        | 2.48        | 0.89        |
|       |          | <b>SD+LD</b> | <b>13</b> | <b>4</b> | <b>0.78</b> | <b>3.03</b> | <b>0.89</b> | <b>1.01</b> | <b>2.31</b> | <b>0.81</b> | <b>0.92</b> | <b>3.00</b> | <b>0.92</b> |
|       |          | SNV+SD       | 5         | 4        | 0.73        | 3.22        | 0.90        | 0.88        | 2.68        | 0.86        | 1.51        | 1.54        | 0.70        |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for 4 °C is highlighted in bold.

Appendix 5. Performance of the TVC PLS-R models developed using NIR (957 - 1664 nm ) data from beef *LD* samples stored at 10 °C, PLS full spectral range on reflectance (R) and logarithmic transformed (log(1/R)) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Pre-treatment | # Bands    | # LV      | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |
|--------------------|---------------|------------|-----------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|
|                    |               |            |           | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |
| PLS                | R             | None       | 102       | 11                | 0.59             | 3.68                        | 0.93               | 1.06              | 2.04                         | 0.77              | 1.90             | 1.16                        | 0.62        |
|                    |               | SNV        | 102       | 5                 | 1.03             | 2.10                        | 0.77               | 1.39              | 1.55                         | 0.60              | 2.19             | 1.23                        | 0.54        |
|                    |               | SD         | 96        | 7                 | 0.71             | 3.07                        | 0.89               | 1.21              | 1.79                         | 0.70              | 2.05             | 0.98                        | 0.47        |
|                    |               | SD+LD      | 96        | 4                 | 1.27             | 1.71                        | 0.66               | 1.52              | 1.43                         | 0.51              | 1.67             | 1.28                        | 0.55        |
|                    |               | SNV+SD     | 96        | 6                 | 0.73             | 2.97                        | 0.89               | 1.07              | 2.02                         | 0.76              | 1.59             | 1.31                        | 0.63        |
|                    | Log(1/R)      | None       | 102       | 11                | 0.55             | 3.91                        | 0.93               | 1.07              | 2.02                         | 0.76              | 2.38             | 0.80                        | 0.35        |
|                    |               | SNV        | 102       | 12                | 0.41             | 5.29                        | 0.96               | 0.90              | 2.41                         | 0.83              | 1.67             | 1.53                        | 0.73        |
|                    |               | SD         | 96        | 7                 | 0.68             | 3.18                        | 0.90               | 1.11              | 1.95                         | 0.74              | 1.38             | 1.33                        | 0.64        |
|                    |               | SD+LD      | 96        | 6                 | 0.79             | 2.75                        | 0.87               | 1.29              | 1.68                         | 0.65              | 1.37             | 1.31                        | 0.63        |
|                    |               | SNV+SD     | 96        | 7                 | 0.61             | 3.56                        | 0.92               | 1.03              | 2.12                         | 0.78              | 1.19             | 1.57                        | 0.72        |
| EMCVS              | R             | None       | 19        | 9                 | 0.68             | 3.19                        | 0.90               | 1.00              | 2.17                         | 0.79              | 1.79             | 1.02                        | 0.51        |
|                    |               | SNV        | 4         | 4                 | 1.00             | 2.10                        | 0.77               | 1.17              | 1.79                         | 0.69              | 1.93             | 1.05                        | 0.41        |
|                    |               | SD         | 8         | 4                 | 0.90             | 2.40                        | 0.83               | 1.04              | 2.08                         | 0.77              | 1.59             | 1.34                        | 0.64        |
|                    |               | SD+LD      | 7         | 4                 | 0.81             | 2.67                        | 0.86               | 0.96              | 2.26                         | 0.81              | 1.37             | 1.31                        | 0.65        |
|                    |               | SNV+SD     | 14        | 3                 | 0.80             | 2.72                        | 0.86               | 0.90              | 2.39                         | 0.83              | 1.64             | 1.43                        | 0.69        |
|                    | Log(1/R)      | None       | 12        | 8                 | 0.63             | 3.46                        | 0.92               | 0.88              | 2.45                         | 0.84              | 2.57             | 0.70                        | 0.31        |
|                    |               | <b>SNV</b> | <b>19</b> | <b>9</b>          | <b>0.44</b>      | <b>4.93</b>                 | <b>0.96</b>        | <b>0.67</b>       | <b>3.22</b>                  | <b>0.90</b>       | <b>1.15</b>      | <b>2.23</b>                 | <b>0.87</b> |
|                    |               | SD         | 12        | 5                 | 0.78             | 2.78                        | 0.87               | 0.96              | 2.25                         | 0.80              | 1.71             | 1.35                        | 0.67        |
|                    |               | SD+LD      | 9         | 4                 | 1.03             | 2.11                        | 0.78               | 1.14              | 1.91                         | 0.73              | 1.49             | 1.15                        | 0.51        |
|                    |               | SNV+SD     | 15        | 5                 | 0.71             | 3.05                        | 0.89               | 0.92              | 2.36                         | 0.82              | 1.45             | 1.30                        | 0.60        |
| SR                 | R             | None       | 1         | 1                 | 2.14             | 1.01                        | 0.03               | 2.32              | 0.93                         | 0.12              | 1.93             | 0.90                        | 0.29        |
|                    |               | SNV        | 7         | 5                 | 1.28             | 1.69                        | 0.65               | 1.58              | 1.37                         | 0.49              | 2.22             | 0.84                        | 0.26        |

|                 |        |    |    |      |      |      |      |      |      |      |             |      |
|-----------------|--------|----|----|------|------|------|------|------|------|------|-------------|------|
|                 | SD     | 2  | 1  | 1.45 | 1.49 | 0.55 | 1.55 | 1.40 | 0.49 | 1.80 | <b>0.96</b> | 0.30 |
|                 | SD+LD  | 1  | 1  | 1.72 | 1.26 | 0.37 | 1.84 | 1.18 | 0.29 | 2.26 | <b>0.77</b> | 0.12 |
|                 | SNV+SD | 1  | 1  | 1.91 | 1.14 | 0.23 | 2.03 | 1.07 | 0.14 | 1.90 | <b>1.04</b> | 0.36 |
|                 | None   | 1  | 1  | 2.14 | 1.01 | 0.02 | 2.32 | 0.93 | 0.15 | 1.95 | <b>0.89</b> | 0.26 |
|                 | SNV    | 1  | 1  | 1.92 | 1.13 | 0.21 | 2.04 | 1.06 | 0.13 | 1.50 | <b>1.23</b> | 0.72 |
| <b>Log(1/R)</b> | SD     | 1  | 1  | 1.91 | 1.13 | 0.22 | 2.00 | 1.08 | 0.15 | 1.74 | <b>0.99</b> | 0.29 |
|                 | SD+LD  | 1  | 1  | 1.91 | 1.14 | 0.23 | 2.00 | 1.09 | 0.16 | 1.73 | <b>1.00</b> | 0.30 |
|                 | SNV+SD | 4  | 3  | 1.49 | 1.46 | 0.53 | 1.78 | 1.22 | 0.36 | 1.82 | <b>1.07</b> | 0.39 |
|                 | None   | 6  | 4  | 1.32 | 1.64 | 0.63 | 1.55 | 1.40 | 0.49 | 2.17 | <b>0.89</b> | 0.28 |
|                 | SNV    | 21 | 8  | 0.74 | 2.92 | 0.88 | 1.14 | 1.90 | 0.74 | 1.95 | <b>1.30</b> | 0.60 |
| <b>R</b>        | SD     | 6  | 4  | 1.07 | 2.02 | 0.76 | 1.22 | 1.78 | 0.69 | 1.47 | <b>1.64</b> | 0.76 |
|                 | SD+LD  | 5  | 3  | 1.40 | 1.55 | 0.58 | 1.59 | 1.36 | 0.47 | 1.91 | <b>1.14</b> | 0.54 |
| <b>VIP</b>      | SNV+SD | 9  | 4  | 0.87 | 2.48 | 0.84 | 1.03 | 2.10 | 0.77 | 1.82 | <b>1.71</b> | 0.77 |
|                 | None   | 13 | 9  | 0.82 | 2.65 | 0.86 | 1.18 | 1.84 | 0.71 | 1.78 | <b>1.79</b> | 0.86 |
|                 | SNV    | 20 | 10 | 0.54 | 4.00 | 0.94 | 1.04 | 2.07 | 0.78 | 1.82 | <b>1.12</b> | 0.53 |
| <b>Log(1/R)</b> | SD     | 24 | 8  | 0.67 | 3.23 | 0.90 | 0.98 | 2.22 | 0.80 | 1.40 | <b>1.35</b> | 0.66 |
|                 | SD+LD  | 22 | 6  | 0.90 | 2.42 | 0.83 | 1.18 | 1.84 | 0.70 | 1.61 | <b>1.15</b> | 0.54 |
|                 | SNV+SD | 31 | 8  | 0.67 | 3.23 | 0.90 | 0.98 | 2.21 | 0.80 | 1.14 | <b>1.65</b> | 0.75 |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for 10 °C is highlighted in bold.

