

1 **Abstract**

2 A series of partial least squares (PLS) models were employed to correlate spectral data from
3 FTIR analysis with beef fillet spoilage during aerobic storage at different temperatures (0, 5,
4 10, 15, and 20°C) using the dataset presented by Argyri et al. (2009). The performance of the
5 PLS models was compared with a three-layer feed-forward artificial neural network (ANN)
6 developed using the same dataset. FTIR spectra were collected from the surface of meat
7 samples in parallel with microbiological analyses to enumerate total viable counts. Sensory
8 evaluation was based on a three point hedonic scale classifying meat samples as fresh, semi-
9 fresh, and spoiled. The purpose of the modelling approach employed in this work was to
10 classify beef samples in the respective quality class as well as to predict their total viable
11 counts directly from FTIR spectra. The results obtained demonstrated that both approaches
12 showed good performance in discriminating meat samples in one of the three predefined
13 sensory classes. The PLS classification models showed performances ranging from 72.0 to
14 98.2% using the training dataset, and from 63.1 to 94.7% using independent testing dataset.
15 The ANN classification model performed equally well in discriminating meat samples, with
16 correct classification rates from 98.2 to 100% and 63.1 to 73.7% in the train and test sessions,
17 respectively. PLS and ANN approaches were also applied to create models for the prediction
18 of microbial counts. The performance of these was based on graphical plots and statistical
19 indices (bias factor, accuracy factor, root mean square error). Furthermore, results
20 demonstrated reasonably good correlation of total viable counts on meat surface with FTIR
21 spectral data with PLS models presenting better performance indices compared to ANN.

22

23 *Keywords: artificial neural networks, aerobic storage, beef fillets, FTIR, machine learning, meat*
24 *spoilage, partial least squares regression, pattern recognition*

25

1 **1. Introduction**

2 One of the most commonly consumed food commodities on a global basis is meat, due to
3 its high nutritional value in the human diet. In the USA alone the retail market of beef
4 industry amounted to \$76 billion in 2008 with an overall consumption of approximately 27.3
5 billion pounds in that year (USDA, 2008). During meat production/processing quality
6 assurance is difficult due to the heterogeneous nature of the raw material, since the chemical
7 composition, technological and sensory attributes are highly influenced by pre-slaughter (e.g.,
8 breed, age, environment) intrinsic (e.g. pH, available nutrients) and extrinsic (e.g., storage
9 method, period and temperature of storage) factors (Damez and Clerjon, 2008; Nychas et al.,
10 2008; Prieto et al., 2009). Consequently, in order to keep the quality standards as close as
11 possible to the preference of the consumer, control procedures must be undertaken including
12 sensory, microbiological and physico-chemical analysis. Today, more than 50 such methods
13 have been employed for the characterization of microbiologically spoiled or contaminated
14 meat (Ellis and Goodacre, 2001; Nychas et al., 2008). However, these methods suffer certain
15 disadvantages as they are time-consuming, destructive, require highly trained personnel,
16 provide retrospective information, and hence they are unsuitable for on-line monitoring
17 (Dainty, 1996; Nychas et al., 1998, 2008; Ellis et al., 2002, 2004; Liu et al., 2004).

18 Nowadays, various rapid, non-invasive methods based on analytical instrumental
19 techniques, such as Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy,
20 near infrared spectroscopy, and electronic nose technology are being researched for their
21 potential as reliable meat quality sensors (Ellis et al., 2005; Rajamäki et al., 2006; Damez and
22 Clerjon, 2008; Ammor et al., 2009; Argyri et al., 2009; Balasubramanian et al., 2009; Prieto et
23 al., 2009). The principle underlying this approach is based on the assumption that the
24 metabolic activity of microorganisms on meat results in biochemical changes with the
25 concurrent formation of metabolic by-products which may indicate or may contribute to

1 spoilage. The quantification of these metabolites constitutes a characteristic fingerprint
2 providing information about the type and rate of spoilage (Ellis and Goodacre, 2001; Nychas
3 et al., 2008).

4 The introduction of converging technologies in the food industry is among the priorities of
5 the 7th Framework Programme and they are anticipated to predominate in the future and result
6 in substantial changes in the manner in which researchers design their research (Hair et al.,
7 1998; NBIC report USA 2002). This can be achieved thorough the integration of modern
8 analytical and high throughput platforms with computational and chemometric techniques.
9 Multivariate statistical analyses (e.g., partial least square regression, discriminant function
10 analysis, cluster analysis) and intelligent methodologies (e.g., artificial neural networks), can
11 result in the development of a decision support system for timely determination of
12 safety/quality of meat products, and also prevent unnecessary economic losses (Mataragas et
13 al., 2007; Nychas et al., 2008; Guillén et al., 2010). Furthermore, the development of
14 computational research platforms and online experimental databases such as Combase
15 (Baranyi and Tamplin, 2004) and Sym'Previus (Leporq et al., 2005), provide research
16 scientists with fast and efficient means of storing and exchanging knowledge despite their
17 geographic distribution.

18 Partial least squares discriminant analysis (PLS-DA) and artificial neural networks
19 (ANNs) are widely employed modelling approaches due to their ability to relate the input and
20 output variables without having any prior knowledge on the system under study, provided that
21 an accurate and adequate amount of data on the system variables is available (Singh et al.,
22 2009). Compared to other areas, the application of ANNs in the field of food science is still in
23 the early development stage. Nevertheless, interest in using ANNs as secondary models in
24 food microbiology is increasing as they have shown promising results in several applications
25 such as growth parameter estimation of microorganisms (Geeraerd et al., 1998; Hervás et al.,

1 2001; García-Gimeno et al., 2005), bacterial heat resistance (Lou and Nakai, 2001; Esnoz et
2 al., 2006), production of metabolites (Poirazi et al., 2007), and simulation of survival curves
3 (Palanichamy et al., 2008; Panagou, 2008). The multi-layer perceptron (MLP) is the most
4 frequently used type of neural network in practical applications (Siripatrawan et al., 2006).
5 The basic structure is comprised of three distinctive layers, the input layer where the data are
6 introduced to the model and computation of the weighted sum of the input is performed, the
7 hidden layer or layers where data processing takes place, and the output layer where the
8 results of the neural network are produced (Bishop, 2004; Huang et al., 2007).

