Metabolomics Application on Bacterial Safety, Spoilage and Adulteration

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Outline of the presentation

INTRODUCTION

- What is Quantitative Food Microbiology?
- How microbes can be measured?
- What is Food Spoilage?

METHODS/TOOLS/RESULTS

- 1^{st} Case Study; Meat (beef, pork, adulteration & marinated poultry)
- 2^{rd} Case Study; Table olives
- 3^{th} Case Study; Pasteurized vanilla cream

CONCLUSION – FUTURE CHALLENGES

INTRODUCTION; Quantitative Food Microbiology

is dealing with the quantification of parameters that can describe the behavior of microbial populations in foods (growth, survival, or death) and is determined by the properties of the food (e.g., water activity and pH) and the storage conditions (e.g., temperature, relative humidity, and atmosphere).

The effect of these properties can be predicted by **mathematical models derived from quantitative studies** on microbial populations and they could be used to allow decisions on the shelf life and safety of foods

McMeekin et al. (1997) Emerg Infect Dis;3(4):541-9.

INTRODUCTION; How bacteria can be measured?

Conventional vs Molecular tools in measuring microorganisms in food microbiology

The use of microbiological methods either conventional or advanced molecular methods in the Food Industry is under consideration

Both are time consuming, (results from 18 hrs to 72 hrs)

Retrospective results, Few samples, Limited reproducibility,

measurements require sophisticated procedures,

highly educated personnel, time and equipment.

INTRODUCTION; Food Spoilage

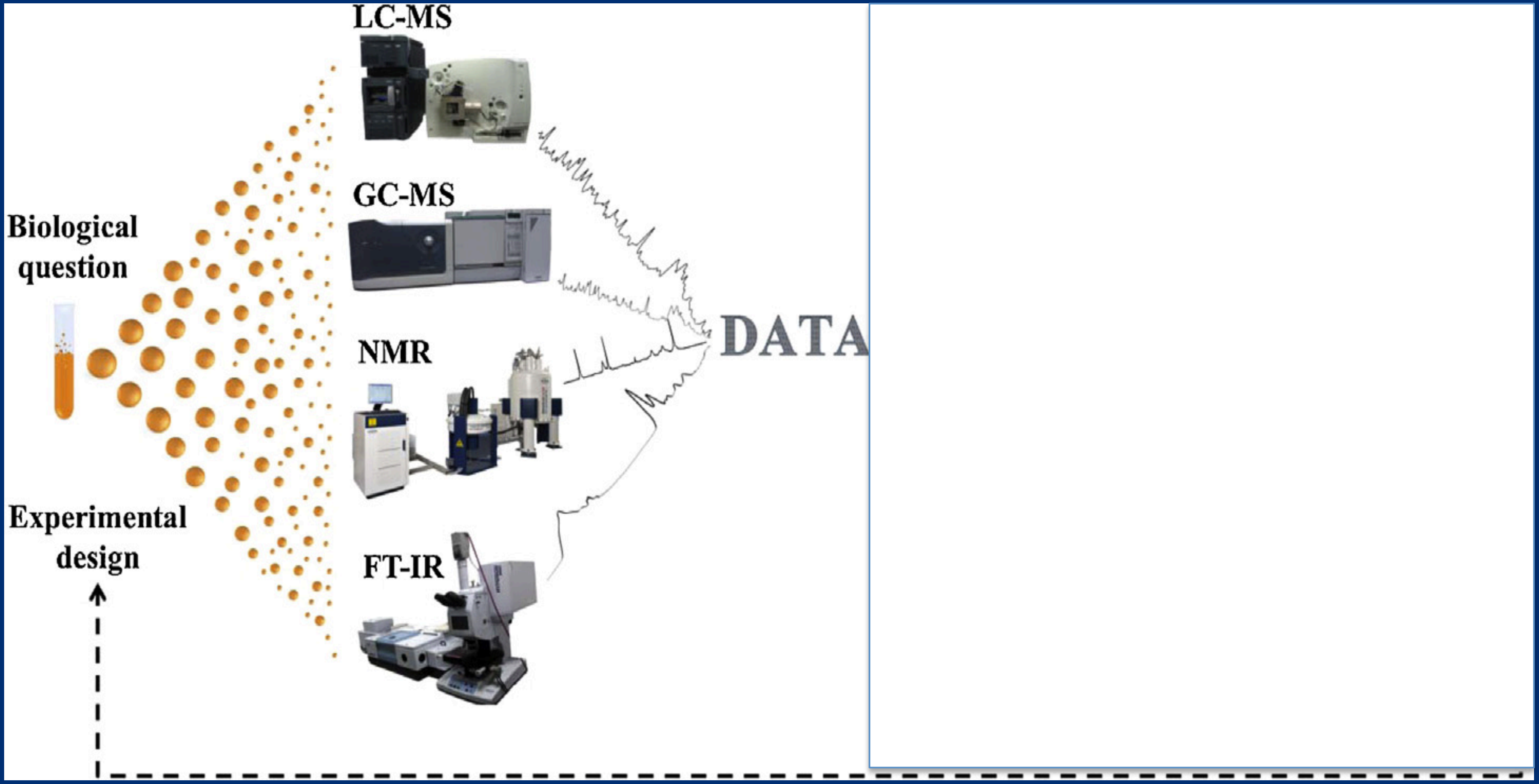
- Spoilage of food can be considered as an ecological phenomenon that encompasses changes in the available components (e.g., low molecular weight compounds) during proliferation of bacteria present in the microbial association of product.

- The correlation between microbial growth and chemical changes during spoilage has been continuously recognised as a means of revealing indicators that may be useful for quantifying the degree of spoilage.

Ellis & Goodacre (2001) Trends in Food Science & Technology 12, 414
Nychas, G.-J.E., et al. (2008) *Meat Science*, 78: 77-89.

METHODS & TOOLS

Graphical representation of the different analytical (GC/MS,HPLC,FTIR,NMR, etc) tools

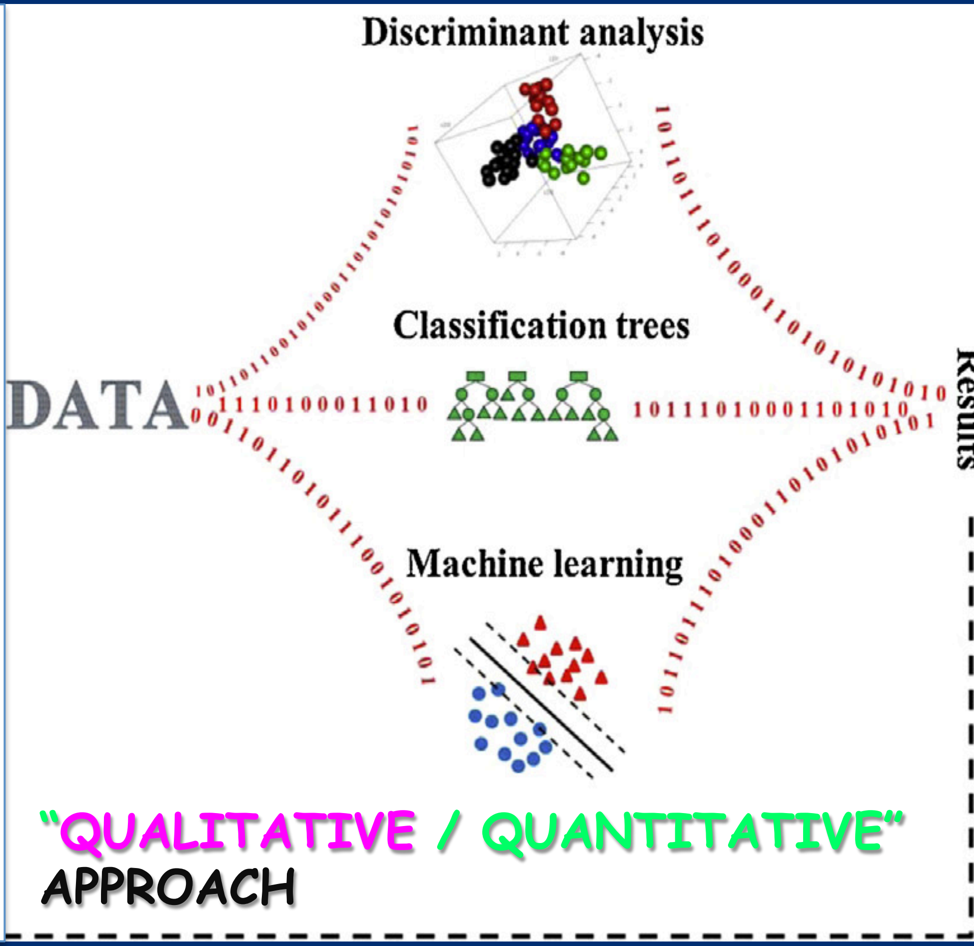


GROMSKI et al. 2015 Analytica Chimica Acta 879, 10-23.

METHODS & TOOLS

Graphical representation of the different analytical (GC/MS,HPLC,FTIR,NMR, etc) tools & informatics techniques/data analysis (discriminant analysis, classification trees, machine learning etc) employed in metabolomics studies;

"QUALITATIVE / QUANTITATIVE" APPROACH



GROMSKI et al. 2015 Analytica Chimica Acta 879, 10-23.