Appendix 6. Performance of the TVC PLS-R models developed using NIR (957 - 1664 nm ) data from beef *LD* samples stored either 4 °C or 10 °C. PLS full spectral range on reflectance (R) and logarithmic transformed ( $\log(1/R)$ ) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands | # LV | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |      |
|--------------------|------------------------|---------|------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|------|
|                    |                        |         |      | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |      |
| PLS                | R                      | None    | 102  | 6                 | 1.36             | 1.72                        | 0.66               | 1.57              | 1.49                         | 0.55              | 2.19             | 0.89                        | 0.29 |
|                    |                        | SNV     | 102  | 13                | 0.86             | 2.72                        | 0.86               | 1.27              | 1.85                         | 0.71              | 2.58             | 1.00                        | 0.44 |
|                    |                        | SD      | 96   | 6                 | 1.19             | 1.97                        | 0.74               | 1.40              | 1.67                         | 0.64              | 1.27             | 1.53                        | 0.71 |
|                    |                        | SNV+SD  | 96   | 7                 | 1.06             | 2.20                        | 0.79               | 1.36              | 1.72                         | 0.67              | 1.58             | 1.25                        | 0.61 |
|                    |                        | SD+LD   | 96   | 6                 | 1.20             | 1.94                        | 0.73               | 1.42              | 1.65                         | 0.64              | 1.29             | 1.52                        | 0.71 |
|                    | Log(1/R)               | None    | 102  | 5                 | 1.51             | 1.55                        | 0.58               | 1.74              | 1.34                         | 0.45              | 2.78             | 0.72                        | 0.14 |
|                    |                        | SNV     | 102  | 13                | 0.84             | 2.79                        | 0.87               | 1.38              | 1.70                         | 0.67              | 1.44             | 1.35                        | 0.64 |
|                    |                        | SD      | 96   | 6                 | 1.18             | 1.98                        | 0.74               | 1.47              | 1.59                         | 0.61              | 1.21             | 1.62                        | 0.74 |
|                    |                        | SNV+SD  | 96   | 6                 | 1.15             | 2.03                        | 0.76               | 1.48              | 1.58                         | 0.61              | 1.29             | 1.51                        | 0.70 |
|                    |                        | SD+LD   | 96   | 6                 | 1.17             | 2.01                        | 0.75               | 1.47              | 1.59                         | 0.61              | 1.18             | 1.66                        | 0.76 |
| VIP                | R                      | None    | 9    | 5                 | 1.41             | 1.65                        | 0.63               | 1.56              | 1.50                         | 0.56              | 2.52             | 0.79                        | 0.22 |
|                    |                        | SNV     | 20   | 13                | 0.92             | 2.53                        | 0.84               | 1.19              | 1.97                         | 0.75              | 1.45             | 1.42                        | 0.68 |
|                    |                        | SD      | 27   | 6                 | 1.18             | 1.99                        | 0.75               | 1.37              | 1.70                         | 0.66              | 1.41             | 1.40                        | 0.65 |
|                    |                        | SNV+SD  | 17   | 6                 | 1.17             | 2.01                        | 0.75               | 1.35              | 1.73                         | 0.67              | 1.41             | 1.41                        | 0.65 |
|                    |                        | SD+LD   | 6    | 4                 | 1.36             | 1.72                        | 0.66               | 1.47              | 1.59                         | 0.60              | 1.34             | 1.46                        | 0.67 |
|                    | Log(1/R)               | None    | 32   | 10                | 1.24             | 1.89                        | 0.72               | 1.52              | 1.54                         | 0.59              | 2.33             | 0.84                        | 0.27 |
|                    |                        | SNV     | 10   | 5                 | 1.35             | 1.73                        | 0.67               | 1.52              | 1.53                         | 0.58              | 1.93             | 1.09                        | 0.44 |
|                    |                        | SD      | 17   | 6                 | 1.23             | 1.90                        | 0.72               | 1.41              | 1.66                         | 0.64              | 1.29             | 1.58                        | 0.72 |
|                    |                        | SNV+SD  | 12   | 6                 | 1.21             | 1.93                        | 0.73               | 1.40              | 1.67                         | 0.65              | 1.17             | 1.66                        | 0.75 |
|                    |                        | SD+LD   | 17   | 6                 | 1.27             | 1.83                        | 0.70               | 1.43              | 1.63                         | 0.63              | 1.30             | 1.51                        | 0.70 |
| SR                 | R                      | None    | 28   | 7                 | 1.40             | 1.67                        | 0.64               | 1.93              | 1.21                         | 0.41              | 1.31             | 1.49                        | 0.70 |
|                    |                        | SNV     | 1    | 1                 | 1.92             | 1.22                        | 0.33               | 1.98              | 1.18                         | 0.28              | 2.19             | 0.89                        | 0.13 |

|          |          |           |           |             |             |             |             |             |             |             |             |             |      |
|----------|----------|-----------|-----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------|
|          | SD       | 1         | 1         | 1.77        | 1.32        | 0.43        | 1.81        | 1.29        | 0.40        | 1.88        | 1.05        | 0.39        |      |
|          | SNV+SD   | 5         | 4         | 1.49        | 1.57        | 0.59        | 1.62        | 1.44        | 0.52        | 1.58        | 1.24        | 0.55        |      |
|          | SD+LD    | 1         | 1         | 1.72        | 1.36        | 0.46        | 1.77        | 1.32        | 0.43        | 1.93        | 1.02        | 0.37        |      |
|          | None     | 27        | 7         | 1.44        | 1.63        | 0.62        | 1.84        | 1.27        | 0.42        | 1.48        | 1.33        | 0.63        |      |
|          | SNV      | 11        | 3         | 1.91        | 1.23        | 0.34        | 2.07        | 1.13        | 0.23        | 2.32        | 0.86        | 0.11        |      |
| Log(1/R) | SD       | 1         | 1         | 1.94        | 1.20        | 0.31        | 1.98        | 1.18        | 0.28        | 1.84        | 1.13        | 0.45        |      |
|          | SNV+SD   | 1         | 1         | 2.10        | 1.12        | 0.20        | 2.16        | 1.08        | 0.15        | 2.14        | 0.92        | 0.18        |      |
|          | SD+LD    | 1         | 1         | 1.93        | 1.21        | 0.32        | 1.97        | 1.19        | 0.29        | 1.83        | 1.14        | 0.46        |      |
| <hr/>    |          |           |           |             |             |             |             |             |             |             |             |             |      |
| EMCVS    | None     | 6         | 4         | 1.42        | 1.65        | 0.63        | 1.55        | 1.52        | 0.57        | 2.12        | 1.00        | 0.37        |      |
|          | SNV      | 19        | 11        | 0.85        | 2.76        | 0.87        | 1.09        | 2.15        | 0.79        | 1.77        | 1.23        | 0.56        |      |
|          | R        | SD        | 10        | 4           | 1.31        | 1.78        | 0.69        | 1.42        | 1.65        | 0.63        | 1.48        | 1.45        | 0.67 |
|          |          | SNV+SD    | 12        | 5           | 1.04        | 2.24        | 0.80        | 1.18        | 1.98        | 0.74        | 1.15        | 1.75        | 0.77 |
|          |          | SD+LD     | 11        | 4           | 1.32        | 1.77        | 0.68        | 1.43        | 1.63        | 0.63        | 1.55        | 1.28        | 0.59 |
|          | None     | 12        | 6         | 1.36        | 1.70        | 0.65        | 1.55        | 1.49        | 0.55        | 2.08        | 0.95        | 0.32        |      |
|          | SNV      | <b>19</b> | <b>11</b> | <b>0.90</b> | <b>2.60</b> | <b>0.85</b> | <b>1.14</b> | <b>2.05</b> | <b>0.77</b> | <b>1.03</b> | <b>1.92</b> | <b>0.81</b> |      |
|          | Log(1/R) | SD        | 5         | 4           | 1.29        | 1.81        | 0.70        | 1.41        | 1.66        | 0.64        | 1.46        | 1.35        | 0.63 |
|          |          | SNV+SD    | 5         | 3           | 1.17        | 1.96        | 0.74        | 1.28        | 1.80        | 0.69        | 1.63        | 1.20        | 0.53 |
|          |          | SD+LD     | 6         | 4           | 1.25        | 1.87        | 0.72        | 1.37        | 1.71        | 0.66        | 1.48        | 1.35        | 0.64 |