9 The purpose of the present study was to compare the performance of a multilayer
10 perceptron (MLP) neural network and partial least squares (PLS) regression models in order
11 to (i) classify beef fillets stored aerobically at different temperatures (0, 5, 10, 15, and 20°C)
12 in terms of quality classes (i.e., fresh, semi-fresh, spoiled), and (ii) predict the total viable
13 counts on the surface of meat samples directly from FTIR data.

14

15 **2. Materials and methods**

16 *2.1 Experimental design*

17 A detailed description of the methodology employed in this work is presented elsewhere
18 (Argyri et al., 2009). In brief, fresh deboned pieces of beef were purchased from a local
19 butcher shop and transported under refrigeration to the laboratory within 30 min. The samples
20 were prepared by cutting meat pieces into portions (40 mm wide x 50 mm long x 10 mm
21 thick) that were subsequently placed into 90 mm Petri dishes and stored at 0, 5, 10, 15, and
22 20°C in high-precision ($\pm 0.5^\circ\text{C}$) incubation chambers until spoilage was evident.

23 For the FTIR measurements, a thin slice (0.5 cm thickness) of the aerobic upper surface of
24 the fillet was excised and used for further analysis. Spectra were collected using a ZnSe 45°
25 ATR (Attenuated Total Reflectance) crystal on a Nicolet 6700 FT-IR Spectrometer, collecting

1 spectra over the wavenumber range of 4,000 to 400 cm^{-1} , by accumulating 100 scans with a
2 resolution of 4 cm^{-1} . The collection time for each sample spectrum was 2 min. Spectra
3 collected between 1800 and 1000 cm^{-1} were initially subjected to smoothing according to the
4 Savitzky-Golay algorithm prior to further analysis.

5 For microbiological analysis a portion (40 mm wide x 50 mm long x 10 mm thick) was
6 added to 150 ml sterile quarter strength Ringer's solution, and homogenized in a stomacher
7 for 60 s at room temperature. Further decimal dilutions were prepared with the same diluent,
8 and duplicate 0.1 ml samples of three appropriate dilutions were spread in triplicate on plate
9 count agar for counts of total viable bacteria, incubated at 30°C for 48 h.

10 Sensory evaluation of meat samples was performed during storage, based on the
11 perception of colour and smell before and after cooking (20 min at 180°C in preheated oven)
12 (Gill and Jeremiah, 1991). Each sensory attribute was scored on a three-point hedonic scale
13 corresponding to: 1=Fresh; 2=Marginal; and 3=Spoiled. Score of 1.5 was characterized as
14 Semi-fresh and it was considered as the early detection of meat spoilage. Overall, 76 meat
15 samples were evaluated by the sensory panel and classified into the selected groups as fresh
16 ($n = 26$), semi-fresh ($n = 16$), and spoiled ($n = 34$).

17

18 *2.2 Partial least squares (PLS) modelling*

19 The partial least squares regression (PLS-R) derives its usefulness from its ability to
20 analyze data with strongly collinear, noisy and numerous variables in the predictor matrix X
21 (i.e., independent variables) and responses Y (i.e., dependent variables) (Eriksson et al., 2001).
22 The PLS-R method projects the initial input-output data down into a latent space, extracting a
23 number of principal factors (also known as latent variables) with an orthogonal structure,
24 while capturing most of the variance in the original data. In brief, it can be expressed as a
25 bilinear decomposition of both X and Y as:

1
$$X = \mathbf{T}\mathbf{W}^T + E_X \tag{1}$$

2 and

3
$$Y = \mathbf{U}\mathbf{Q}^T + E_Y \tag{2}$$

4 Therefore, the scores in the X -matrix and the scores of the yet unexplained part of Y have
5 maximum covariance. In equations (1) and (2), \mathbf{T} and \mathbf{W} , \mathbf{U} and \mathbf{Q} are the vectors of X and Y
6 PLS scores and loadings, respectively, and E_X , E_Y are the X and Y residuals (Singh et al.,
7 2009). The aim of PLS method is to find a linear (or polynomial) relationship between X and
8 Y matrices, so that:

9
$$Y = bX + E \tag{3}$$

10 where b is the regression coefficient. The PLS models are developed in two stages; the initial
11 dataset is divided into training and testing subsets. The former dataset is used to build the
12 models and compute a set of regression coefficients (\mathbf{b}_{PLS}), which are subsequently used to
13 make a prediction of the dependent variable in the test subset. The initial dataset consisted of
14 74 beef fillet spectral patterns corresponding to different storage temperatures (0, 5, 10, 15,
15 and 20°C) and storage times (up to 350 hours depending on storage temperature). The
16 database was randomly partitioned into a training and testing subset representing 75% ($n =$
17 57) and 25% ($n = 19$) of the data, respectively. Test data were not employed in any step of
18 training the PLS model but they were used exclusively to determine its performance. A series
19 of PLS models were created using a number of latent variables ranging from 1 to 25, hence 25
20 models were developed in total. The performance of each generated model was calculated
21 using leave-one-out cross validation. The optimum numbers of components were used to
22 build the final model. The resulting model was then tested with the independent data set.
23 This procedure was repeated two times for predicting the predefined sensory class: *i*) based on
24 storage time and temperature as two input variables in addition to the FTIR dataset, and *ii*)
25 based entirely on the FTIR data where no storage condition data was included to build the

1 models. Similarly, two sets of models were developed to predict the total viable counts
2 (TVC), firstly based on including the storage conditions as additional input variables, and
3 secondly based entirely on the FTIR data. Therefore four sets of models were developed in
4 total.