METHODS & TOOLS

1^{st} CASE STUDY ;

Pork or beef meat stored under different storage and temperatures conditions

The aim was to investigate the potential of GC/MS data of Volatile Compounds (VOCs), as a quick analytical method, in combination with an appropriate data analysis strategy to:

1. Define spoilage indices of pork and beef meat during storage at different temperatures (0, 5, 10, 15, and 20°C) &

2. Discriminate among different quality classes of minced beef samples during storage at different temperatures and packaging conditions (aerobic, MAP, MAP+EO).

3. Correlate **(estimate)** the microbial load of different microbial groups REGRDLESS of storage temperature.

METHODS & TOOLS

Product : pork / beef

Packaging : Aerobic, MAP (40% CO_2, 30% O_2,30% N_2),
MAP + oregano essential oil (2% v/w)

Storage temperature : 0, 5, 10, 15 & 20°C

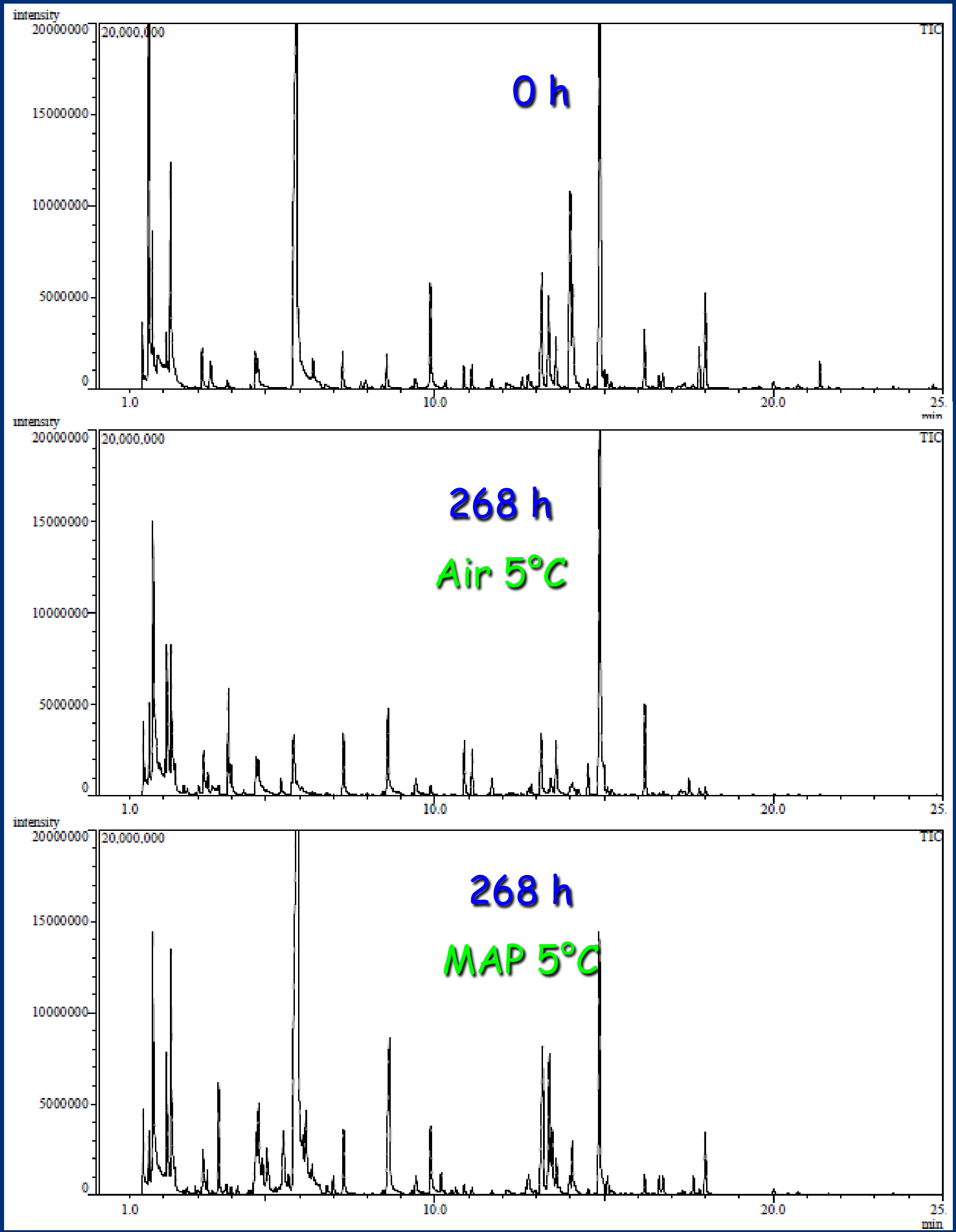
Microbiological analysis : Total viable counts, *Pseudomonas* spp, *Enterobacteriaceae*, lactic acid bacteria, *Br thermosphacta*, and yeasts

pH monitoring

Organoleptic assessment : Spoilage detection based on changes in colour, odour and taste based on a taste panel
(Score range 1-3; 1=Fresh, 1.5 Semi-Fresh, 2-3 Spoiled)

GC/MS – HPLC analysis : Collection of data from the GC/MS and HPLC to monitor biochemical changes in meat during storage.

RESULTS; GC/MS



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RESULTS; GC/MS

Compound	AIR				MAP			
	0	5	10	15	0	5	10	15
Alcohols								
Ethanol *	+	+	+	+	+	+	+	+
Propanol	+	+	+	+	+	+	+	+
2-Butanol	+	+	+	+	+	+	+	+
1-Butanol	+	+	+	+	+	+	+	+
1-Penten-3-ol *	+	+	+	+	+	+	+	+
Isoamyl alcohol (3-Methyl-1-butanol) *	+	+	+	+	+	+	+	+
2-Methyl-1-butanol *	+	+	+	+	+	+	+	+
Amyl alcohol (pentanol) *	+	+	+	+	+	+	+	+
2,3-Butanediol (1)	+	+	+	+	+	+	+	+
2,3-Butanediol (2)	+	+	+	+	+	+	+	+
1-Hexanol *	+	+	+	+	+	+	+	+
Heptanol *	+	+	+	+	+	+	+	+
1-octen-3-ol *	+	+	+	+	+	+	+	+
3-Octanol	+	+	+	+	+	+	+	+
2-Ethyl-1-hexanol	+	+	+	+	+	+	+	+
2-Octen-1-ol *	+	+	+	+	+	+	+	+
1-Octanol *	+	+	+	+	+	+	+	+
Nonanol	+	+	+	+	+	+	+	+
4-Carvomenthenol (Terpinen-4-ol)	+	+	+	+	+	+	+	+
Aldehydes								
Acetaldehyde	+	+	+	+	+	+	+	+
3-Methylbutanal (Isovaleraldehyde)	+	+	+	+	+	+	+	+
2-Methylbutanal	+	+	+	+	+	+	+	+
Pentanal *	+	+	+	+	+	+	+	+
Hexanal *	+	+	+	+	+	+	+	+
trans-2-Hexenal	+	+	+	+	+	+	+	+
cis-4-Heptenal *	+	+	+	+	+	+	+	+
Heptanal *	+	+	+	+	+	+	+	+
Benzaldehyde	+	+	+	+	+	+	+	+

RESULTS; GC/MS

Compound	AIR				MAP			
	0	5	10	15	0	5	10	15
Aldehydes								
Octanal *	+	+	+	+	+	+	+	+
trans-2-octenal *	+	+	+	+	+	+	+	+
Nonanal *	+	+	+	+	+	+	+	+
trans-2-Nonenal *	+	+	+	+	+	+	+	+
3-Phenylpropionaldehyde	+	+	+	+	+	+	+	+
cis-4-Decenal	+	+	+	+	+	+	+	+
n-decanal *	+	+	+	+	+	+	+	+
trans,trans-2,4-Nonadienal	+	+	+	+	+	+	+	+
trans-2-Decenal	+	+	+	+	+	+	+	+
trans,trans-2,4-Decadienal (1)	+	+	+	+	+	+	+	+
trans,trans-2,4-Decadienal (2)	+	+	+	+	+	+	+	+
Ketones								
Diacetyl (3-hydroxy-2-butanone) *	+	+	+	+	+	+	+	+
Methyl ethyl ketone (2-Butanone) *	+	+	+	+	+	+	+	+
2-Pentanone *	+	+	+	+	+	+	+	+
Acetyl propionyl (2,3-Pentanedione) *	+	+	+	+	+	+	+	+
Acetoin (3-Hydroxy-2-butanone) *	+	+	+	+	+	+	+	+
3-Methyl-2-pentanone	+	+	+	+	-	-	-	-
2-Heptanone *	+	+	+	+	+	+	+	+
6-Methyl-2-heptanone	+	+	+	+	+	+	+	+
2,3-Octanedione or 2,5- *	+	+	+	+	+	+	+	+
3-Octanone *	+	+	+	+	+	+	+	+
2-Octanone *	+	+	+	+	+	+	+	+
3-Octen-2-one	+	+	+	+	+	+	+	+
Acetophenone	+	+	+	+	+	+	+	+
2-Nonanone *	+	+	+	+	+	+	+	+
trans,trans -3,5-Octadien-2-one	+	+	+	+	+	+	+	+