Appendix 7. Performance of the best TVC PLS-R models developed using the LL data fusion of VIS-SWNIR (445 - 970 nm ) and NIR (957 - 1664 nm) HSI data from beef LD samples stored at 4 °C. PLS full spectral range on reflectance (R) and logarithmic transformed ( $\log(1/R)$ ) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands  | # LV      | Calibration        |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |      |
|--------------------|------------------------|----------|-----------|--------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|------|
|                    |                        |          |           | RMSE <sub>cv</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |      |
| PLS                | R                      | None     | 208       | 7                  | 0.87             | 2.85                        | 0.88               | 1.53              | 1.63                         | 0.66              | 1.73             | 1.23                        | 0.68        |      |
|                    |                        | SNV      | 208       | 7                  | 0.81             | 3.06                        | 0.89               | 1.34              | 1.86                         | 0.73              | 1.69             | 1.30                        | 0.67        |      |
|                    |                        | SD       | 202       | 6                  | 0.84             | 2.97                        | 0.89               | 1.35              | 1.86                         | 0.71              | 1.18             | 1.75                        | 0.86        |      |
|                    |                        | SD+LD    | 202       | 6                  | 0.85             | 2.94                        | 0.88               | 1.38              | 1.81                         | 0.70              | 1.17             | 1.76                        | 0.86        |      |
|                    |                        | SNV+SD   | 202       | 6                  | 0.82             | 3.05                        | 0.89               | 1.15              | 2.17                         | 0.79              | 1.35             | 1.52                        | 0.77        |      |
|                    |                        | None     | 198       | 6                  | 0.75             | 3.30                        | 0.91               | 1.45              | 1.74                         | 0.67              | 1.42             | 1.51                        | 0.78        |      |
|                    |                        | SNV      | 208       | 6                  | 0.75             | 3.32                        | 0.91               | 1.06              | 2.35                         | 0.82              | 1.36             | 1.57                        | 0.75        |      |
|                    |                        | Log(1/R) | SD        | 208                | 7                | 0.71                        | 3.49               | 0.92              | 1.11                         | 2.25              | 0.80             | 1.32                        | 1.66        | 0.78 |
|                    |                        |          | SD+LD     | 208                | 9                | 0.71                        | 3.51               | 0.92              | 1.28                         | 1.95              | 0.75             | 1.38                        | 1.86        | 0.85 |
|                    |                        |          | SNV+SD    | 202                | 6                | 0.72                        | 3.44               | 0.92              | 1.17                         | 2.13              | 0.78             | 1.25                        | 1.66        | 0.83 |
| VIP                | R                      | None     | 4         | 3                  | 1.11             | 2.25                        | 0.80               | 1.23              | 2.03                         | 0.76              | 1.62             | 1.45                        | 0.71        |      |
|                    |                        | SNV      | 24        | 5                  | 0.97             | 2.56                        | 0.85               | 1.26              | 1.97                         | 0.74              | 1.74             | 1.27                        | 0.63        |      |
|                    |                        | SD       | 22        | 11                 | 0.56             | 4.42                        | 0.95               | 1.11              | 2.27                         | 0.81              | 1.74             | 1.65                        | 0.83        |      |
|                    |                        | SD+LD    | <b>22</b> | <b>8</b>           | <b>0.76</b>      | <b>3.28</b>                 | <b>0.91</b>        | <b>1.09</b>       | <b>2.30</b>                  | <b>0.81</b>       | <b>1.16</b>      | <b>1.90</b>                 | <b>0.88</b> |      |
|                    |                        | SNV+SD   | 32        | 6                  | 0.90             | 2.78                        | 0.87               | 1.23              | 2.03                         | 0.76              | 1.22             | 1.87                        | 0.82        |      |
|                    |                        | None     | 10        | 7                  | 0.88             | 2.82                        | 0.87               | 1.31              | 1.91                         | 0.75              | 1.48             | 1.52                        | 0.72        |      |
|                    |                        | SNV      | 18        | 12                 | 0.52             | 4.82                        | 0.96               | 0.97              | 2.56                         | 0.87              | 1.51             | 1.45                        | 0.75        |      |
|                    |                        | Log(1/R) | SD        | 35                 | 9                | 0.57                        | 4.35               | 0.95              | 1.00                         | 2.50              | 0.84             | 1.45                        | 1.56        | 0.75 |
|                    |                        |          | SD+LD     | 29                 | 12               | 0.50                        | 4.99               | 0.96              | 0.95                         | 2.64              | 0.86             | 1.58                        | 1.61        | 0.74 |
|                    |                        |          | SNV+SD    | 10                 | 7                | 0.86                        | 2.90               | 0.88              | 1.32                         | 1.90              | 0.72             | 1.34                        | 1.71        | 0.77 |
| SR                 | R                      | None     | 15        | 7                  | 1.07             | 2.34                        | 0.82               | 1.56              | 1.60                         | 0.66              | 1.53             | 1.62                        | 0.79        |      |

|                 |                 |        |    |      |      |      |      |      |      |      |             |             |      |
|-----------------|-----------------|--------|----|------|------|------|------|------|------|------|-------------|-------------|------|
|                 | SNV             | 17     | 9  | 0.92 | 2.72 | 0.87 | 1.36 | 1.83 | 0.71 | 1.00 | <b>2.22</b> | 0.87        |      |
|                 | SD              | 8      | 4  | 1.00 | 2.49 | 0.84 | 1.27 | 1.96 | 0.74 | 1.60 | <b>1.37</b> | 0.68        |      |
|                 | SD+LD           | 8      | 3  | 1.11 | 2.25 | 0.80 | 1.29 | 1.94 | 0.73 | 1.72 | <b>1.28</b> | 0.66        |      |
|                 | SNV+SD          | 2      | 1  | 1.35 | 1.85 | 0.71 | 1.45 | 1.72 | 0.66 | 1.77 | <b>1.29</b> | 0.66        |      |
|                 | None            | 15     | 8  | 0.91 | 2.73 | 0.87 | 1.39 | 1.80 | 0.73 | 1.52 | <b>1.48</b> | 0.74        |      |
| <b>Log(1/R)</b> | SNV             | 21     | 6  | 1.14 | 2.19 | 0.79 | 1.58 | 1.59 | 0.62 | 1.41 | <b>1.58</b> | 0.77        |      |
|                 | SD              | 7      | 6  | 0.85 | 2.94 | 0.88 | 1.09 | 2.29 | 0.81 | 2.64 | <b>1.35</b> | 0.64        |      |
|                 | SD+LD           | 1      | 1  | 1.24 | 2.01 | 0.75 | 1.31 | 1.90 | 0.72 | 2.08 | <b>1.05</b> | 0.44        |      |
|                 | SNV+SD          | 8      | 5  | 0.91 | 2.72 | 0.87 | 1.13 | 2.21 | 0.80 | 1.97 | <b>1.78</b> | 0.83        |      |
| <b>EMCVS</b>    | None            | 9      | 7  | 0.97 | 2.58 | 0.85 | 1.28 | 1.95 | 0.75 | 1.33 | <b>1.66</b> | 0.76        |      |
|                 | SNV             | 5      | 4  | 1.02 | 2.32 | 0.81 | 1.15 | 2.06 | 0.76 | 1.74 | <b>1.29</b> | 0.58        |      |
|                 | SD              | 9      | 6  | 0.71 | 3.51 | 0.92 | 0.91 | 2.74 | 0.87 | 1.71 | <b>1.29</b> | 0.81        |      |
|                 | SD+LD           | 10     | 6  | 0.74 | 3.36 | 0.91 | 0.94 | 2.64 | 0.86 | 1.69 | <b>1.36</b> | 0.76        |      |
|                 | SNV+SD          | 28     | 4  | 0.92 | 2.72 | 0.86 | 1.08 | 2.30 | 0.81 | 1.28 | <b>1.81</b> | 0.82        |      |
|                 | None            | 25     | 11 | 0.53 | 4.73 | 0.96 | 0.93 | 2.68 | 0.87 | 3.12 | <b>1.30</b> | 0.60        |      |
|                 | SNV             | 11     | 4  | 0.70 | 3.54 | 0.92 | 0.94 | 2.66 | 0.86 | 1.94 | <b>1.34</b> | 0.61        |      |
|                 | <b>Log(1/R)</b> | SD     | 6  | 4    | 0.77 | 3.22 | 0.90 | 0.92 | 2.72 | 0.87 | 1.54        | <b>1.43</b> | 0.68 |
|                 |                 | SD+LD  | 5  | 4    | 0.85 | 2.93 | 0.88 | 0.98 | 2.54 | 0.85 | 1.33        | <b>1.66</b> | 0.80 |
|                 |                 | SNV+SD | 8  | 5    | 0.75 | 3.32 | 0.91 | 0.92 | 2.72 | 0.87 | 1.30        | <b>1.71</b> | 0.77 |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for the LL data fusion of 4 °C data is highlighted in bold.



Appendix 8. Performance of the best TVC PLS-R models developed using the LL data fusion of VIS-SWNIR (445 - 970 nm ) and NIR (957 - 1664 nm) HSI data from beef LD samples stored at 10 °C. PLS full spectral range on reflectance (R) and logarithmic transformed ( $\log(1/R)$ ) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Chemometric method | Spectral Pre-treatment | # Bands     | # LV      | Calibration        |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |
|--------------------|------------------------|-------------|-----------|--------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|
|                    |                        |             |           | RMSE <sub>cv</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |
| PLS                | R                      | None        | 208       | 8                  | 0.43             | 5.04                        | 0.96               | 0.76              | 2.87                         | 0.88              | 1.39             | 1.61                        | 0.73        |
|                    |                        | SNV         | 208       | 7                  | 0.42             | 5.20                        | 0.96               | 0.67              | 3.25                         | 0.91              | 1.41             | 1.87                        | 0.79        |
|                    |                        | SD          | 202       | 7                  | 0.58             | 3.72                        | 0.93               | 0.95              | 2.28                         | 0.81              | 1.11             | 1.86                        | 0.79        |
|                    |                        | SD+LD       | 202       | 7                  | 0.58             | 3.73                        | 0.93               | 0.95              | 2.29                         | 0.81              | 1.10             | 1.87                        | 0.79        |
|                    |                        | SNV+SD      | 202       | 4                  | 0.70             | 3.08                        | 0.89               | 0.93              | 2.32                         | 0.82              | 0.88             | 2.46                        | 0.89        |
|                    | Log(1/R)               | None        | 208       | 8                  | 0.44             | 4.90                        | 0.96               | 0.77              | 2.82                         | 0.88              | 1.64             | 1.59                        | 0.76        |
|                    |                        | SNV         | 208       | 6                  | 0.55             | 3.95                        | 0.94               | 0.83              | 2.61                         | 0.85              | 1.33             | 1.97                        | 0.81        |
|                    |                        | SD          | 202       | 6                  | 0.54             | 4.02                        | 0.94               | 0.84              | 2.59                         | 0.85              | 1.41             | 1.75                        | 0.79        |
|                    |                        | SD+LD       | 202       | 6                  | 0.54             | 4.05                        | 0.94               | 0.83              | 2.61                         | 0.85              | 1.39             | 1.78                        | 0.80        |
|                    |                        | SNV+SD      | 202       | 6                  | 0.48             | 4.49                        | 0.95               | 0.76              | 2.85                         | 0.88              | 1.23             | 1.97                        | 0.83        |
| EMCVS              | R                      | None        | 20        | 6                  | 0.43             | 5.09                        | 0.96               | 0.59              | 3.68                         | 0.93              | 1.26             | 1.89                        | 0.81        |
|                    |                        | SNV         | 128       | 6                  | 0.42             | 5.11                        | 0.96               | 0.61              | 3.54                         | 0.92              | 1.30             | 1.92                        | 0.82        |
|                    |                        | SD          | 9         | 6                  | 0.52             | 4.16                        | 0.94               | 0.65              | 3.36                         | 0.91              | 0.86             | 2.09                        | 0.84        |
|                    |                        | SD+LD       | 10        | 7                  | 0.49             | 4.45                        | 0.95               | 0.64              | 3.40                         | 0.91              | 0.97             | 1.98                        | 0.84        |
|                    |                        | SNV+SD      | 12        | 5                  | 0.49             | 4.39                        | 0.95               | 0.68              | 3.17                         | 0.90              | 1.20             | 1.76                        | 0.77        |
|                    | Log(1/R)               | <b>None</b> | <b>11</b> | <b>6</b>           | <b>0.46</b>      | <b>4.66</b>                 | <b>0.95</b>        | <b>0.58</b>       | <b>3.71</b>                  | <b>0.93</b>       | <b>0.94</b>      | <b>3.03</b>                 | <b>0.94</b> |
|                    |                        | SNV         | 7         | 5                  | 0.59             | 3.69                        | 0.93               | 0.75              | 2.90                         | 0.88              | 1.13             | 2.22                        | 0.86        |
|                    |                        | SD          | 7         | 3                  | 0.62             | 3.49                        | 0.92               | 0.71              | 3.04                         | 0.89              | 0.98             | 2.05                        | 0.84        |
|                    |                        | SD+LD       | 20        | 3                  | 0.63             | 3.41                        | 0.91               | 0.73              | 2.96                         | 0.89              | 1.11             | 1.87                        | 0.82        |
|                    |                        | SNV+SD      | 9         | 4                  | 0.55             | 3.94                        | 0.94               | 0.66              | 3.30                         | 0.91              | 1.03             | 2.12                        | 0.85        |
| SR                 | R                      | None        | 8         | 5                  | 1.07             | 2.02                        | 0.75               | 1.30              | 1.66                         | 0.65              | 0.82             | 2.67                        | 0.93        |
|                    |                        | SNV         | 20        | 8                  | 0.65             | 3.32                        | 0.91               | 0.98              | 2.21                         | 0.80              | 0.89             | 2.56                        | 0.91        |