5

6 *2.3 Artificial neural networks modelling*

7 Mean-centered and standardized spectral data were initially subjected to principal
8 components analysis (PCA) for dimensionality reduction, and the variables (wavenumbers)
9 for which communality values were less than 0.6 were excluded from further analysis, as they
10 were considered to contain not enough information to explain the variance of spectral data.
11 The remaining wavenumbers (from 1718 to 1203 cm^{-1} and 1020 to 1001 cm^{-1}) were subjected
12 to a second PCA, where the total variance (100%) of the dataset was cumulatively explained
13 by 37 principal components (PCs). The scores of the first five PCs were extracted and used in
14 further analysis as they explained a cumulative variance of 98.08% of the dataset.

15 The selected network was a multilayer perceptron (MLP) based on backpropagation. The
16 basic element in an MLP is the “neuron” that receives a set of input signals (x_i) with weight
17 (w_i), calculates their impact using the summation function ($I = \sum x_i \cdot w_i$), and finally
18 produces an output using some activation function ($y = f(I)$). The determination of the
19 weights is achieved through training of the system. Normally, supervised training is
20 performed in such a way as to minimize the difference between the network output and the
21 measured value:

$$22 \quad MSE = \frac{1}{n} \sum_{i=1}^n (y_{predicted,i} - y_{observed,i})^2 \quad (4)$$

23 where, $y_{predicted,i}$ and $y_{observed,i}$ represent the predicted and observed values of the variable,
24 respectively, and n is the number of observations. Back propagation (BP) is the most

1 commonly used training algorithm in neural networks, also employed in this work. It works
2 on the principle that after the information has gone through the network in a forward direction
3 and an output has been produced, the error associated with this output is redistributed
4 backwards through the model and weights are adjusted accordingly. Minimization of the error
5 occurs through several iterations (training cycles) (Ham and Kostanic, 2001).

6 Two separate networks were developed in this work comprising of an input layer with
7 seven nodes, one for temperature and storage time, respectively, and the remaining five for
8 each one of the five PCs. The output layer contained one node for the prediction of either
9 meat quality class (i.e., F, SF, S) or total viable counts on the surface of meat samples (\log_{10}
10 cfu cm^{-2}). In addition two other similar neural networks were developed in which storage time
11 and temperature were excluded from the input layer as dependent variables, in an attempt to
12 investigate the performance of the network to discriminate meat samples based only on FTIR
13 data. Therefore four neural networks were developed in total. Based on previous work (Argyri
14 et al., 2009) the best performance of the network was obtained with 10 neurons in the hidden
15 layer. To facilitate comparison between the two models, the database was also randomly
16 divided into a training subset with 75% of the data, and a test subset with the remaining 25%.
17 These data were not employed at all in the training session of the network but they were used
18 to assess its capability to foresee for unknown cases. The MLP network was developed using
19 NeuralTools version 1.0 (Palisade Corp., Ithaca, NY, USA).

20

21 *2.5 Evaluation of model performance*

22 The classification accuracy of the neural network and PLS model was determined by the
23 number of correctly classified meat samples in each sensory class divided by the total number
24 of samples in the class. The overall correct classification (accuracy, %) of the model was
25 determined as the number of correct classifications in all classes divided by the total number

1 of samples analyzed (Panigrahi et al., 2006). For the prediction of total viable counts (TVC)
 2 in each meat sample three performance indices were calculated, namely the bias (B_f) and
 3 accuracy (A_f) factors (Ross, 1996) and the root mean squared error ($RMSE$).

4 The bias factor (B_f) indicates whether, on average, the observed TVC counts are above or
 5 below the line of equity ($y = x$), and if so, by how much. The index is defined as:

$$6 \quad B_f = 10^{\left(\frac{\sum \log \left(\frac{\log N(t)_{predicted}}{\log N(t)_{observed}} \right)}{n} \right)} \quad (5)$$

7 where n is the number of observations. A bias factor = 1 indicates a perfect model where the
 8 predictions are in full agreement with observations. Values < 1 indicate that the observed total
 9 viable counts are larger than predicted ones.

10 The accuracy factor is a measure of the average deviation between predictions and
 11 observations, i.e. how close predictions are to observations.

$$12 \quad A_f = 10^{\left(\frac{\sum \log \left(\left| \frac{\log N(t)_{predicted}}{\log N(t)_{observed}} \right| \right)}{n} \right)} \quad (6)$$

13 The values of this index are ≥ 1 . The larger the value the less accurate is the average estimate.

14 The goodness of fit of the modelling approach was also evaluated by the root mean square
 15 error ($RMSE$), which measures the average deviation between observed and predicted values
 16 (Ratkowsky, 2004). The smaller the value of this index the better the fit of the model to the
 17 experimental data:

$$18 \quad RMSE = \sqrt{\frac{\sum (\log N(t)_{predicted} - \log N(t)_{observed})^2}{n}} \quad (7)$$

19 where n is the number of observations.

20

21

1 3. Results

2 Typical FTIR spectral data from 1000 to 1800 cm^{-1} collected from beef fillets stored at
3 0°C for different storage times are presented in Figure 1. The selected spectra correspond to
4 each one of the three quality classes (i.e., fresh, semi-fresh, spoiled) employed in this work.
5 Based on Figure 1, a major peak at 1640 cm^{-1} was apparent in the meat sample due to the
6 presence of moisture (O-H stretch) with an underlying contribution from amide I, whereas a
7 second peak at 1550 cm^{-1} appeared due to the absorbance of amide II (N-H bend, C-N
8 stretch). A second amide vibration was observed at 1400 cm^{-1} (C-N stretch), followed by
9 amide III peaks at 1315 and at 1240 (C-N stretch, N-H bend, C-O stretch, O=C-N bend). The
10 peaks at 1460, 1240 and 1175 cm^{-1} can be attributed also to fat. Finally, the peaks arising
11 from 1025 to 1140 could be absorbance due to amines (C-N stretch) (Chen et al., 1998; Ellis
12 et al., 2002, 2004; Ammor et al., 2009; Argyri et al., 2009).