RESULTS; GC/MS

Compound	AIR				MAP			
	0	5	10	15	0	5	10	15
Hydrocarbons								
Hexane	+	+	+	+	+	+	+	+
Benzene	+	+	+	+	+	+	+	+
Heptane	+	+	+	+	+	+	+	+
Cyclohexane, methyl	+	+	+	+	+	+	+	+
Cyclopentane, ethyl	-	-	-	-	+	+	+	+
Alkane 1	-	-	-	-	+	+	+	+
Alkane 2	-	-	-	-	+	+	+	+
Alkane 3	-	-	-	-	+	+	+	+
Toluene	+	+	+	+	+	+	+	+
Alkane 4	+	+	+	+	+	+	+	+
Alkane 5	+	+	+	+	+	+	+	+
Isomer of Alkane 5	+	+	+	+	+	+	+	+
Alkane 6	+	+	+	+	+	+	+	+
1-Octene	+	+	+	+	+	+	+	+
Alkane 7	+	+	+	+	+	+	+	+
Alkane 8	+	+	+	+	+	+	+	+
n-Octane	+	+	+	+	+	+	+	+
Trans-4-Octene	+	+	+	+	+	+	+	+
Alkane 10	+	+	+	+	+	+	+	+
cis-2-Octene	+	+	+	+	+	+	+	+
Cyclohexane, ethyl	+	+	+	+	+	+	+	+
Ethyl benzene	+	+	+	+	+	+	+	+
Xylene 1	+	+	+	+	+	+	+	+
Styrene	+	+	+	+	+	+	+	+
Xylene 2	+	+	+	+	+	+	+	+
n-Nonane	+	+	+	+	+	+	+	+
Alkane 11	+	+	+	+	+	+	+	+
n-Decane	+	+	+	+	+	+	+	+
Benzene, 1,2,3-trimethyl	+	+	+	+	+	+	+	+
Indane	+	+	+	+	+	+	+	+
3a,4,5,6,7,7a-Hexahydro-4,7-	+	+	+	+	+	+	+	+
1-Undecene	+	+	+	+	-	-	-	-

RESULTS: GC/MS

Compound	AIR				MAP			
	0	5	10	15	0	5	10	15
Hydrocarbons								
n-Dodecane	+	+	+	+	+	+	+	+
Tridecane	+	+	+	+	+	+	+	+
n-Tetradecane	+	+	+	+	+	+	+	+
Terpenes								
a -Thujene	+	+	+	+	+	+	+	+
a -Pinene	+	+	+	+	+	+	+	+
Camphene	+	+	+	+	+	+	+	+
trans-2-Heptenal	+	+	+	+	+	+	+	+
Sabinene	+	+	+	+	+	+	+	+
Myrcene	+	+	+	+	+	+	+	+
a -Phellandrene	+	+	+	+	+	+	+	+
delta-3-carene	+	+	+	+	+	+	+	+
a -Terpinene	+	+	+	+	+	+	+	+
p-Cymene	+	+	+	+	+	+	+	+
Limonene	+	+	+	+	+	+	+	+
Eucalyptol	+	+	+	+	+	+	+	+
Ocimene (cis)	+	+	+	+	+	+	+	+
γ-Terpinene	+	+	+	+	+	+	+	+
Linaloloxide (cis, isomer B)	+	+	+	+	+	+	+	+
Terpinolene	+	+	+	+	+	+	+	+
4,7-Methano-1H-indene, octahydro-	+	+	+	+	+	+	+	+
Linalol	+	+	+	+	+	+	+	+
Esters								
Methyl acetate	+	+	+	+	+	+	+	+
Ethyl acetate *	+	+	+	+	+	+	+	+
Ethyl propionate *	+	+	+	+	+	+	+	+
n-Propyl acetate	-	-	-	-	+	+	+	+
Methyl butyrate	+	+	+	+	+	+	+	+
Ethyl isobutyrate	+	+	+	+	+	+	+	+
Ethyl butyrate (butanoate) *	+	+	+	+	+	+	+	+
Ethyl lactate *	+	+	+	+	+	+	+	+
Ethyl 2-methylbutyrate	+	+	+	+	+	+	+	+

RESULTS; GC/MS

Compound	AIR				MAP			
	0	5	10	15	0	5	10	15
Esters								
Isoamyl acetate	+	+	+	+	+	+	+	+
Ethyl pentanoate	+	+	+	+	+	+	+	+
Pentyl acetate	+	+	+	+	+	+	+	+
Methyl caproate (methyl hexanoate)	+	+	+	+	+	+	+	+
Ethyl hexanoate *	+	+	+	+	+	+	+	+
Hexyl acetate	+	+	+	+	+	+	+	+
Ethyl heptanoate	+	+	+	+	+	+	+	+
Ethyl octanoate	+	+	+	+	+	+	+	+
Ethyl nonanoate	+	+	+	+	+	+	+	+
Miscellaneous								
Dimethyl sulfide	+	+	+	+	+	+	+	+
Furan, 2-methyl	+	+	+	+	+	+	+	+
Furan, 3-methyl	+	+	+	+	+	+	+	+
Furan 2-ethyl	+	+	+	+	+	+	+	+
2-n-Butyl furan	+	+	+	+	+	+	+	+
Furan, 2,5-diethyltetrahydro	+	+	+	+	+	+	+	+
Unknown 1	-	-	-	-	+	+	+	+
Unknown 2	-	-	-	-	+	+	+	+
Furan 2-pentyl	+	+	+	+	+	+	+	+
2,3,5,6-Tetramethylpyrazine	+	+	+	+	-	-	+	+
Unknown 3	+	+	+	+	+	+	+	+

METHODS & TOOLS

QUANTITATIVE APPROACH

Pork or beef stored under air, MAP & active packaging (0, 5, 10, and 15°C)

Collection of GC/MS spectral data

↓

Principal components analysis (PCA)

(Investigation of the variables that significantly contribute during storage) (Dimensionality reduction)

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RESULTS; QUANTITATIVE APPROACH - GC/MS

Principal Component Analysis

Fresh & Semi-fresh samples

beef	pork
PENTANAL	***PENTANAL***
HEXANAL	***HEXANAL***
trans-2-heptanal	Heptanal
trans-2-octenal	Nonanal
2-butanone	Octanal
2, 3-pentanedione	2-heptenal
2, 5-octanedione	1-pentanol
	1-penten-3-ol
	1-octen-3-one
	2, 5-octanedione

(decreasing trend during storage)

Spoiled samples

beef	pork
ETHANOL	*ETHANOL*
2-METHYL-1-BUTANOL	*2-METHYL-1-BUTANOL*
3-METHYL-1-BUTANOL	*3-METHYL-1-BUTANOL*
2-PENTANONE	***2-PENTANONE***
2-NONANONE	***2-NONANONE***
3-OCTANONE	***3-OCTANONE***
diacetyl	2-butanone
acetoin	Ethyl 3 methyl butyrate
2-heptanone	***ETHYL ACETATE***
ethyl lactate	***ETHYL HEXANOATE***
ETHYL ACETATE	***ETHYL PROPANOATE***
ETHYL HEXANOATE	Dimethyl sulfide
ETHYL PROPANOATE	Dimethyl trisulfite
	Disulfitde dimethyl

(increasing trend during storage)

Aldehydes; Ketones; Esters; Alcohols; ; Sulfur compounds

METHODS & TOOLS; QUANTITATIVE APPROACH

Pork or beef stored under air, MAP & active packaging
(0, 5, 10, and 15°C)

Collection of GC/MS spectral data
(Areas under peaks)

1st Principal components analysis (PCA)
(Investigation of the variables that significantly fluctuate during storage)

Partial least squares regression
(PLS-R with storage time) Define spoilage indices based on storage time