|                 |                 |        |    |      |      |      |      |      |      |      |             |             |      |
|-----------------|-----------------|--------|----|------|------|------|------|------|------|------|-------------|-------------|------|
|                 | SD              | 13     | 6  | 0.67 | 3.25 | 0.91 | 0.92 | 2.35 | 0.82 | 1.00 | <b>2.07</b> | 0.87        |      |
|                 | SD+LD           | 23     | 7  | 0.74 | 2.93 | 0.88 | 1.08 | 2.01 | 0.75 | 0.74 | <b>2.51</b> | 0.90        |      |
|                 | SNV+SD          | 11     | 6  | 0.73 | 2.96 | 0.89 | 0.97 | 2.24 | 0.80 | 1.20 | <b>1.81</b> | 0.84        |      |
|                 | None            | 8      | 5  | 0.90 | 2.39 | 0.83 | 1.12 | 1.93 | 0.73 | 1.07 | <b>2.12</b> | 0.86        |      |
|                 | SNV             | 25     | 8  | 0.70 | 3.08 | 0.89 | 1.14 | 1.91 | 0.73 | 1.50 | <b>1.40</b> | 0.84        |      |
| <b>Log(1/R)</b> | SD              | 25     | 5  | 0.54 | 4.04 | 0.94 | 0.80 | 2.70 | 0.86 | 1.13 | <b>2.02</b> | 0.83        |      |
|                 | SD+LD           | 10     | 8  | 0.53 | 4.11 | 0.94 | 0.80 | 2.71 | 0.86 | 1.20 | <b>1.86</b> | 0.80        |      |
|                 | SNV+SD          | 24     | 5  | 0.55 | 3.95 | 0.94 | 0.77 | 2.82 | 0.87 | 1.02 | <b>2.20</b> | 0.86        |      |
| <b>VIP</b>      | None            | 21     | 10 | 0.40 | 5.48 | 0.97 | 0.59 | 3.68 | 0.93 | 1.21 | <b>1.77</b> | 0.78        |      |
|                 | SNV             | 27     | 5  | 0.48 | 4.48 | 0.95 | 0.68 | 3.20 | 0.90 | 1.04 | <b>2.15</b> | 0.86        |      |
|                 | <b>R</b>        | SD     | 20 | 8    | 0.60 | 3.62 | 0.92 | 0.88 | 2.47 | 0.84 | 1.21        | <b>1.72</b> | 0.77 |
|                 |                 | SD+LD  | 16 | 8    | 0.61 | 3.56 | 0.92 | 0.89 | 2.43 | 0.83 | 1.24        | <b>1.66</b> | 0.75 |
|                 |                 | SNV+SD | 14 | 5    | 0.73 | 2.97 | 0.89 | 0.94 | 2.31 | 0.81 | 0.84        | <b>2.50</b> | 0.89 |
|                 | None            | 14     | 7  | 0.48 | 4.52 | 0.95 | 0.68 | 3.17 | 0.90 | 1.11 | <b>2.35</b> | 0.87        |      |
|                 | SNV             | 7      | 5  | 0.61 | 3.57 | 0.92 | 0.75 | 2.88 | 0.88 | 1.10 | <b>2.42</b> | 0.88        |      |
|                 | <b>Log(1/R)</b> | SD     | 10 | 5    | 0.63 | 3.44 | 0.92 | 0.80 | 2.70 | 0.86 | 1.12        | <b>1.94</b> | 0.83 |
|                 |                 | SD+LD  | 14 | 4    | 0.63 | 3.43 | 0.92 | 0.80 | 2.70 | 0.86 | 1.16        | <b>1.85</b> | 0.82 |
|                 |                 | SNV+SD | 10 | 5    | 0.58 | 3.72 | 0.93 | 0.74 | 2.92 | 0.88 | 1.01        | <b>2.12</b> | 0.85 |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for the LLDF of 10 °C data is highlighted in bold.

Appendix 9. Performance of the best TVC PLS-R models developed using the LL data fusion of VIS-SWNIR (445 - 970 nm ) and NIR (957 - 1664 nm) HSI data from beef *LD* samples stored at either 4 °C or 10 °C. PLS full spectral range on reflectance (R) and logarithmic transformed (log(1/R)) spectral data is compared with spectral pre-treatments (SNV, SD, SD+LD, SNV+SD) and band selection methods (VIP, SR and EMCVS).

| Regression Model | Pre-treatment | # Bands  | # LV   | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |      |      |
|------------------|---------------|----------|--------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|------|------|
|                  |               |          |        | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |      |      |
| PLS              | R             | None     | 208    | 8                 | 0.86             | 2.72                        | 0.86               | 1.06              | 2.21                         | 0.8               | 1.38             | 1.43                        | 0.72 |      |
|                  |               | SNV      | 208    | 7                 | 0.79             | 2.95                        | 0.89               | 1.01              | 2.32                         | 0.82              | 1.42             | 1.38                        | 0.70 |      |
|                  |               | SD       | 202    | 6                 | 0.96             | 2.45                        | 0.83               | 1.20              | 1.95                         | 0.74              | 0.95             | 2.08                        | 0.85 |      |
|                  |               | SD+LD    | 202    | 7                 | 0.89             | 2.64                        | 0.86               | 1.16              | 2.02                         | 0.75              | 1.00             | 2.04                        | 0.85 |      |
|                  |               | SNV+SD   | 202    | 7                 | 0.83             | 2.82                        | 0.87               | 1.07              | 2.19                         | 0.79              | 1.12             | 1.86                        | 0.81 |      |
|                  |               | None     | 208    | 8                 | 0.83             | 2.81                        | 0.87               | 1.12              | 2.09                         | 0.78              | 1.44             | 1.36                        | 0.66 |      |
|                  |               | SNV      | 208    | 5                 | 0.94             | 2.50                        | 0.84               | 1.09              | 2.14                         | 0.78              | 1.33             | 1.49                        | 0.71 |      |
|                  |               | Log(1/R) | SD     | 202               | 6                | 0.88                        | 2.66               | 0.86              | 1.10                         | 2.13              | 0.78             | 1.17                        | 1.71 | 0.77 |
|                  |               |          | SD+LD  | 202               | 6                | 0.89                        | 2.63               | 0.86              | 1.11                         | 2.11              | 0.78             | 1.15                        | 1.76 | 0.78 |
|                  |               |          | SNV+SD | 202               | 5                | 0.93                        | 2.52               | 0.84              | 1.14                         | 2.06              | 0.76             | 1.18                        | 1.75 | 0.78 |
| VIP              | R             | None     | 30     | 8                 | 0.96             | 2.44                        | 0.83               | 1.09              | 2.15                         | 0.78              | 1.48             | 1.43                        | 0.69 |      |
|                  |               | SNV      | 13     | 7                 | 0.96             | 2.45                        | 0.83               | 1.09              | 2.15                         | 0.78              | 1.40             | 1.44                        | 0.73 |      |
|                  |               | SD       | 15     | 7                 | 1.03             | 2.27                        | 0.81               | 1.22              | 1.91                         | 0.73              | 1.07             | 1.86                        | 0.80 |      |
|                  |               | SD+LD    | 11     | 6                 | 1.02             | 2.30                        | 0.81               | 1.18              | 1.98                         | 0.75              | 1.15             | 1.73                        | 0.79 |      |
|                  |               | SNV+SD   | 29     | 10                | 0.82             | 2.84                        | 0.88               | 1.10              | 2.13                         | 0.78              | 1.09             | 1.83                        | 0.81 |      |
|                  |               | None     | 10     | 4                 | 1.06             | 2.21                        | 0.8                | 1.14              | 2.06                         | 0.76              | 1.49             | 1.35                        | 0.66 |      |
|                  |               | SNV      | 22     | 6                 | 0.92             | 2.55                        | 0.85               | 1.04              | 2.24                         | 0.8               | 1.31             | 1.53                        | 0.73 |      |
|                  |               | Log(1/R) | SD     | 6                 | 4                | 1.10                        | 2.12               | 0.78              | 1.19                         | 1.97              | 0.74             | 1.18                        | 1.74 | 0.77 |
|                  |               |          | SD+LD  | 6                 | 3                | 1.08                        | 2.17               | 0.79              | 1.12                         | 2.10              | 0.77             | 1.21                        | 1.67 | 0.75 |
|                  |               |          | SNV+SD | 10                | 4                | 1.04                        | 2.25               | 0.8               | 1.17                         | 2.00              | 0.75             | 1.27                        | 1.66 | 0.75 |
| SR               | R             | None     | 7      | 5                 | 1.41             | 1.66                        | 0.64               | 1.59              | 1.47                         | 0.54              | 1.44             | 1.60                        | 0.74 |      |