13 A PLS model performance evaluation was performed using leave-one-out cross validation
14 for the prediction of sensory class of beef samples. The number of latent variables (LVs) was
15 selected on the basis of the highest number of correctly classified samples of the testing
16 subset. For this reason, different models were developed with the LVs ranging from 1 to 25.
17 For each model, the number of correctly classified samples in both the training and test
18 dataset was calculated. When the PLS models were built based entirely on the FTIR data (*i.e.*
19 no storage time and temperature was included), a number of 21 LVs was finally selected
20 presenting the highest correct classification (%) in the training (98.2%) and test (68.4%)
21 subsets (Fig. 2, Table 1). For the training subset, the PLS approach provided 100% correct
22 classification for fresh and semi-fresh meat samples, whereas for spoiled samples the
23 respective number was 96.1%, representing 1 misclassification out of 26 spoiled samples
24 (Table 1). However, for the testing subset the relative percentages were lower, which is not
25 unusual as these data were not involved at all in model development but provided as unknown

1 cases for prediction. Specifically, the highest correct classification was observed in spoiled
2 (71.4%) and fresh (75%) samples, with 2 samples misclassified as semi-fresh out of 7 and 8
3 samples, respectively. The lowest performance was obtained in semi-fresh samples with 2
4 misclassifications out of 4 samples. However, the performance was slightly improved when
5 storage time and temperature were associated with the training data prior to building the
6 model. The best performance in this case was monitored when 20 LVs (Fig. 2), showing a
7 performance of 94.7% on the training and 70.0% on the independent testing dataset. For the
8 training dataset, the PLS approach provided 18 out of 20 correct classification for fresh meat
9 samples (Table 2), whereas for semi-fresh and spoiled samples, the respective numbers were
10 5 and 6 misclassifications out of 15 semi-fresh and 22 spoiled samples, respectively.

11 Similar performance was obtained for the ANN model developed entirely on the FTIR
12 dataset (*i.e.* storage time and temperature were excluded from model development as
13 dependent variables). The obtained correct classifications were 98.2% and 63.1% for the
14 training and test datasets, respectively (Table 1). Within each sensory class in the training
15 dataset, the ANN model provided 100% correct discrimination for fresh and semi-fresh
16 samples, whereas for spoiled samples there was 1 misclassification out of 27 meat samples
17 (96.3%). However, for the test dataset the performance of the ANN was lower but still
18 comparable with the PLS model. Specifically, the highest correct classification was obtained
19 for the fresh and spoiled sensory class where 2 samples were misclassified as spoiled and
20 fresh, respectively (Table 1). Less consistent results were obtained for the semi-fresh class
21 with 3 misclassifications out of 5 samples which is quite reasonable taking into account that
22 sensorial discrimination of this class is rather difficult and requires highly trained taste panels.
23 The performance of the ANN model was slightly improved when storage time and
24 temperature were included as additional inputs in model development (Table 2). The obtained
25 results indicated that correct classification increased by approximately 2% and 10% for the

1 training and test datasets, respectively. In this case, the ANN provided 100% correct
2 classification for all sensory classes in the training dataset. With regard to the test dataset,
3 classification performance was improved by approximately 14% for the spoiled meat samples,
4 compared with the ANN model developed on FTIR data only, with 1 misclassification out of
5 7 samples. For fresh and semi-fresh meat samples, the calculated correct classifications were
6 71.4% and 60.0%, representing 2 misclassifications out of 5 semi-fresh and 7 spoiled meat
7 samples, respectively (Table 2).

8 The PLS approach was also used to associate spectral data with total viable counts (TVC)
9 on the surface of meat samples. The model was developed on the assumption that when the
10 difference between individual predictions and observations was higher than a threshold value
11 of 1 log unit, then the prediction was false. When PLS was applied using only the FTIR data
12 (i.e. no storage time and temperature was included within the input matrix), the model
13 correctly predicted 87.7% of the training data, and 60% of the independent testing data. In the
14 case of including the storage time and temperature within the input dataset, the model showed
15 an increase in performance, reaching 100% and 84.2% for the training and testing,
16 respectively.

17 For models developed on FTIR data only, the calculated value of the bias factor for the
18 ANN training dataset was close to 1 indicating no systematic bias (under or overprediction)
19 (Table 3), whereas for PLS model a slight underestimation was evident (B_f 0.967). The values
20 of bias factor were improved when storage time and temperature were included as inputs in
21 model development, especially for the PLS approach (Table 4). For the test datasets,
22 underprediction ($B_f < 1$) was observed for the PLS models whereas overprediction ($B_f > 1$)
23 was evident in ANN models, regardless of the approach employed in model development
24 (i.e., inclusion or not of storage time and temperature as inputs). These calculations were also

1 graphically verified by the comparison of the observed vs. predicted total viable counts (TVC)
2 plots (Figs. 3 and 4).

3 Moreover, based on the calculated indices for the test datasets between ANN and PLS
4 models that were developed on FTIR data only, it can be concluded that the PLS model
5 presented a comparatively better performance as it yielded lower values for accuracy factor
6 (1.321) and root mean square error (1.993) (Table 3). However, when storage time and
7 temperature were included as input parameters to the models, then the best performance was
8 obtained for ANN based on the comparison of the same indices (Table 4).

9

10 **4. Discussion**

11 So far the assessment of meat quality and safety is based on sensory and retrospective
12 microbiological analyses (Nychas et al., 2008). Sensory analysis is an important and common
13 method to evaluate quality of food commodities since the consumer is the ultimate judge of
14 quality of a product (Lee and O'Mahony, 2005). However, the method has certain
15 disadvantages as it relies on highly trained taste panels, a procedure which makes it costly and
16 unattractive for daily analysis. In addition, a limited number of samples can be analysed daily
17 due to the fatigue of the senses of the panellists. Finally, sensory evaluation has a subjective
18 connotation, although this effect could be reduced by applying scientific protocols under
19 carefully controlled conditions. On the other hand, microbiological analyses are laborious,
20 time-consuming, costly and highly technical (molecular tools), as well as destructive to
21 products analysed, requiring in most cases a complex process of sample preparation, while
22 not able to give the 'immediate answer required' (McMeekin et al., 2007).