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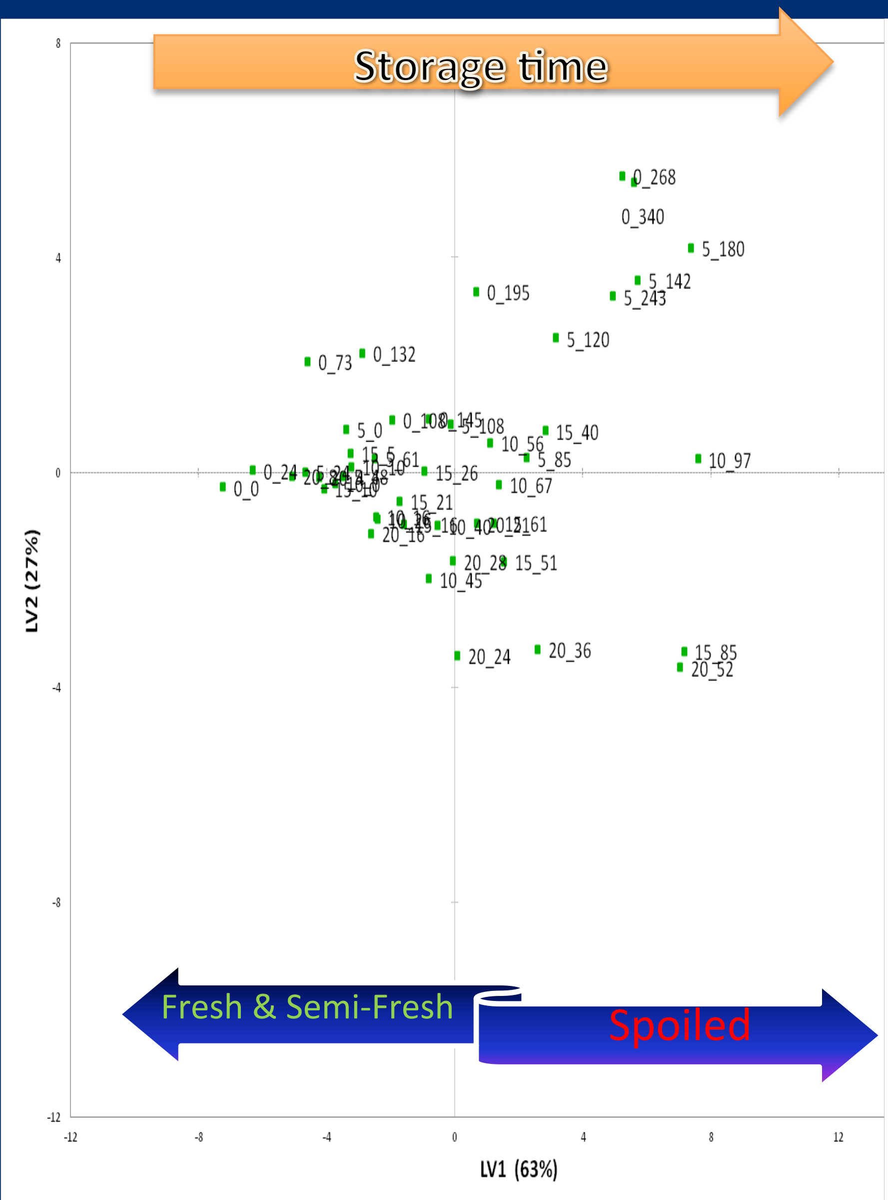
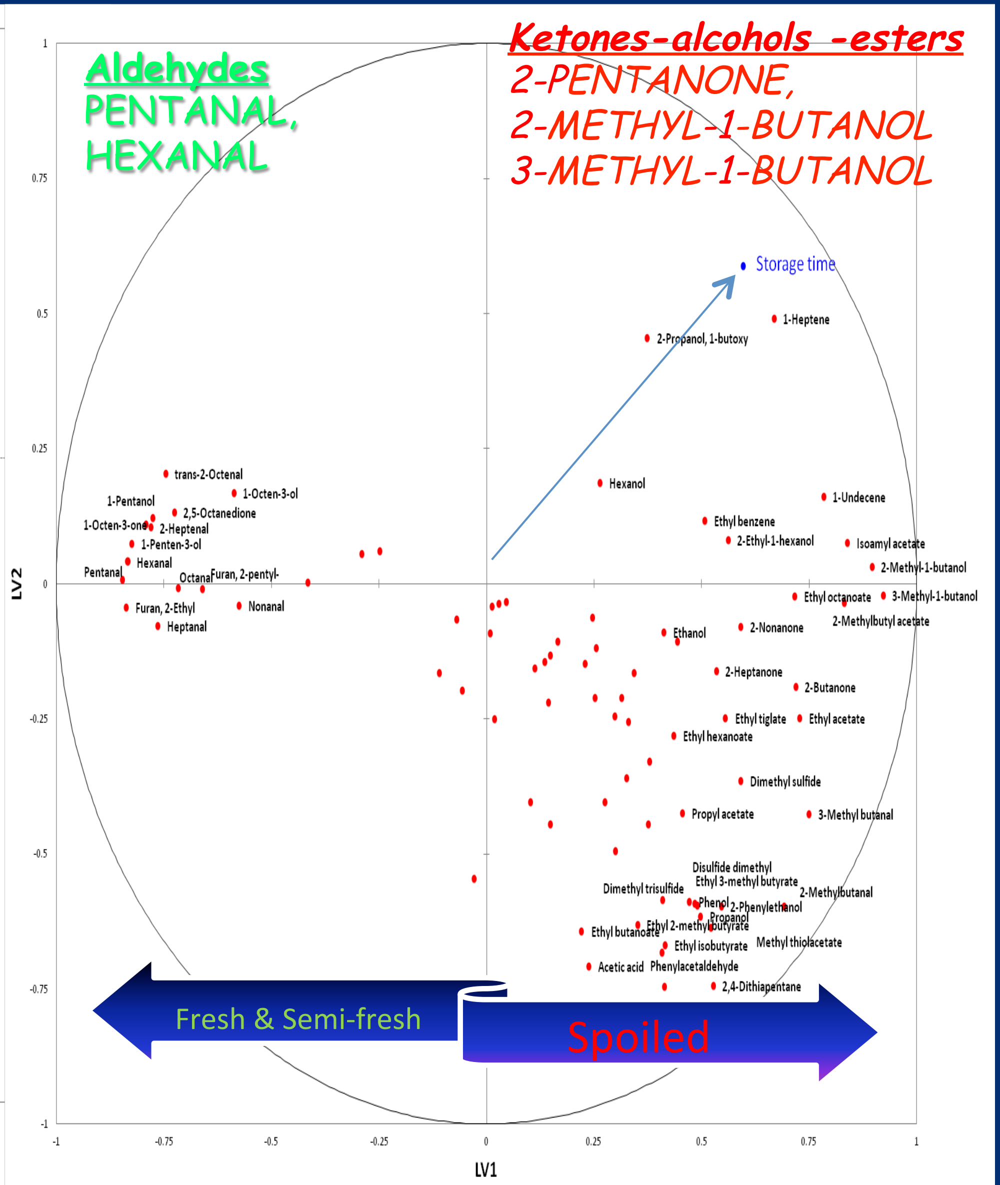
RESULTS; PLS analysis; Plot of scores vs loadings

QUANTITATIVE APPROACH





METHODS & TOOLS; QUANTITATIVE APPROACH

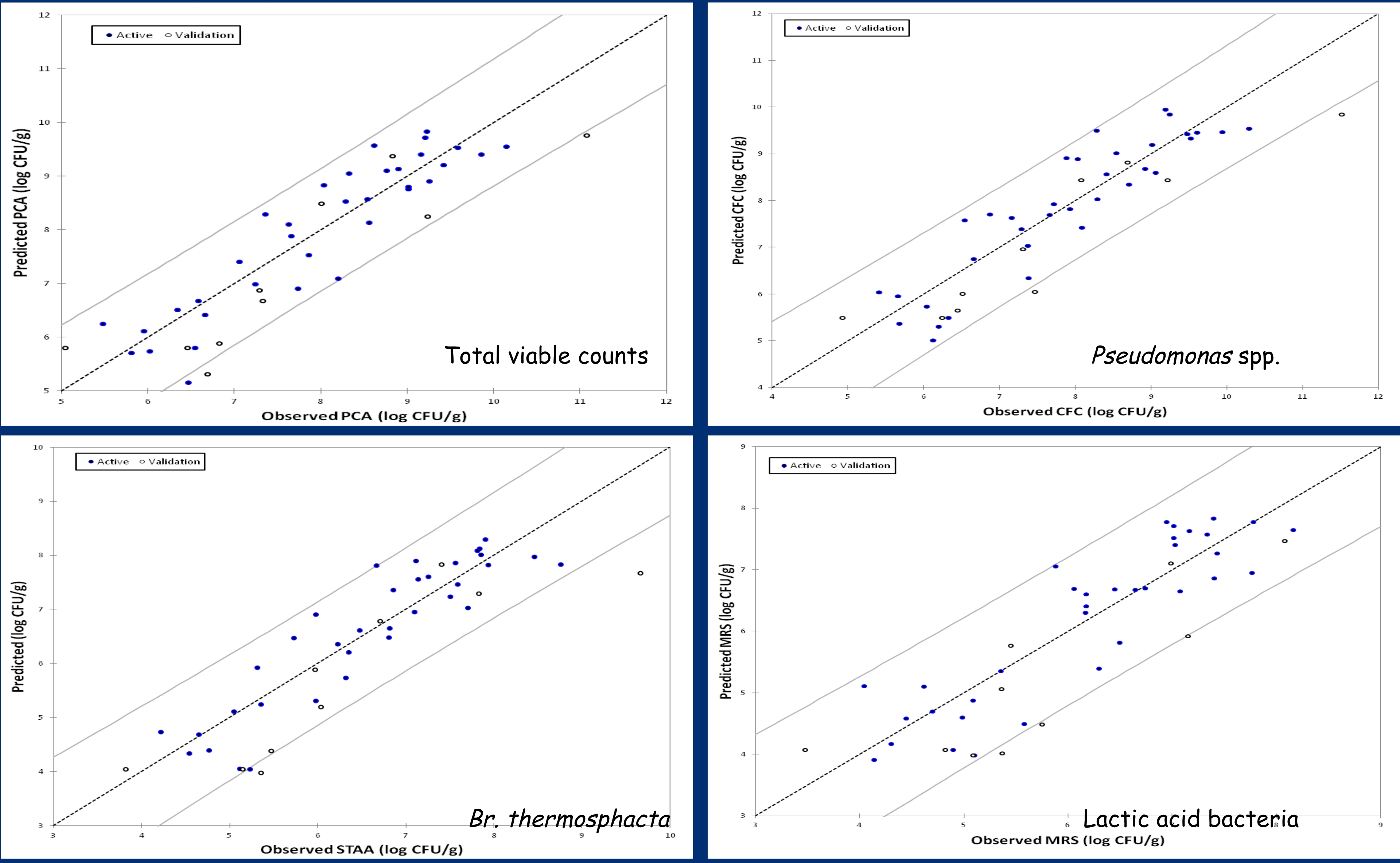
Pork or beef stored under air, MAP & active packaging
(0, 5, 10, and 15°C)