|          |             |           |          |             |             |             |             |             |             |             |             |             |
|----------|-------------|-----------|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|          | SNV         | 20        | 9        | 0.97        | 2.42        | 0.83        | 1.33        | 1.75        | 0.68        | 1.24        | 1.75        | 0.78        |
|          | SD          | 12        | 8        | 1.05        | 2.23        | 0.80        | 1.23        | 1.91        | 0.73        | 1.06        | 1.87        | 0.82        |
|          | SD+LD       | 24        | 6        | 1.07        | 2.19        | 0.79        | 1.23        | 1.90        | 0.72        | 1.24        | 1.61        | 0.75        |
|          | SNV+SD      | 11        | 6        | 1.13        | 2.06        | 0.76        | 1.32        | 1.78        | 0.69        | 1.33        | 1.50        | 0.71        |
|          | None        | 14        | 7        | 1.02        | 2.3         | 0.81        | 1.23        | 1.90        | 0.73        | 1.27        | 1.63        | 0.74        |
| Log(1/R) | SNV         | 18        | 8        | 1.09        | 2.15        | 0.78        | 1.31        | 1.79        | 0.69        | 1.19        | 1.96        | 0.82        |
|          | SD          | 13        | 7        | 0.97        | 2.4         | 0.83        | 1.15        | 2.03        | 0.76        | 1.23        | 1.70        | 0.76        |
|          | SD+LD       | 19        | 5        | 0.98        | 2.38        | 0.82        | 1.1         | 2.12        | 0.78        | 1.25        | 1.61        | 0.74        |
|          | SNV+SD      | 15        | 7        | 0.95        | 2.46        | 0.84        | 1.15        | 2.04        | 0.76        | 1.36        | 1.59        | 0.72        |
| EMCVS    | None        | 15        | 5        | 0.93        | 2.51        | 0.84        | 1.07        | 2.18        | 0.79        | 1.32        | 1.63        | 0.77        |
|          | SNV         | 52        | 6        | 0.86        | 2.73        | 0.87        | 0.98        | 2.4         | 0.83        | 1.37        | 1.48        | 0.73        |
|          | R SD        | 6         | 3        | 1.06        | 2.21        | 0.80        | 1.13        | 2.06        | 0.76        | 1.15        | 1.73        | 0.79        |
|          | SD+LD       | <b>35</b> | <b>4</b> | <b>0.96</b> | <b>2.45</b> | <b>0.83</b> | <b>1.12</b> | <b>2.08</b> | <b>0.77</b> | <b>0.87</b> | <b>2.27</b> | <b>0.88</b> |
|          | SNV+SD      | 15        | 4        | 0.90        | 2.61        | 0.85        | 0.99        | 2.36        | 0.82        | 1.03        | 2.10        | 0.85        |
|          | None        | 7         | 5        | 0.97        | 2.40        | 0.83        | 1.06        | 2.21        | 0.8         | 1.58        | 1.37        | 0.65        |
|          | SNV         | 17        | 8        | 0.87        | 2.68        | 0.86        | 1.03        | 2.26        | 0.81        | 1.32        | 1.70        | 0.76        |
|          | Log(1/R) SD | 6         | 3        | 0.99        | 2.36        | 0.82        | 1.07        | 2.18        | 0.79        | 1.04        | 1.91        | 0.81        |
|          | SD+LD       | 5         | 5        | 0.93        | 2.51        | 0.84        | 1.01        | 2.31        | 0.81        | 0.98        | 2.09        | 0.84        |
| SNV+SD   | 3           | 2         | 1.04     | 2.18        | 0.79        | 1.08        | 2.10        | 0.77        | 1.24        | 1.60        | 0.73        |             |

SR, selectivity ratio; VIP, variable importance projection; EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; LD, linear detrend; #Bands, wavelengths used for model development; #LVs, latent variables. The overall best model for the LLDF of 4 and 10 °C combine data is highlighted in bold.

- 1 Table 1. TVC of beef *LD* samples (log CFU/g) stored at 4 and 10 °C. Average value  $\pm$  standard deviation (n = 3). Superscripts show the  
 2 statistical significance between samples obtained with Tukey-Kramer test at  $\alpha = 0.05$ .

| Temperature | Time (hours) | Sample id. /TVC                    |                                      |                                 |                                 |                                 |                                |
|-------------|--------------|------------------------------------|--------------------------------------|---------------------------------|---------------------------------|---------------------------------|--------------------------------|
|             |              | S1                                 | S2                                   | S3                              | S7                              | S8                              | S9                             |
| 4 °C        | 0            | 7.1 $\pm$ 0.4 <sup>a,c</sup>       | 6.9 $\pm$ 0.2 <sup>a,c</sup>         | 7.0 $\pm$ 0.5 <sup>a,b</sup>    | 5.3 $\pm$ 0.1 <sup>a</sup>      | 5.3 $\pm$ 0.4 <sup>a</sup>      | 3.4 $\pm$ 0.5 <sup>a</sup>     |
|             | 24           | 7.1 $\pm$ 0.3 <sup>a,c</sup>       | 6.9 $\pm$ 0.4 <sup>a,c</sup>         | 7.2 $\pm$ 0.6 <sup>a,b</sup>    | 5.3 $\pm$ 0.2 <sup>a</sup>      | 5.1 $\pm$ 0.4 <sup>a</sup>      | 3.3 $\pm$ 0.0 <sup>a</sup>     |
|             | 96           | 8.9 $\pm$ 0.1 <sup>b,c,d,e</sup>   | 8.6 $\pm$ 0.2 <sup>b,c,d,f,g</sup>   | 8.3 $\pm$ 0.3 <sup>a,b,c</sup>  | 6.6 $\pm$ 0.4 <sup>b</sup>      | 7.1 $\pm$ 0.7 <sup>b</sup>      | 4.1 $\pm$ 0.3 <sup>a</sup>     |
|             | 120          | 8.1 $\pm$ 0.0 <sup>a,b,c,e</sup>   | 7.7 $\pm$ 0.1 <sup>a,b,c,d,g</sup>   | 8.1 $\pm$ 0.6 <sup>a,b,c</sup>  | 8.7 $\pm$ 0.6 <sup>c</sup>      | 8.3 $\pm$ 0.2 <sup>c</sup>      | 5.6 $\pm$ 0.0 <sup>b</sup>     |
|             | 192          | 8.8 $\pm$ 0.4 <sup>b,c,d,e</sup>   | 9.1 $\pm$ 0.2 <sup>b,c,d,e,f,g</sup> | 8.4 $\pm$ 0.3 <sup>a,b,c</sup>  | 9.4 $\pm$ 0.1 <sup>c</sup>      | 9.4 $\pm$ 0.2 <sup>c</sup>      | 7.7 $\pm$ 0.5 <sup>c,d</sup>   |
|             | 264          | 10.1 $\pm$ 0.7 <sup>b,d,e,f</sup>  | 10.5 $\pm$ 0.7 <sup>d,e,f</sup>      | 9.0 $\pm$ 0.1 <sup>b,c,d</sup>  | 10.9 $\pm$ 0.8 <sup>d</sup>     | 12.2 $\pm$ 0.1 <sup>d,e</sup>   | 8.9 $\pm$ 0.1 <sup>c,d,e</sup> |
|             | 288          | 9.5 $\pm$ 0.3 <sup>b,c,d,e,f</sup> | 9.7 $\pm$ 0.6 <sup>b,d,e,f,g,h</sup> | 10.2 $\pm$ 0.3 <sup>c,d,e</sup> | 12.2 $\pm$ 0.3 <sup>e,f</sup>   | 12.1 $\pm$ 0.3 <sup>d,e,f</sup> | 9.2 $\pm$ 0.2 <sup>c,d,e</sup> |
|             | 312          | 9.7 $\pm$ 1.2 <sup>b,c,d,e,f</sup> | 9.0 $\pm$ 1.0 <sup>b,c,d,f,g,h</sup> | 10.6 $\pm$ 0.7 <sup>d,e</sup>   | -                               | -                               | -                              |
|             | 336          | -                                  | -                                    | -                               | 13.2 $\pm$ 0.2 <sup>e,f,g</sup> | 13.5 $\pm$ 0.7 <sup>e,f</sup>   | 10.5 $\pm$ 1.3 <sup>d,c</sup>  |
|             | 360          | 10.6 $\pm$ 0.5 <sup>d,e,f</sup>    | 11.1 $\pm$ 0.3 <sup>f,h</sup>        | 11.4 $\pm$ 1.0 <sup>d,e</sup>   | 14.1 $\pm$ 0.3 <sup>f,g</sup>   | 14.1 $\pm$ 0.1 <sup>f,g</sup>   | -                              |
| Temperature | Time (hours) | Sample id. /TVC                    |                                      |                                 |                                 |                                 |                                |
|             |              | S4                                 | S5                                   | S6                              | S7                              | S8                              | S9                             |
| 10 °C       | 0            | 6.1 $\pm$ 0.1 <sup>a</sup>         | 6.7 $\pm$ 0.1 <sup>a</sup>           | 6.7 $\pm$ 0.3 <sup>a,b</sup>    | 5.3 $\pm$ 0.1 <sup>a</sup>      | 5.3 $\pm$ 0.4 <sup>a</sup>      | 3.4 $\pm$ 0.5 <sup>a</sup>     |
|             | 12           | 6.7 $\pm$ 0.3 <sup>b,c</sup>       | 7.7 $\pm$ 0.2 <sup>b</sup>           | 6.9 $\pm$ 0.1 <sup>a,b</sup>    | -                               | -                               | -                              |
|             | 24           | 6.8 $\pm$ 0.2 <sup>b,c</sup>       | 7.3 $\pm$ 0.1 <sup>b</sup>           | 7.1 $\pm$ 0.1 <sup>a,b,c</sup>  | 6.0 $\pm$ 0.3 <sup>a</sup>      | 6.1 $\pm$ 0.8 <sup>a</sup>      | 3.4 $\pm$ 0.5 <sup>a</sup>     |
|             | 36           | 6.9 $\pm$ 4.0 <sup>b,c,d</sup>     | 7.7 $\pm$ 0.1 <sup>b</sup>           | 7.1 $\pm$ 0.2 <sup>a,b,c</sup>  | -                               | -                               | -                              |
|             | 48           | 7.4 $\pm$ 0.1 <sup>c,d</sup>       | 7.6 $\pm$ 0.1 <sup>b</sup>           | 7.5 $\pm$ 0.1 <sup>b,c</sup>    | -                               | -                               | -                              |
|             | 84           | 9.2 $\pm$ 0.1 <sup>e,f,h</sup>     | 9.4 $\pm$ 0.1 <sup>c,d,e,g</sup>     | 9.3 $\pm$ 0.2 <sup>d,e</sup>    | -                               | -                               | -                              |
|             | 96           | 9.4 $\pm$ 0.2 <sup>e,f,h,i</sup>   | 9.1 $\pm$ 0.2 <sup>c,d</sup>         | 9.3 $\pm$ 0.1 <sup>d,e</sup>    | 8.8 $\pm$ 0.2 <sup>b,c</sup>    | 9.0 $\pm$ 0.1 <sup>b</sup>      | 7.6 $\pm$ 0.1 <sup>b</sup>     |
|             | 108          | 9.9 $\pm$ 0.1 <sup>g,h,i</sup>     | 9.8 $\pm$ 0.2 <sup>c,e,f,g</sup>     | 9.6 $\pm$ 0.1 <sup>d,e,f</sup>  | -                               | -                               | -                              |
|             | 120          | 9.6 $\pm$ 0.2 <sup>e,f,g,h,i</sup> | 9.8 $\pm$ 0.1 <sup>c,e,f,g</sup>     | 9.8 $\pm$ 0.1 <sup>e,f</sup>    | 10.5 $\pm$ 0.4 <sup>b,c,d</sup> | 10.2 $\pm$ 0.1 <sup>c</sup>     | 9.3 $\pm$ 0.5 <sup>c</sup>     |
|             | 132          | 10.1 $\pm$ 0.2 <sup>g,h,i</sup>    | 10.0 $\pm$ 0.1 <sup>e,f,g</sup>      | 9.9 $\pm$ 0.1 <sup>e,f</sup>    | -                               | -                               | -                              |
|             | 144          | 9.8 $\pm$ 0.1 <sup>f,g,h,i</sup>   | 9.9 $\pm$ 0.1 <sup>c,e,f,g</sup>     | 10.0 $\pm$ 0.2 <sup>e,f</sup>   | 11.6 $\pm$ 1.4 <sup>c,d</sup>   | 12.2 $\pm$ 0.2 <sup>d</sup>     | 11.1 $\pm$ 0.2 <sup>d</sup>    |
|             | 168          | -                                  | -                                    | -                               | 12.3 $\pm$ 0.0 <sup>c,d</sup>   | 13.1 $\pm$ 0.1 <sup>d</sup>     | 12.3 $\pm$ 0.3 <sup>e</sup>    |