23 A major challenge of the meat industry in the 21st century is to obtain reliable information
24 on meat quality and safety throughout the production, processing, and distribution chain, and
25 finally turn this information into practical management support systems to ensure high quality

1 final products for the consumer (Damez and Clerjon, 2008; Sofos, 2008). These systems must
2 be readily available to the industry, and easy-to-use without requiring special expertise from
3 the end-users. Certain databases are available today, such as the Combase (www.combase.cc)
4 and Sym'Previus (www.symprevius.net) providing information on growth/death kinetics of
5 microorganisms in order to define the shelf-life of various foods incorporating mathematical
6 models (Baranyi and Tamplin, 2004; Leporq et al., 2005). It must be stressed however, that
7 the existing predictive microbiology spoilage models tend to underestimate important factors
8 such as microbial interaction among the members of the microbial association as well as with
9 the food matrix (Wilson et al., 2002; Koutsoumanis et al., 2004). In the latter case the changes
10 in the concentration of microbial metabolites on meat surface due to microbial activity can be
11 used to monitor quality deterioration. There is thus a need to replace, or at least limit, the
12 number and extent of microbiological analyses, with (bio)chemical analyses in an attempt to
13 define metabolic indices as potential indicators of spoilage. The concept is not new and it was
14 proposed as a promising alternative to monitor meat spoilage in the late 80s and 90s
15 (McMeekin, 1982; Gill, 1986; Nychas et al., 1988; Kakouri and Nychas, 1994; Dainty, 1996).
16 However, the idea of a single biochemical substance as spoilage indicator put forward at that
17 time, has been replaced today by the metabolomic concept which is based on a holistic
18 approach of spoilage profile (Goodacre et al., 2004; Nychas et al., 2008).

19 Recent developments in sensor technologies and data analysis procedures have stimulated
20 interest in developing rapid and non-invasive techniques to monitor changes in meat quality.
21 Among these, spectroscopic methods are widely used for muscle food quality assessment and
22 control, in both laboratory and meat industry installations (Hildrum et al., 2006). In contrast to
23 conventional methods for the determination of meat quality parameters, Fourier transform
24 infrared spectroscopy (FTIR) is a sensitive, rapid and non-destructive analytical technique,
25 with simplicity in sample preparation, allowing simultaneous assessment of numerous meat

1 properties. This technique has found numerous applications in foods such as olive oil (Maggio
2 et al., 2010), honey (Kelly et al., 2006), wine (Versari et al., 2010), coffee (Briandet et al.,
3 1996). Ellis et al. (2002, 2004) have been the pioneers to report that FTIR spectral data
4 collected directly from the surface of meat could be used as biochemical interpretable
5 “fingerprints” to provide information on early detection of microbial spoilage of chicken
6 breast and rump steaks. However, the amount of information provided by spectral data require
7 special data mining techniques based on multivariate statistical analysis (e.g. cluster analysis,
8 principal components analysis, discriminant function analysis, partial least squares regression)
9 and/or soft computing methodologies (e.g. artificial neural networks, genetic algorithms,
10 support vector machines) to provide information related to (a) the responses of specific
11 spoilage microorganisms in meat and (b) the discrimination of meat samples in quality classes
12 (Goodacre, 2000; Mataragas et al., 2007; Verouden et al., 2009).

13 In the present work, FTIR spectral data from beef fillets stored under aerobic conditions at
14 five different storage temperatures were analyzed by partial least squares regression in an
15 effort to classify meat samples in three sensorial categories (fresh, semi-fresh, spoiled) as
16 defined by a taste panel. The performance of the PLS approach was compared with a multi-
17 layer perceptron (MLP) neural network. Two different approaches were followed in model
18 development. Firstly, storage time and temperature were treated as input variables and
19 associated with FTIR spectral data during model development. However, in practice, the
20 history of a meat sample in terms of storage temperature and time is not always known, and
21 hence meat quality must be assessed by spectral data only. To cope with this issue separate
22 models were developed based on the FTIR data only and the two approaches were compared.

23 Results showed relatively better performance when storage time and temperature were
24 included as inputs in model development, as a more precise dataset was used for the training
25 of models. Good classification accuracies were obtained for fresh and spoiled meat samples,

1 demonstrating the effectiveness of the method to discriminate samples between these two
2 classes (Table 1 and 2). The high classification rate of both models (i.e., PLS and ANN) could
3 be associated to the beginning of proteolysis in meat (Nychas and Tassou, 1997) resulting in
4 changes in the concentration of amides and amines (Ellis and Goodacre, 2001), as well as to
5 glucose consumption and the resulting changes in the levels of organic acids (Dainty, 1996;
6 Nychas et al., 1998). It must be emphasized however that the number of examined samples
7 within each class was not equal due to the different spoilage rate of beef samples at different
8 storage temperatures resulting in variable number of samples in each class. This may have
9 affected the training process which is basically a data driven approach (Basheer and Hajmeer,
10 2000), and could thus account for the lower classification accuracies observed in certain
11 classes (e.g. fresh and semi-fresh) (Table 1 and 2). Finally, the lower accuracies observed in
12 the semi-fresh class could also be attributed to the performance of the taste panel, as the
13 difference between “fresh/semi-fresh” and “semi-fresh/spoiled” is sometimes subjective and
14 affects the overall classification, as the developed models are based on supervised training for
15 parameter optimization.