Collection of GC/MS spectral data
(Areas under peaks)

1st Principal components analysis (PCA)
(Investigation of the variables that significantly fluctuate during storage)

Partial least squares regression (PLS-R)
Predict the counts of the different microbial groups

RESULTS; QUANTITATIVE APPROACH - Estimation of microbial counts based on VOCs



Blue points; calibration data set – White points; validation data set.
The majority are within the 95% confidence interval

METHODS & TOOLS; QUALITATIVE APPROACH

Pork or beef stored under air, MAP & active packaging (0, 5, 10, and 15°C)

Collection of GC/MS spectral data (Areas under peaks)

↓

1st Principal components analysis (PCA)

(Investigation of the variables that significantly fluctuate during storage)

↙

Factorial Discriminant Analysis (FDA)

Predict the spoilage status of a sample; fresh, semi-fresh, and spoiled

RESULTS; GC/MS (beef)

QUALITATIVE APPROACH

Qualitative discrimination of the classes- Factorial Discriminant Analysis

True class	Estimated class			Sensitivity (%)
	Fresh	Semi-fresh	Spoiled	
Fresh (*n* = 27)	**21**	0	6	77.78
Semi-fresh (*n* = 16)	1	**10**	5	62.50
Spoiled (*n* = 29)	1	2	**26**	89.66

Total correct classification: 79.17%

This is a simple method for data analysis but when apply non-linear statistical approaches the sensitivity is increased

METHODS & TOOLS; minced beef

QUANTITATIVE APPROACH

Pork or beef stored under air, MAP & active packaging
(0, 5, 10, and 15°C)

Collection of the HPLC or GC/MS spectral data (Areas under peaks)

↓

1st Principal components analysis (PCA)

(Investigation of the variables that significantly fluctuate during storage)

↘

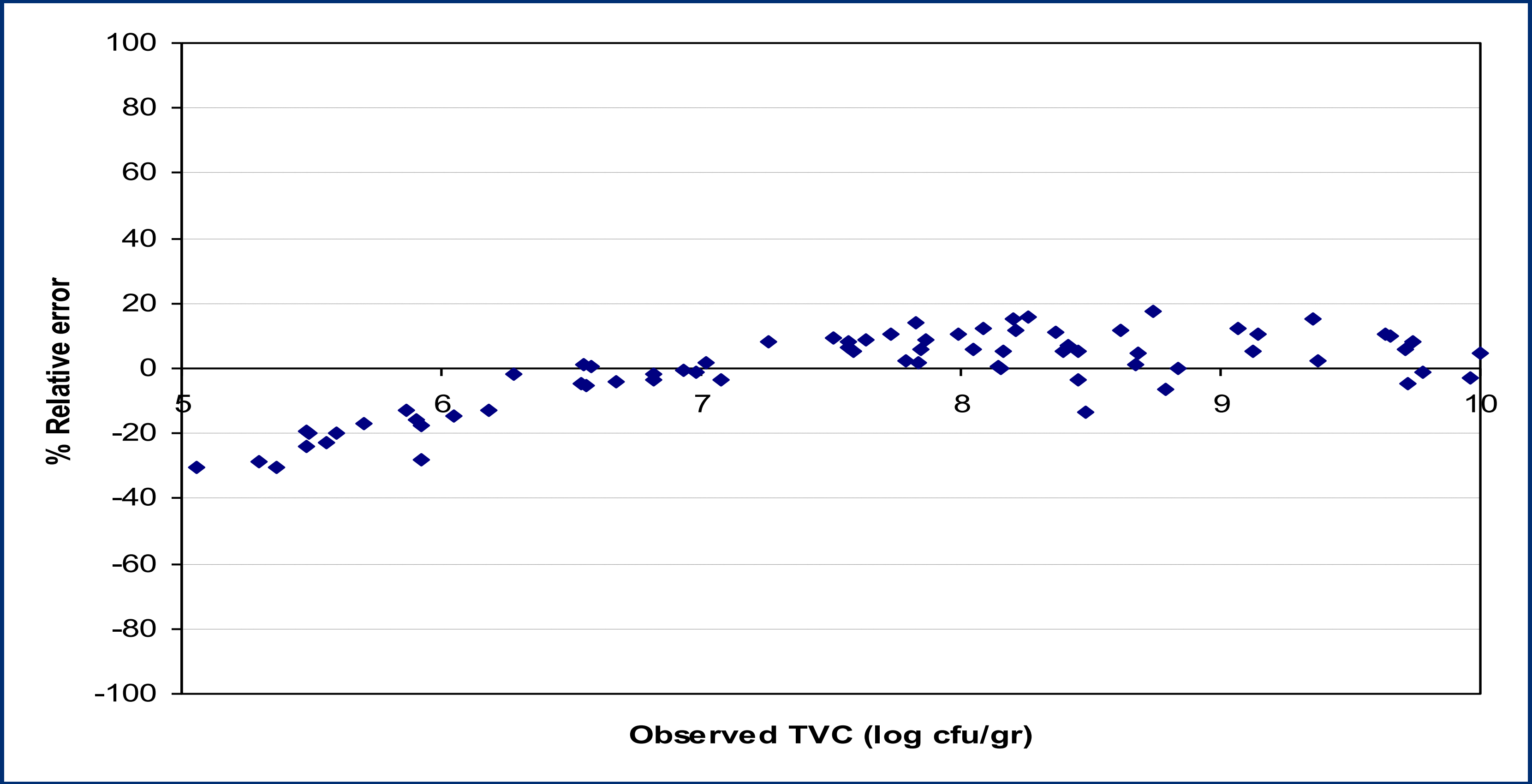
Partial least squares regression (PLS-R)

Predict the counts of the different microbial groups

RESULTS; GC/MS (beef)

QUANTITATIVE APPROACH

Estimation of the microbial population – TVC



Percent relative errors (% RE) between Observed and Predicted counts of the total viable counts (TVC) as estimated from the full cross validated values of the PLS-R model

91.78 % of the estimated values lies between the ± 20% RE

RESULTS; GC/MS

QUANTITATIVE APPROACH

The performance of the models using the cross-validated estimates from the PLS-R models

Microbial group	B_f [a]	A_f [b]	% of the samples in ±20% RE[c] zone	% of the samples in ±10% RE zone	RMSE[d]
TVC	1.001	1.093	91.78	76.71	0.81
Pseudomonas spp	1.012	1.125	83.56	60.27	0.97
Br. thermosphacta	1.010	1.140	75.34	58.90	0.94
LAB	1.008	1.099	90.41	65.75	0.81
Enterobacteriaceae	1.008	1.112	80.82	65.75	0.84
Yeasts and moulds	1.009	1.111	84.93	78.08	0.78