- 3 Values followed by different letters in the same column are significantly different using ANOVA and Tukey test (p < 0.05).

4 Table 2. Performance of the best TVC PLS-R models developed for beef *LD* samples stored at 4 °C using the full spectral range and optimum  
 5 band selection method evaluated for VIS-SWNIR (445 - 970 nm ) and NIR (957 - 1664 nm) HSI data.

| Regression model     | Pre-treatment   |                 | # Bands     | # LV      | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |
|----------------------|-----------------|-----------------|-------------|-----------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|
|                      | 1 <sup>st</sup> | 2 <sup>nd</sup> |             |           | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |
| <b>445 - 970 nm</b>  |                 |                 |             |           |                   |                  |                             |                    |                   |                              |                   |                  |                             |             |
| PLS                  | R               | SNV             | SD          | 100       | 6                 | 0.79             | 3.15                        | 0.9                | 1.34              | 1.86                         | 0.74              | 1.35             | 1.61                        | 0.81        |
| EMCVS                | log(1/R)        | SNV             | SD          | 6         | 5                 | 0.88             | 2.83                        | 0.88               | 1.03              | 2.42                         | 0.83              | 1.17             | 1.88                        | 0.83        |
| <b>957 - 1664 nm</b> |                 |                 |             |           |                   |                  |                             |                    |                   |                              |                   |                  |                             |             |
| PLS                  | log(1/R)        | SD              | AsLs        | 96        | 9                 | 0.42             | 5.63                        | 0.97               | 1.03              | 2.29                         | 0.81              | 0.99             | 2.26                        | 0.94        |
| <b>EMCVS</b>         | <b>log(1/R)</b> | <b>SD</b>       | <b>AsLs</b> | <b>17</b> | <b>7</b>          | <b>0.5</b>       | <b>4.71</b>                 | <b>0.95</b>        | <b>0.7</b>        | <b>3.37</b>                  | <b>0.91</b>       | <b>0.81</b>      | <b>3.09</b>                 | <b>0.95</b> |

6 EMCVS, ensemble Monte Carlo variable selection; SD, second derivative; SNV, standard normal variate; AsLs, asymmetric least squares;  
 7 #Bands, wavelengths used for model development; #LVs, latent variables. The best overall model for 4 °C is highlighted in bold.

8

9 Table 3. Performance of the best TVC PLS-R models developed for beef *LD* samples stored at 10 °C using the full spectral range and optimum  
 10 band selection method evaluated for VIS-SWNIR (445 - 970 nm ) and NIR (957 - 1664 nm) HSI data.

| Regression model     | Pre-treatment   |                 | # Bands | # LV      | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |
|----------------------|-----------------|-----------------|---------|-----------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|
|                      | 1 <sup>st</sup> | 2 <sup>nd</sup> |         |           | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |
| <b>445 - 970 nm</b>  |                 |                 |         |           |                   |                  |                             |                    |                   |                              |                   |                  |                             |             |
| PLS                  | R               | SD              | MS      | 100       | 6                 | 0.48             | 4.52                        | 0.95               | 0.7               | 3.08                         | 0.89              | 1.09             | 2.84                        | 0.92        |
| EMCVS                | R               | SD              | MS      | <b>46</b> | <b>6</b>          | <b>0.47</b>      | <b>4.60</b>                 | <b>0.95</b>        | <b>0.69</b>       | <b>3.16</b>                  | <b>0.90</b>       | <b>0.96</b>      | <b>3.32</b>                 | <b>0.94</b> |
| <b>957 - 1664 nm</b> |                 |                 |         |           |                   |                  |                             |                    |                   |                              |                   |                  |                             |             |
| PLS                  | log(1/R)        | SD              | SNV     | 96        | 7                 | 0.62             | 3.49                        | 0.92               | 1.03              | 2.11                         | 0.78              | 1.2              | 1.59                        | 0.72        |
| EMCVS                | log(1/R)        | SNV             |         | 19        | 9                 | 0.44             | 4.93                        | 0.96               | 0.67              | 3.22                         | 0.90              | 1.15             | 2.23                        | 0.87        |

11 EMCVS, ensemble Monte Carlo variable selection; MS, median scaled; SD, second derivative; SNV, standard normal variate; #Bands,  
 12 wavelengths used for model development; #LVs, latent variables. The best overall model for 10 °C is highlighted in bold.

13

14 Table 4. Performance of the best TVC PLS-R models developed for beef *LD* samples stored at either 4 °C or 10 °C using the full spectral range  
 15 and optimum band selection method evaluated for VIS-SWNIR (445 - 970 nm ) and NIR (957 - 1664 nm) HSI data.

| Regression model     | Pre-treatment   |                 | # Bands   | # LV     | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |             |
|----------------------|-----------------|-----------------|-----------|----------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|-------------|
|                      | 1 <sup>st</sup> | 2 <sup>nd</sup> |           |          | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |             |
| <b>445 - 970 nm</b>  |                 |                 |           |          |                   |                  |                             |                    |                   |                              |                   |                  |                             |             |
| PLS                  | R               | SNV             | SD        | 100      | 7                 | 0.86             | 2.72                        | 0.87               | 1.09              | 2.15                         | 0.78              | 0.98             | <b>1.99</b>                 | 0.84        |
| <b>EMCVS</b>         | <b>R</b>        | <b>SNV</b>      | <b>SD</b> | <b>8</b> | <b>4</b>          | <b>0.94</b>      | <b>2.48</b>                 | <b>0.84</b>        | <b>1.05</b>       | <b>2.22</b>                  | <b>0.80</b>       | <b>0.95</b>      | <b>2.10</b>                 | <b>0.85</b> |
| <b>957 - 1664 nm</b> |                 |                 |           |          |                   |                  |                             |                    |                   |                              |                   |                  |                             |             |
| PLS                  | log(1/R)        | SD              | LD        | 202      | 4                 | 1.17             | 2.01                        | 0.75               | 1.47              | 1.59                         | 0.61              | 1.18             | <b>1.66</b>                 | 0.76        |
| EMCVS                | R               | SNV             | SD        | 96       | 6                 | 1.04             | 2.24                        | 0.80               | 1.18              | 1.98                         | 0.74              | 1.15             | <b>1.75</b>                 | 0.77        |

16 EMCVS, ensemble Monte Carlo variable selection; SNV, standard normal variate; LD, linear detrend; SD, second derivative; #Bands,  
 17 wavelengths used for model development; #LVs, latent variables. The overall best model for the combined data of both temperatures is  
 18 highlighted in bold.