16 Another interesting perspective from a microbiological point of view would be the
17 correlation of FTIR spectra to bacterial population counts on the surface of meat samples. In
18 this way laborious and time consuming microbiological analyses could be replaced in the long
19 term by spectral data in order to provide rapid, low cost and non-invasive microbiological
20 analyses (Nychas et al., 2008). The graphical plots between observed and predicted total
21 viable counts as well as the calculated performance indices showed that for models developed
22 on FTIR spectral data alone better performance was obtained by the PLS model (Table 3; Fig.
23 3) although the model had a tendency to underestimate total viable counts. However, when
24 storage time and temperature were included in model development together with FTIR data
25 the best performance was obtained by ANN (Table 4; Fig. 4). Generally, ANN models tended

1 to overestimate microbial counts ($B_f > 1$) in contrast to PLS models where underestimation of
2 total viable counts was evident ($B_f < 1$). An interesting alternative approach to evaluate the
3 effectiveness of FTIR spectral data in the determination of sensory rating and total viable
4 counts prediction in meat samples, would be the implementation of experimental studies in
5 which meat samples would have been artificially contaminated with spoilage bacteria at
6 different initial populations. Further research is needed in this direction as results from such
7 studies would be valuable in the evaluation of the robustness of the FTIR approach.

8 In conclusion, the correlation between microbial growth and chemical changes during
9 storage has been recognized as a way to identify indicators that could be employed to quantify
10 quality as well as the degree of spoilage. Spectral data collected from FTIR analysis
11 combined with an appropriate machine learning strategy (partial least squares regression,
12 artificial neural networks) could become an interesting tool to monitor beef fillets spoilage
13 through the measurement of biochemical changes occurring in meat substrate. Future work
14 should also focus on the association of specific microbial groups (e.g. lactic acid bacteria,
15 pseudomonads, enterobacteria) with FTIR spectral data in an attempt to increase the
16 prediction performance of the models.

17

18

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1 **Fig. 1.** Typical FTIR spectra in the range of 1800 to 1000 cm^{-1} collected from beef fillets
2 stored at 0°C at the beginning of storage (A; Fresh), after 96 h (B; Semi-fresh), and 216 h (C;
3 Spoiled).

4
5 **Fig. 2.** Optimization of the PLS-DA classification models using latent variables ranging from
6 1 to 25 for the training (grey line) and test (black line) subsets after leave-one-out cross
7 validation. (A) sensory class prediction based on FTIR data; (B) total viable counts prediction
8 based on FTIR data; (C) sensory class prediction based on FTIR data plus storage time and
9 temperature as additional inputs; (D) total viable counts prediction based on FTIR data plus
10 storage time and temperature as additional inputs

11
12 **Fig. 3.** Comparison between observed and predicted total viable counts (TVC) of beef fillets
13 by the ANN (a) and the PLS-DA (b) model based on FTIR spectral data (open symbols:
14 training data; solid symbols: test data; dotted lines are ± 1 log units area).

15
16 **Fig. 4.** Comparison between observed and predicted total viable counts (TVC) of beef fillets
17 by the ANN (a) and the PLS-DA (b) model based on FTIR spectral data with storage time and
18 temperature as additional inputs to the models (open symbols: training data; solid symbols:
19 test data; dotted lines are ± 1 log units area).

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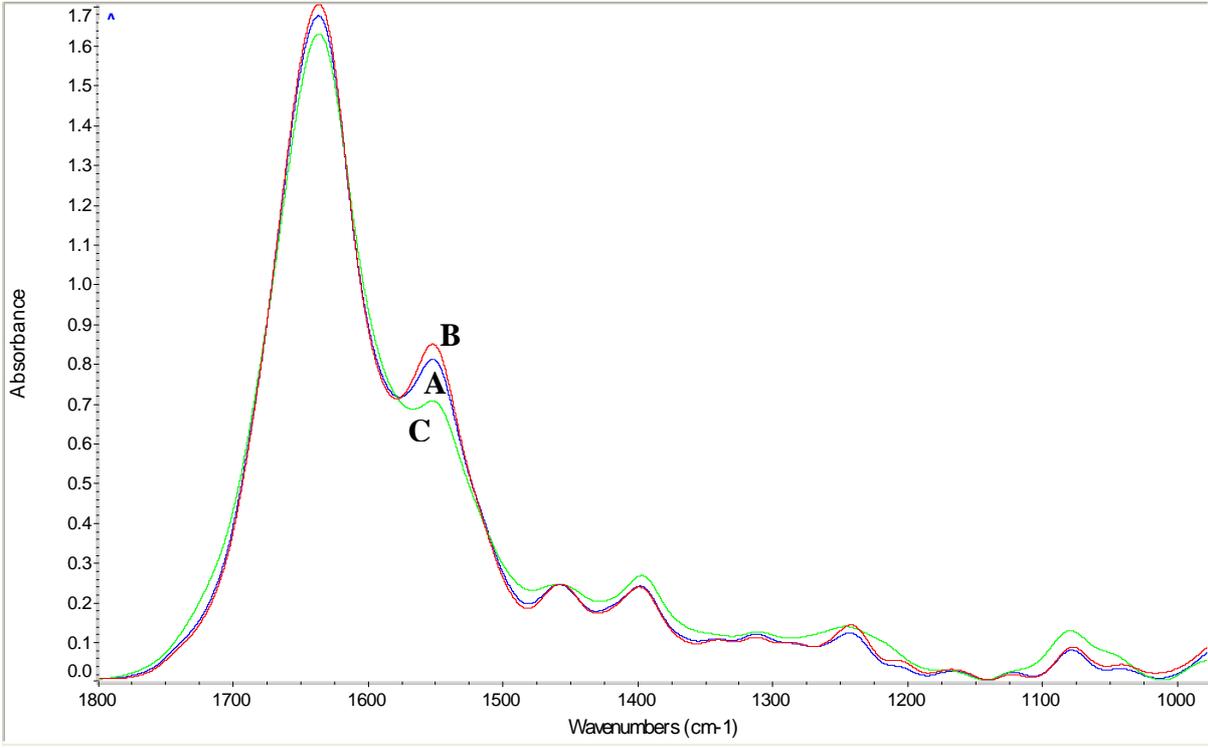
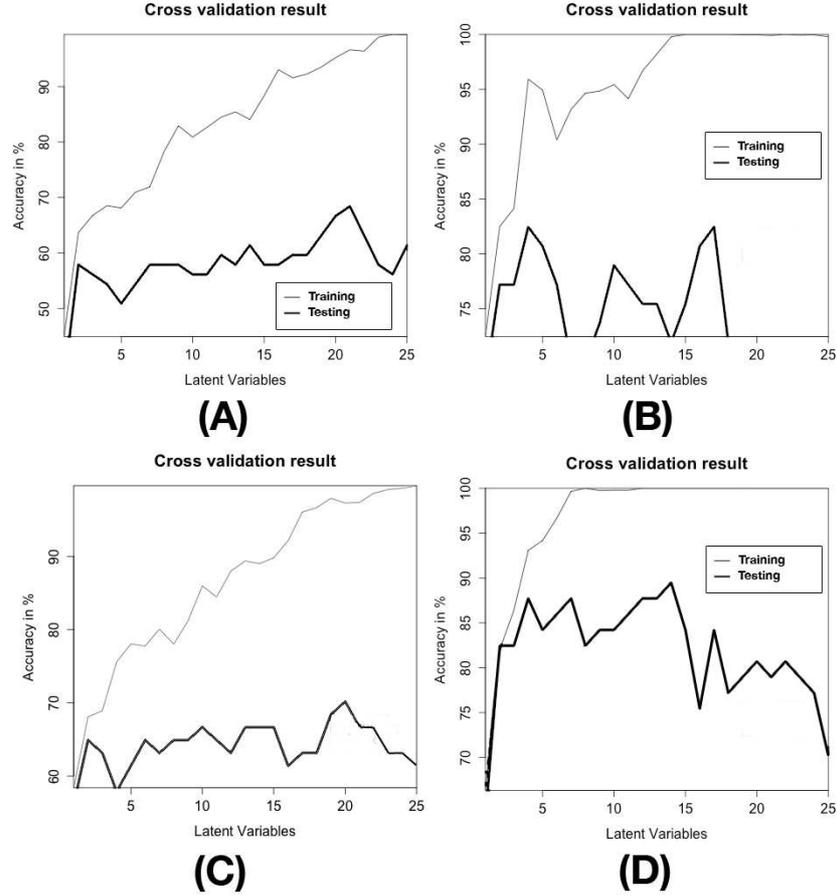