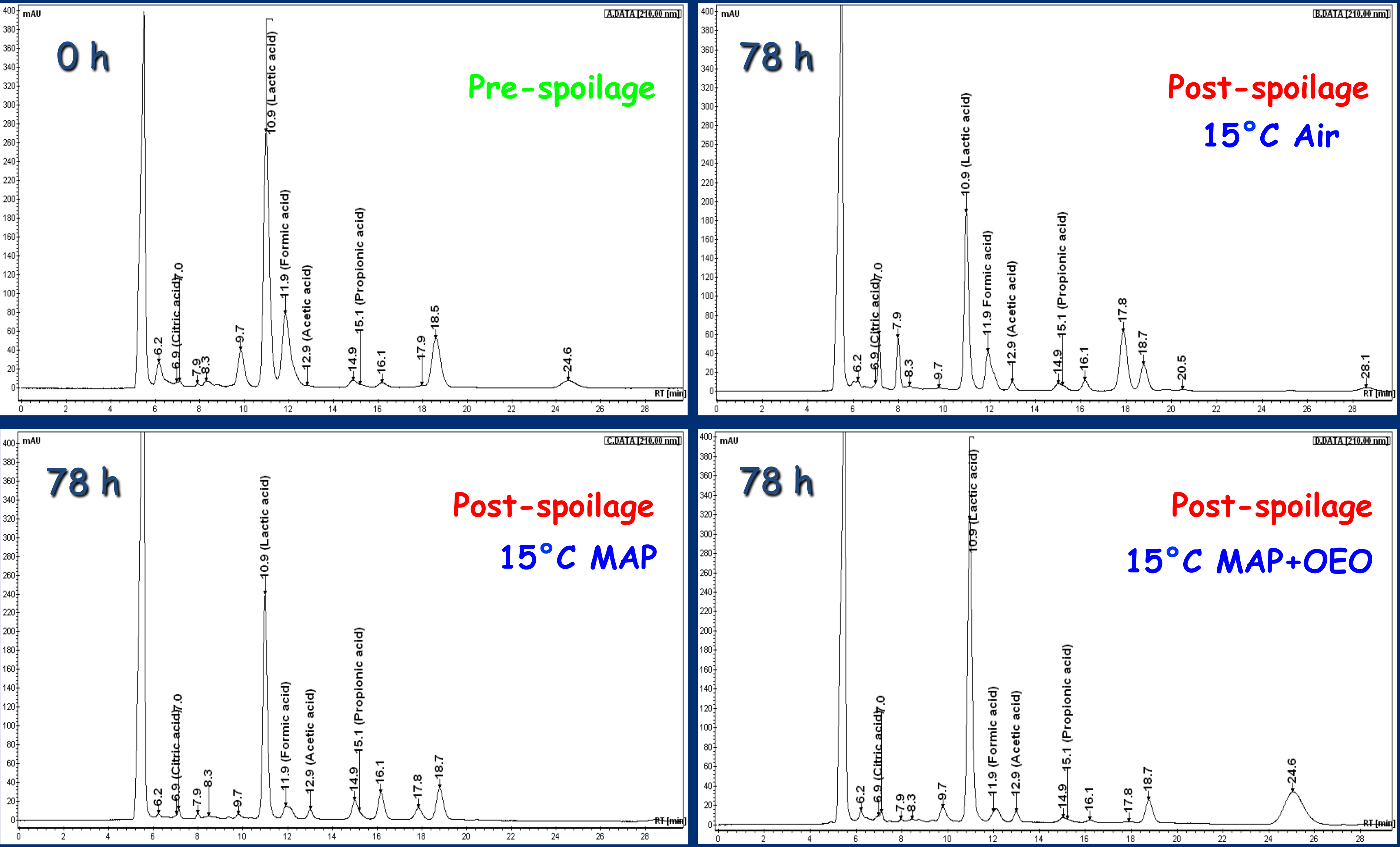
[a] Bias Factor, [b] Accuracy Factor, [c] Relative Error (%), [d] Root Mean Square Error

Conclusions; GC/MS

- Many of the identified and semi-quantified compounds were correlated with the sensory scores, depicting possible spoilage indicators

- The HS/SPME- GC/MS analysis of the volatile compounds of meat could be a potential analytical technique for monitoring the quality and the microbial load of meat regardless of storage conditions

RESULTS; HPLC (beef)



17 pure peaks were selected for analysis ; RT of 6.2, 6.9 (citric acid), 7.0, 7.9, 8.3, 9.7, 10.9 (lactic acid), 11.9 (formic acid), 12.9 (acetic acid), 14.9, 15.1 (propionic acid), 16.1, 17.8, 18.6, 20.5, 24.6 and 28.1.

RESULTS; HPLC (beef) QUALITATIVE APPROACH

Applying Discriminant Function Analysis (DFA) on HPLC data;

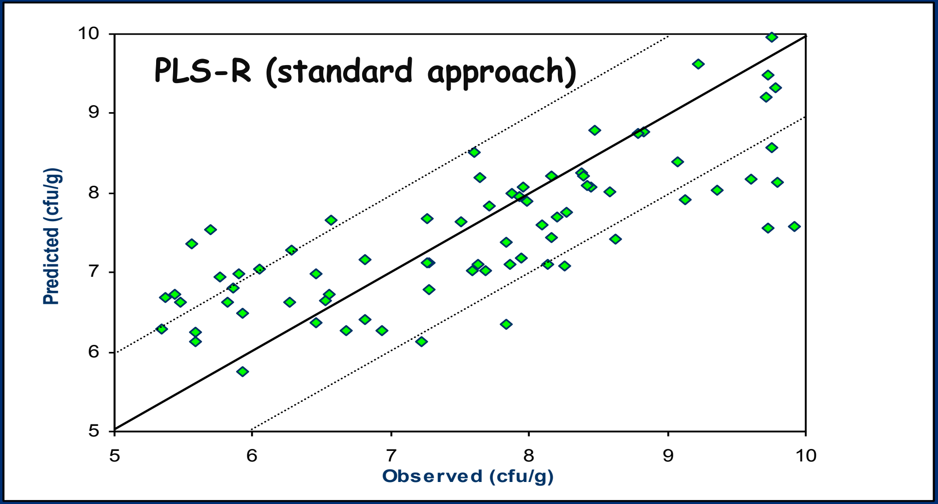
Confusion matrix for the cross-validation

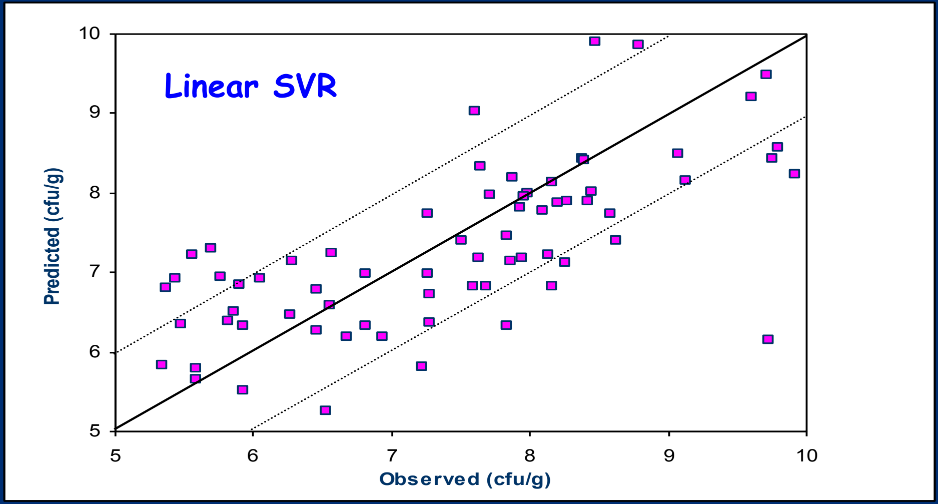
True class	Predicted class: Fresh	Predicted class: Semi-fresh	Predicted class: Spoiled	Sensitivity (%)
Fresh (*n* = 26)	**23**	2	1	88.46
Semi-fresh (*n* = 11)	0	**10**	1	90.91
Spoiled (*n* = 38)	2	2	**34**	89.47

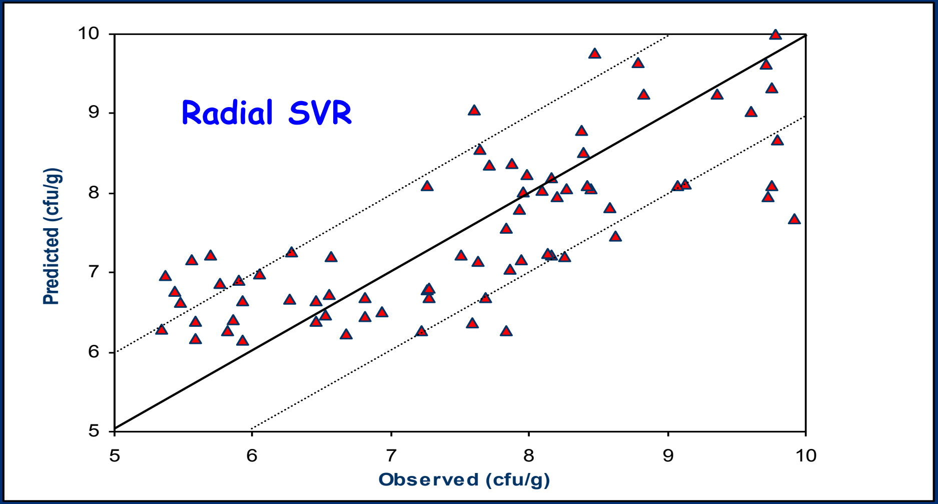
Overall correct classification (accuracy): 89.33%

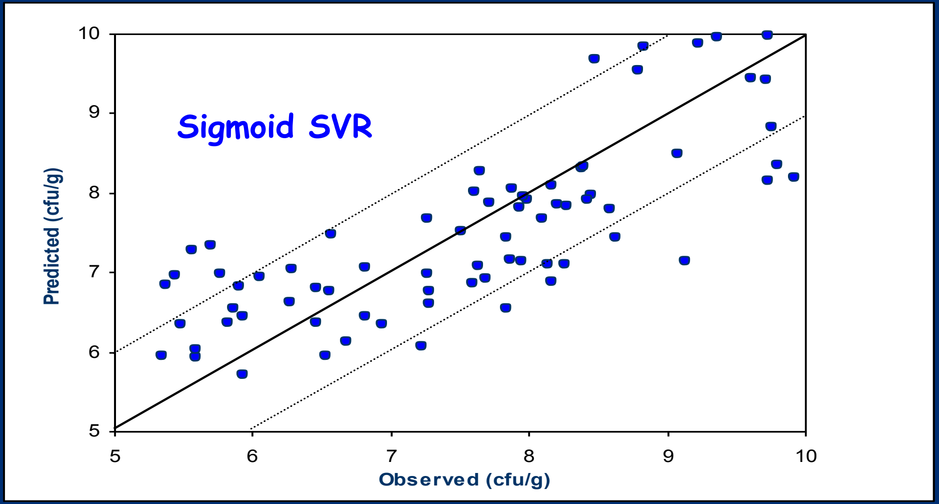
RESULTS; Comparison of the estimated microbial counts using Support Vector Machines (SVM) regression vs. PLS-R (beef)

QUANTITATIVE APPROACH









By applying different computational analysis methods we do not get always better results that can explain the phenomenon.