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20 Table 5. Performance of the best TVC PLS-R models developed using VIS-SWNIR (445 - 970 nm) and NIR (957 - 1664 nm) HSI data from  
 21 beef *LD* samples stored at (i) 4 °C, (ii) 10 °C and (iii) either 4 °C or 10 °C using the optimum band selection method and LL, ML and HL data  
 22 fusion

| Regression model      |       |          | Pre-treatment   |                 | # Bands | # LV | Calibration       |                  |                             | Cross validation   |                   |                              | Prediction        |                  |                             |
|-----------------------|-------|----------|-----------------|-----------------|---------|------|-------------------|------------------|-----------------------------|--------------------|-------------------|------------------------------|-------------------|------------------|-----------------------------|
|                       |       |          | 1 <sup>st</sup> | 2 <sup>nd</sup> |         |      | RMSE <sub>c</sub> | RPD <sub>c</sub> | R <sup>2</sup> <sub>c</sub> | RMSE <sub>cv</sub> | RPD <sub>cv</sub> | R <sup>2</sup> <sub>cv</sub> | RMSE <sub>p</sub> | RPD <sub>p</sub> | R <sup>2</sup> <sub>p</sub> |
| <b>4 °C</b>           |       |          |                 |                 |         |      |                   |                  |                             |                    |                   |                              |                   |                  |                             |
| VIS-SWNIR             | EMCVS | log(1/R) | SNV             | SD              | 6       | 5    | 0.88              | 2.83             | 0.88                        | 1.03               | 2.42              | 0.83                         | 1.17              | 1.88             | 0.83                        |
| NIR                   | EMCVS | log(1/R) | SD              | AsLs            | 17      | 7    | 0.50              | 4.71             | 0.95                        | 0.70               | 3.37              | 0.91                         | 0.81              | 3.09             | 0.95                        |
| LL                    | VIP   | R        | SD              | LD              | 22      | 8    | 0.76              | 3.28             | 0.91                        | 1.09               | 2.30              | 0.81                         | 1.16              | 1.90             | 0.88                        |
| ML                    |       |          |                 |                 |         | 11   | 0.50              | 4.66             | 0.95                        | 0.92               | 2.55              | 0.85                         | 0.80              | 2.41             | 0.93                        |
| HL                    |       |          |                 |                 |         |      | <b>0.83</b>       | <b>2.82</b>      | <b>0.87</b>                 | <b>0.91</b>        | <b>2.58</b>       | <b>0.85</b>                  | <b>0.58</b>       | <b>4.13</b>      | <b>0.96</b>                 |
| <b>10 °C</b>          |       |          |                 |                 |         |      |                   |                  |                             |                    |                   |                              |                   |                  |                             |
| VIS-SWNIR             | EMCVS | R        | SD              | MS              | 46      | 6    | <b>0.47</b>       | <b>4.60</b>      | <b>0.95</b>                 | <b>0.69</b>        | <b>3.16</b>       | <b>0.90</b>                  | <b>0.96</b>       | <b>3.32</b>      | <b>0.94</b>                 |
| NIR                   | EMCVS | log(1/R) | SNV             |                 | 19      | 9    | 0.44              | 4.93             | 0.96                        | 0.67               | 3.22              | 0.90                         | 1.15              | 2.23             | 0.87                        |
| LL                    | EMCVS | log(1/R) | None            |                 | 11      | 6    | 0.46              | 4.66             | 0.95                        | 0.58               | 3.71              | 0.93                         | 0.94              | 3.03             | 0.94                        |
| ML                    |       |          |                 |                 |         | 6    | 0.47              | 4.64             | 0.95                        | 0.75               | 2.89              | 0.88                         | 1.17              | 2.17             | 0.84                        |
| HL                    |       |          |                 |                 |         |      | <b>0.36</b>       | <b>6.07</b>      | <b>0.97</b>                 | <b>0.51</b>        | <b>4.30</b>       | <b>0.95</b>                  | <b>0.97</b>       | <b>3.28</b>      | <b>0.94</b>                 |
| <b>4 °C and 10 °C</b> |       |          |                 |                 |         |      |                   |                  |                             |                    |                   |                              |                   |                  |                             |
| VIS-SWNIR             | EMCVS | R        | SNV             | SD              | 8       | 4    | 0.94              | 2.48             | 0.84                        | 1.05               | 2.22              | 0.80                         | 0.95              | 2.10             | 0.85                        |
| NIR                   | EMCVS | R        | SNV             | SD              | 96      | 6    | 1.04              | 2.24             | 0.80                        | 1.18               | 1.98              | 0.74                         | 1.15              | 1.75             | 0.77                        |
| LL                    | EMCVS | R        | SD              | LD              | 35      | 4    | <b>0.96</b>       | <b>2.45</b>      | <b>0.83</b>                 | <b>1.12</b>        | <b>2.08</b>       | <b>0.77</b>                  | <b>0.87</b>       | <b>2.27</b>      | <b>0.88</b>                 |
| ML                    |       |          |                 |                 |         | 5    | 0.79              | 2.96             | 0.89                        | 0.93               | 2.51              | 0.84                         | 1.32              | 1.49             | 0.74                        |
| HL                    |       |          |                 |                 |         |      | <b>0.84</b>       | <b>2.79</b>      | <b>0.88</b>                 | <b>0.94</b>        | <b>2.47</b>       | <b>0.84</b>                  | <b>0.89</b>       | <b>2.27</b>      | <b>0.86</b>                 |

23 EMCVS, ensemble Monte Carlo variable selection; VIP, variable importance projection ; SD, second derivative; SNV, standard normal variate;  
 24 AsLs, asymmetric least squares; LD, linear detrend; MS, medium scaled: #Bands, wavelengths used for model development; #LVs, latent  
 25 variables. The best model for each storage temperature is highlighted in bold.

26

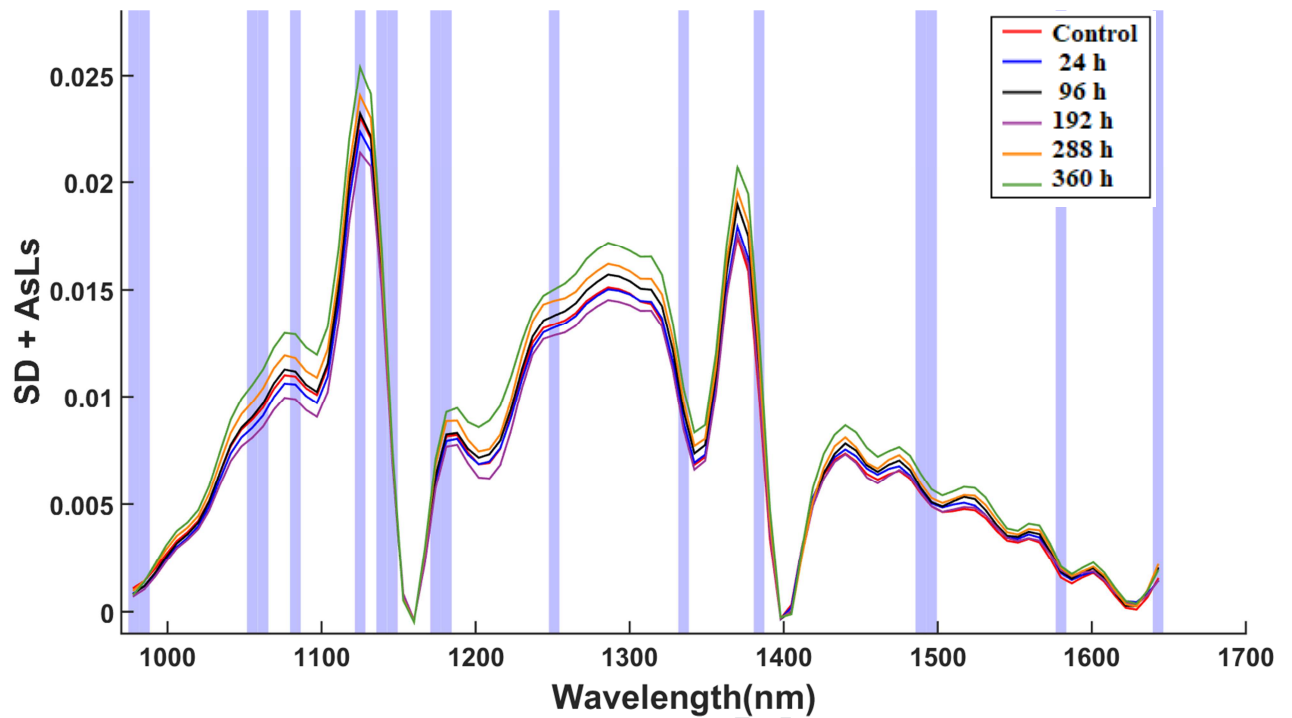


Fig. 1. Log (1/R) NIR pre-treated (SD+AsLs) spectra of beef *LD* samples stored at 4 °C for selected storage times. Bands selected by the EMCVS method to predict TVC of samples are highlighted in blue.