Fig. 1.



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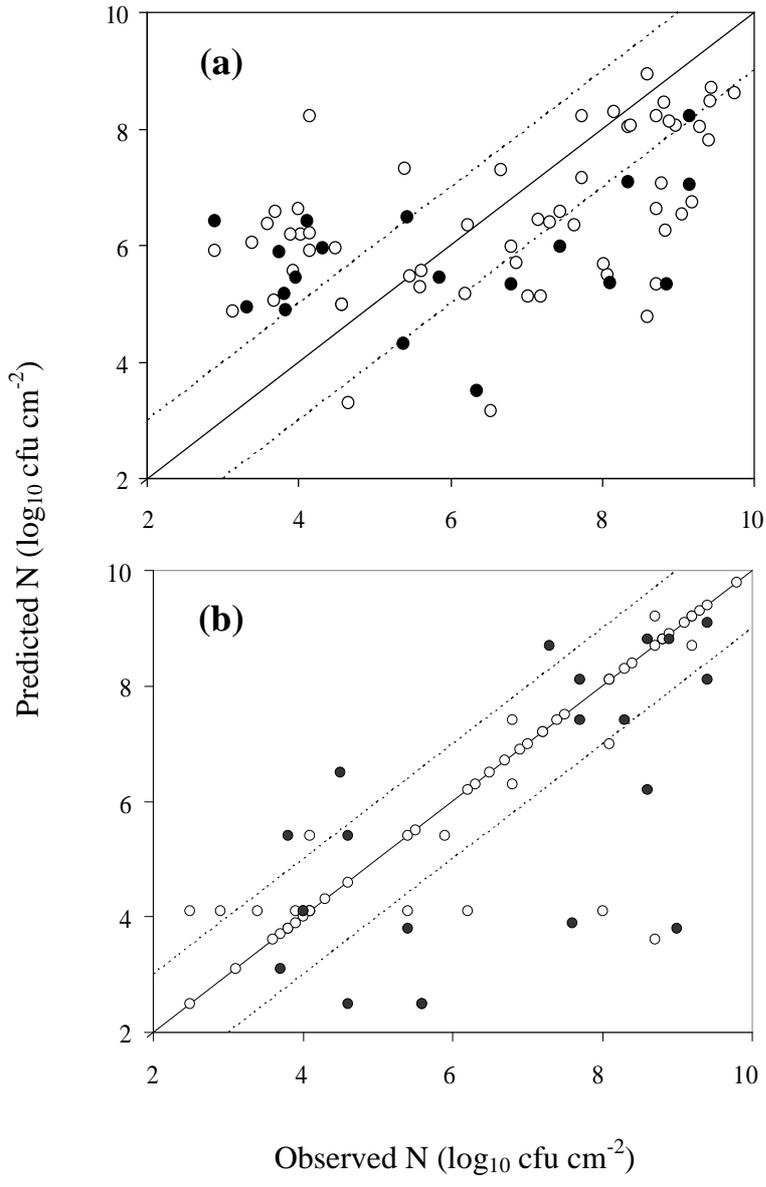