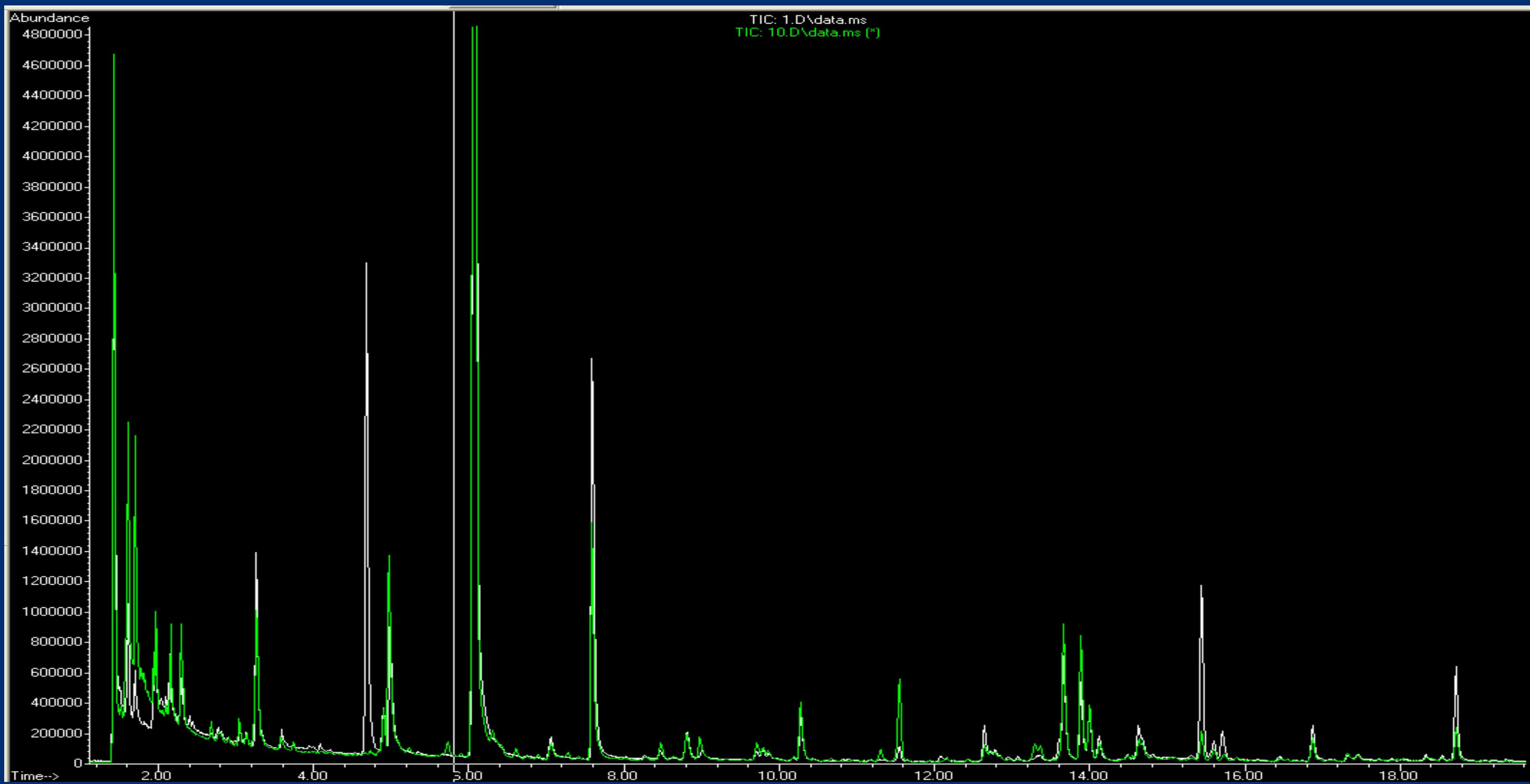
Conclusions; HPLC

- Good correlation of the sensorial evaluation of spoilage with the dynamic changes of the chromatographic areas of organic acids at different time intervals.

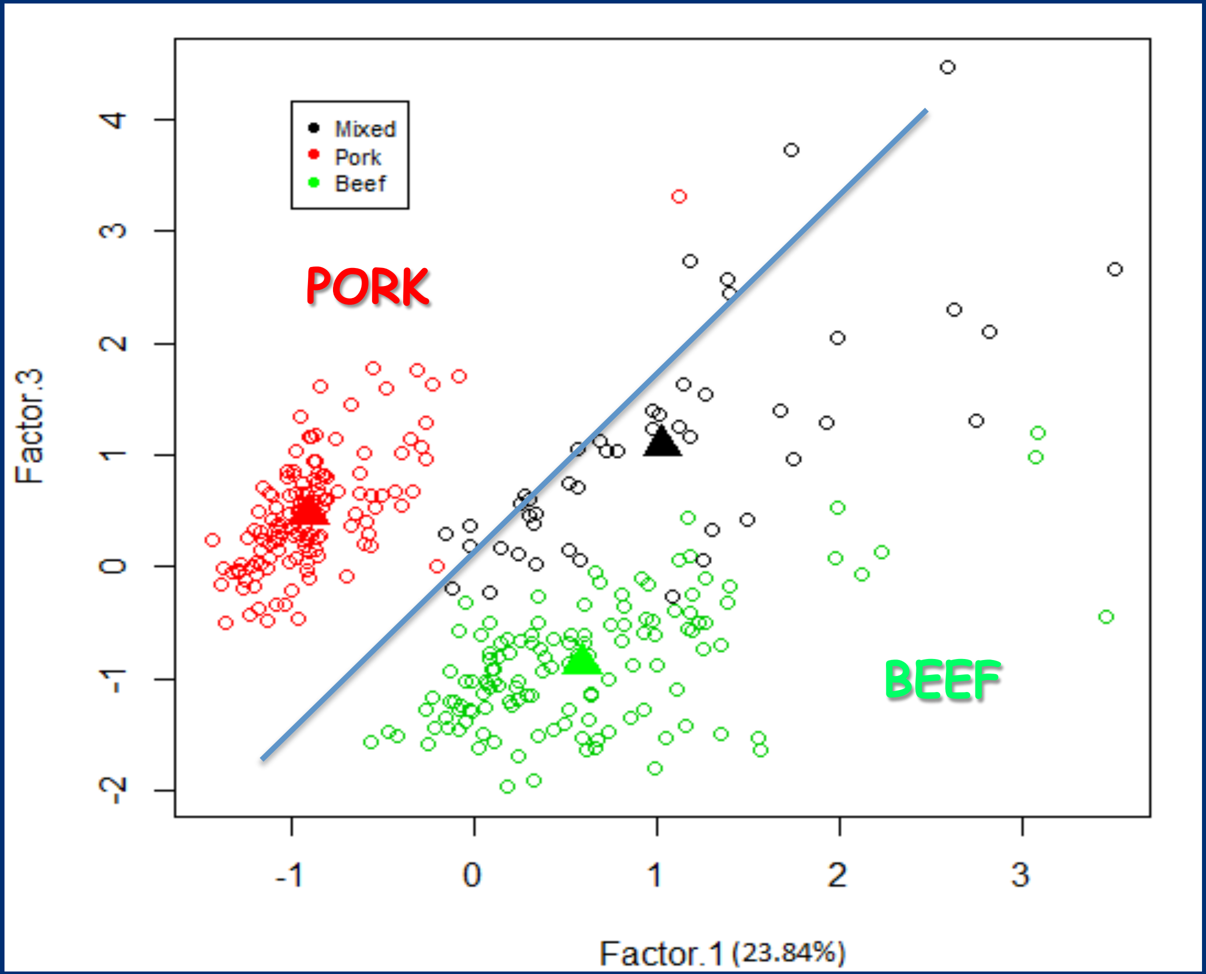
- HPLC analysis of organic acids can be proved as a potential technique for meat analysis in predicting the spoilage status and the microbial load of a meat sample regardless of the storage conditions.