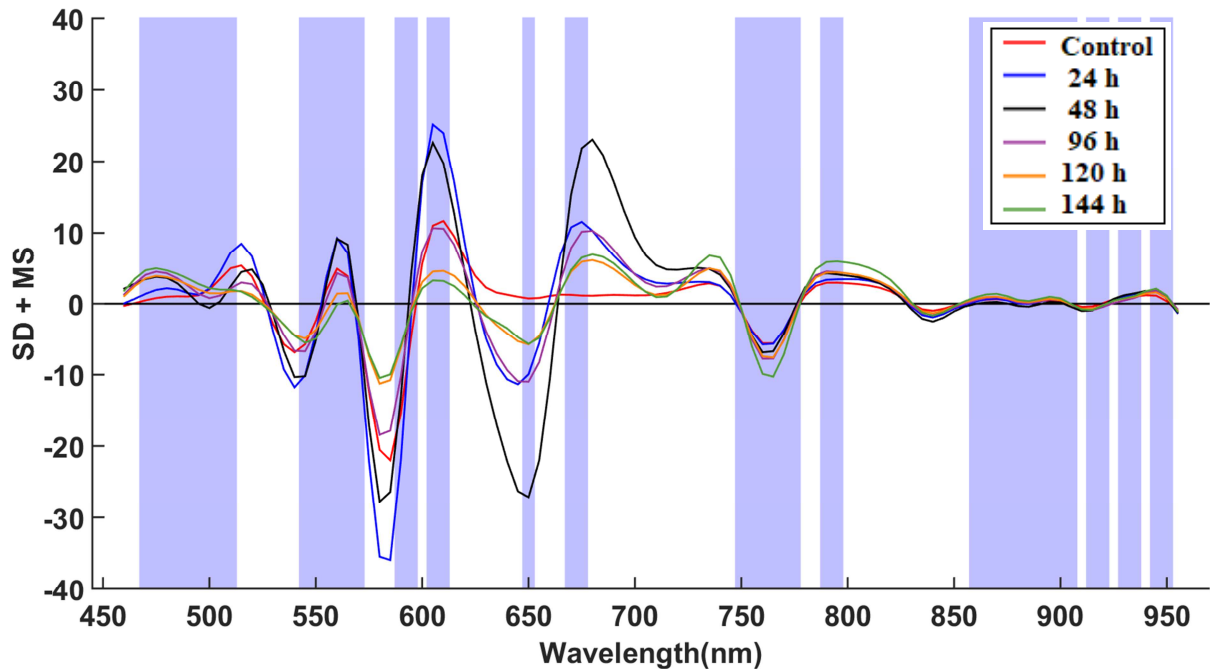


Fig. 2. Reflectance VIS-SWNIR pre-treated (SD+MS) spectra of beef *LD* samples stored at 10 °C for selected storage times. Bands selected by the EMCVS method to predict TVC of samples are highlighted in blue.

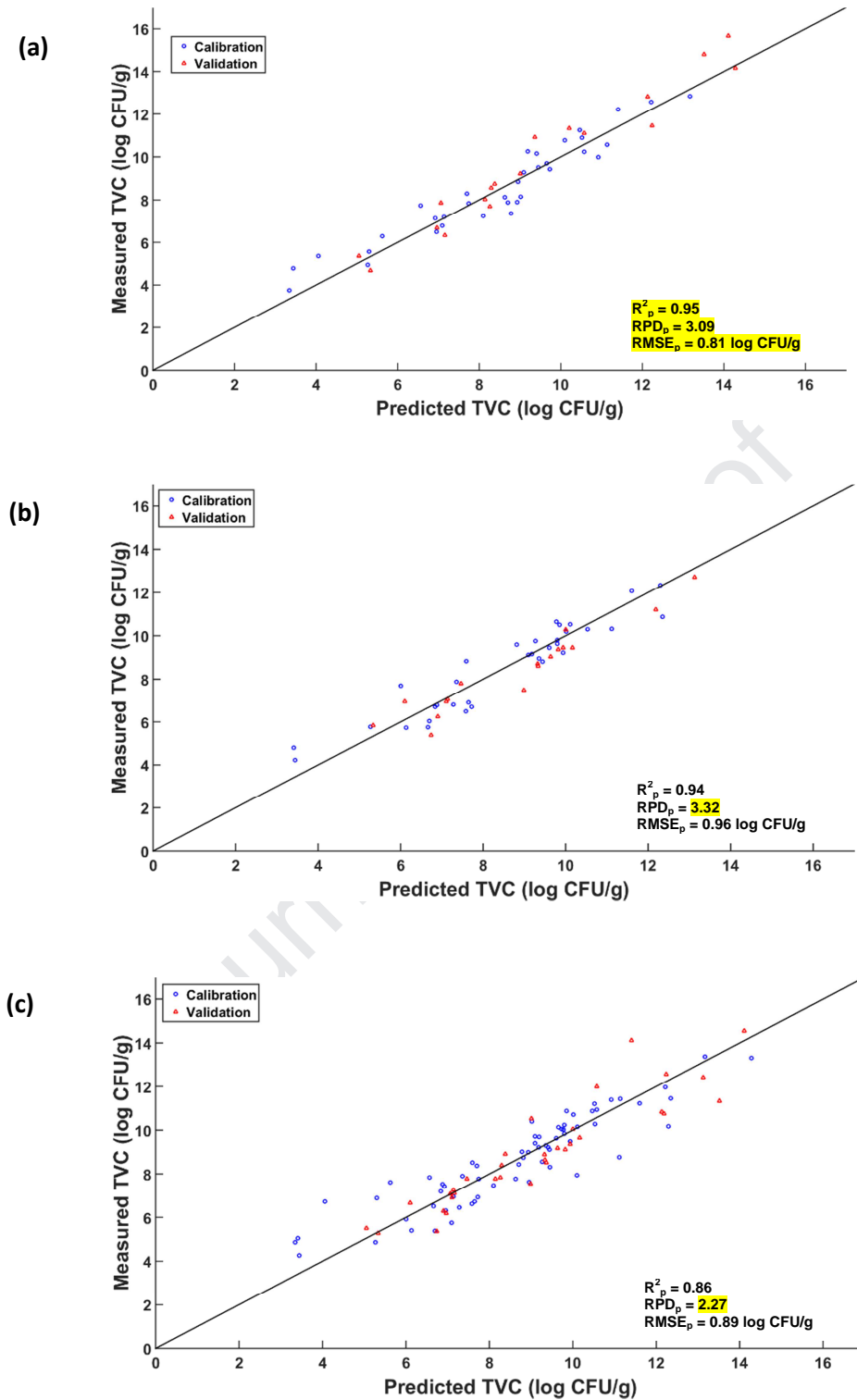


Fig. 3. Measured vs predicted TVC for the best performing PLS-R models developed for beef LD samples stored at (a) 4 °C, (b) 10 °C and (c) either 4 °C or 10 °C.

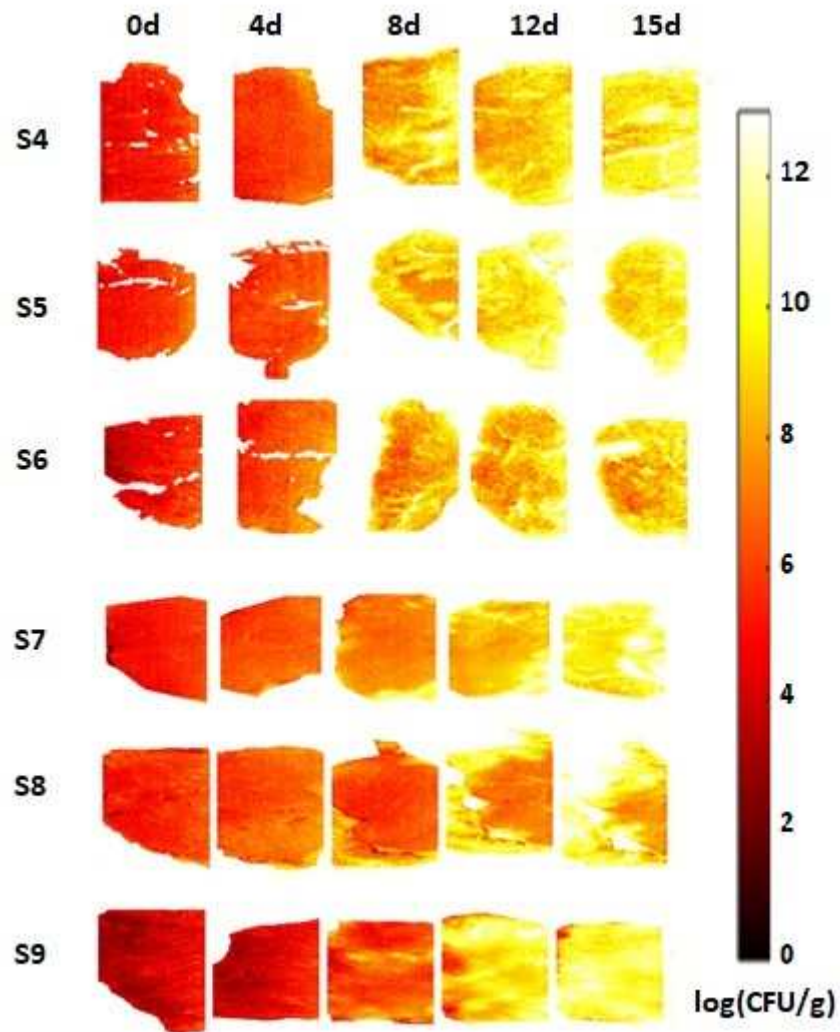


Fig. 4. Prediction maps for TVC of beef *LD* samples (log CFU/g) stored at 10 °C for selected times using the reflectance VIS-SWNIR pre-treated (SD+MS) spectra which selected 46 bands).

- Microbial quality of beef stored under normal or abuse conditions can be predicted
- Spectral pre-treatments, band selection and data fusion methods are key for robust model development
- Hyperspectral imaging and chemometrics have potential for real-time monitoring of microbial quality

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