Fig. 3

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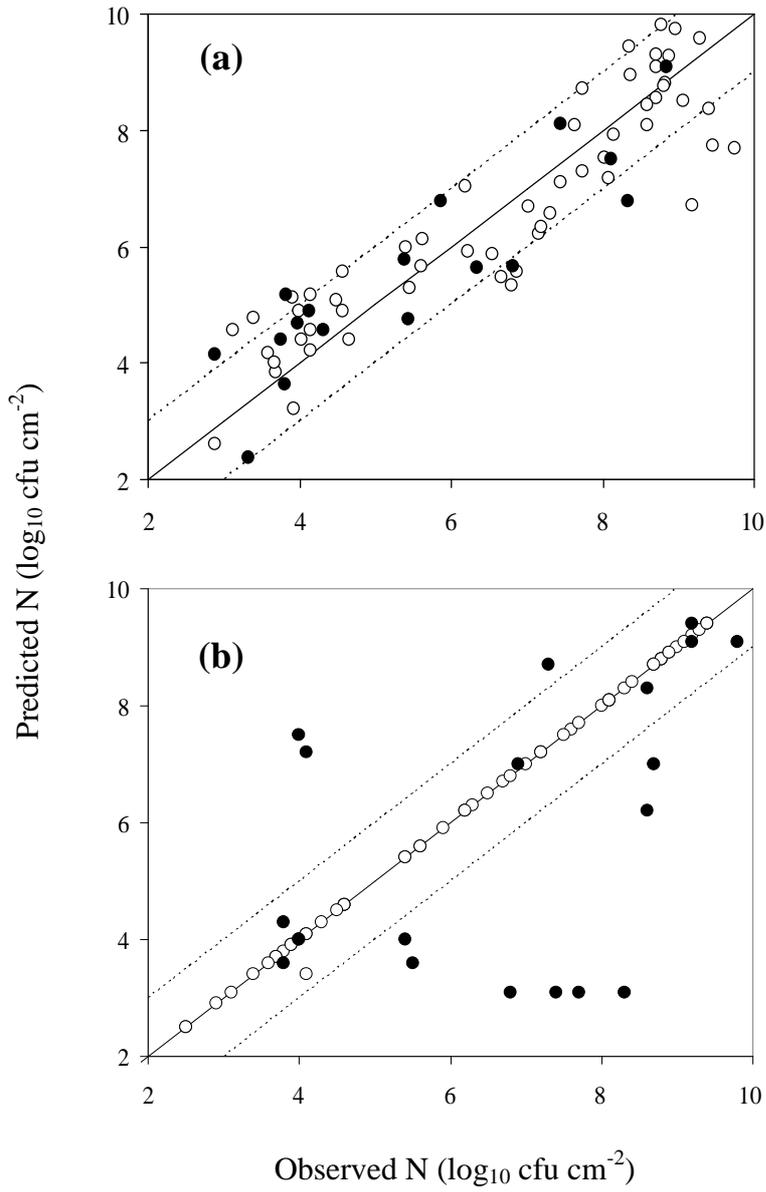


Fig. 4

1 **Table 1.** Confusion matrix of the ANN classifier and the PLS model regarding sensory
 2 quality discrimination of beef fillets based on FTIR spectral data.

3

From/to	ANN training (<i>n</i> = 57)				
	Fresh	Semi-fresh	Spoiled	Total	Correct (%)
Fresh	19	0	0	19	100
Semi-fresh	0	11	0	11	100
Spoiled	1	0	26	27	96.3
	ANN testing (<i>n</i> = 19)				
Fresh	5	0	2	7	71.4
Semi-fresh	2	2	1	5	40.0
Spoiled	2	0	5	7	71.4
	PLS training (<i>n</i> = 57)				
Fresh	18	0	0	18	100
Semi-fresh	0	13	0	13	100
Spoiled	0	1	25	26	96.1
	PLS testing (<i>n</i> = 19)				
Fresh	6	2	0	8	75.0
Semi-fresh	2	2	0	4	50.0
Spoiled	0	2	5	7	71.4

4

5 Overall correct classification (accuracy) for ANN train and test datasets: 98.2% and 63.1%,
 6 respectively.

7 Overall correct classification (accuracy) for PLS train and test datasets: 98.2% and 68.4%,
 8 respectively.

1 **Table 2.** Confusion matrix of the ANN classifier and the PLS model regarding sensory
 2 quality discrimination of beef fillets based on FTIR spectral data together with storage time
 3 and temperature as additional inputs to the models.
 4

From/to	ANN training ($n = 57$)				
	Fresh	Semi-fresh	Spoiled	Total	Correct (%)
Fresh	19	0	0	19	100
Semi-fresh	0	11	0	11	100
Spoiled	0	0	27	27	100
	ANN testing ($n = 19$)				
Fresh	5	0	2	7	71.4
Semi-fresh	2	3	0	5	60.0
Spoiled	1	0	6	7	85.7
	PLS training ($n = 57$)				
Fresh	18	2	0	20	90.0
Semi-fresh	2	10	3	15	66.7
Spoiled	1	5	16	22	72.7
	PLS testing ($n = 19$)				
Fresh	5	1	0	6	83.4
Semi-fresh	0	1	1	2	50.0
Spoiled	2	1	8	11	72.7

5
 6 Overall correct classification (accuracy) for ANN train and test datasets: 100.0% and 73.7%,
 7 respectively.

8 Overall correct classification (accuracy) for PLS train and test datasets: 77.2% and 73.6%,
 9 respectively.

10

1 **Table 3.** Comparison of validation indices between the PLS and ANN models for total viable
2 counts (TVC) predictions in meat samples based on FTIR spectral data.

3

Parameter	ANN		PLS model	
	Train	Test	Train	Test
Bias factor (B_f)	1.002	1.034	0.967	0.854
Accuracy factor (A_f)	1.291	1.390	1.090	1.321
RMSE	1.821	1.978	1.073	1.993

4

5

1 **Table 4.** Comparison of validation indices between the PLS and ANN models for total viable
2 counts (TVC) prediction in meat samples based on FTIR spectral data together with storage
3 time and temperature as additional inputs to the model.

Parameter	ANN		PLS model	
	Train	Test	Train	Test
Bias factor (B_f)	1.008	1.038	0.996	0.833
Accuracy factor (A_f)	1.118	1.166	1.003	1.409
RMSE	0.852	0.921	0.092	2.501

5
6

A comparison of artificial neural networks and partial least squares modelling for the rapid detection of the microbial spoilage of beef fillets based on Fourier transform infrared spectral fingerprints

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