Minced Beef adulterated with minced pork meat

AUA



Typical GC/MS chromatogram; Green line Pork samples – white line beef samples

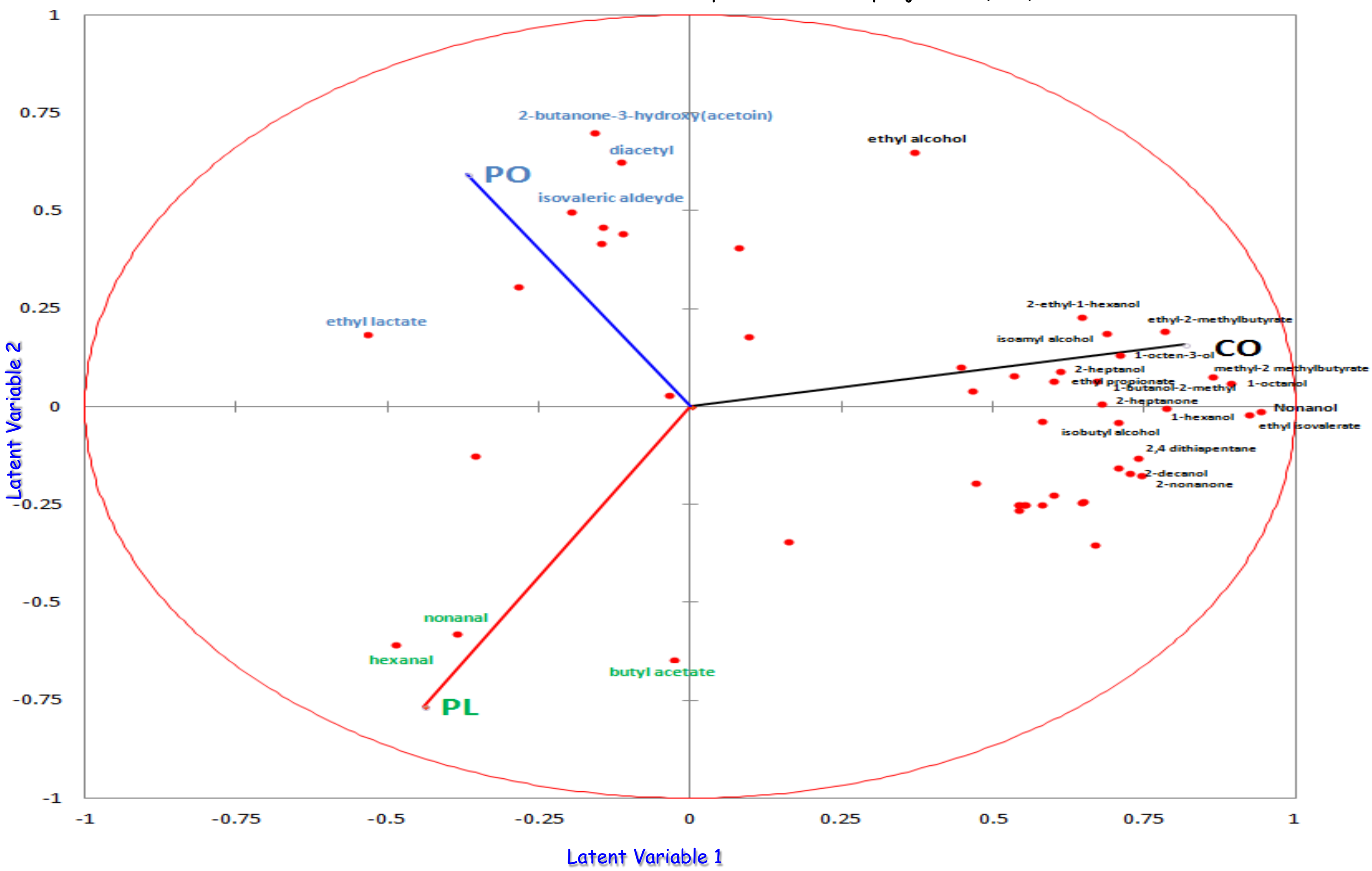


Principal Component Analysis on Autoscaled values of Calibration
Red circles: Pork Samples,
Black: Mixed/Adulterated,
Green: Beef Samples;

Calibration data; 317samples
Validation data; 140 samples
Overall correct classification 99,3%

Discriminating different Marinated poultry products

Variable importance in the projection (VIP) > 1.0



Bi-plot of marination treatments and VOCs by the first two latent variables after PLS-DA analysis indicating potential biomarkers for chicken samples marinated in pomegranate juice (PO), pomegranate and lemon juices (PL), and without marination (CO).

2nd CASE STUDY ;

olive fermentation

Purpose: To investigate the effect of different acidification treatments on the microbiological and biochemical profile of fermentation processes.

Fermentation of green table olives

- ✓ Olives: Conservolea variety, Spanish style processing
- ✓ Lye treatment: 1.7% (w/v) NaOH for 10-12 hrs
- ✓ Brine: Initial salt concentration 10% (w/v, NaCl)
- ✓ Washing scheme: 4, 8, 12 hrs (traditional) vs. 4 and 12 hrs (alternative)
- ✓ Fermentation process: Spontaneous fermentation
- ✓ Acidification treatments: (a) CO_2 flux @ 1 L/min for 1 hr
  - (b) 0.1% (v/v) lactic acid + 0.014% (v/v) HCl
  - (c) no acidification (control)

Experimental procedure – Analyses

Brine

- Microbiological Analysis
  - Lactic acid bacteria (MRS)
  - Yeasts (RBC)
  - *Enterobacteriaceae* (VRBGA
- Physicochemical Analysis
  - pH, titratable acidity
  - Organic acids (HPLC)
  - Volatile compounds (headspace GC)
- Organoleptic Assessment
  - Off-Odour, Saltiness, Bitterness, Acidity, Firmness

Application of multivariate analysis in the fermentation process

X-matrix (independent variables)

Variables determined during the course of fermentation

Microbiological data
Lactic acid bacteria, Yeasts

Organic acids
Lactic acid, Acetic acid
Citric acid, Succinic acid, Malic acid

Volatile compounds
Ethanol, Methanol, 2-Butanol, Propanol, Acetaldehyde, Ethyl-acetate, Dimethyl-sulphite

→

Unsupervised & Supervised

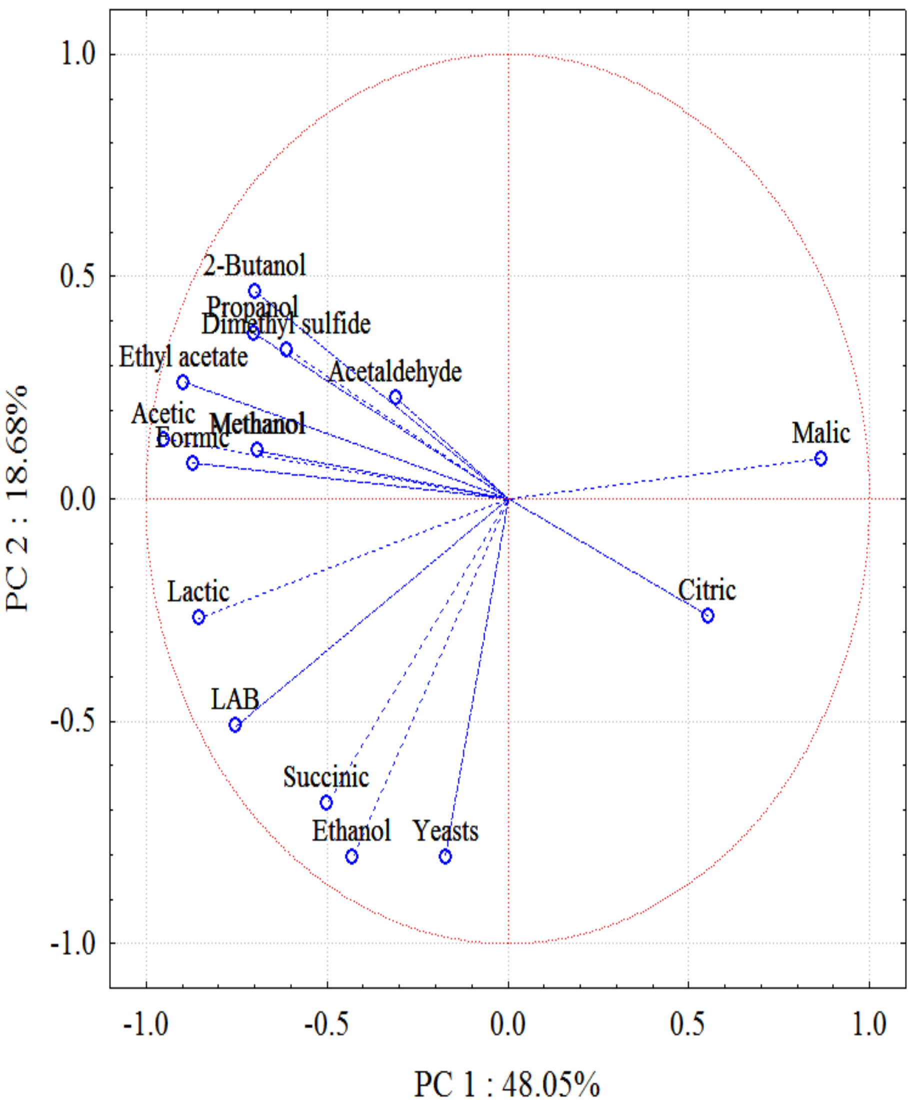
Principal Components Analysis (PCA)

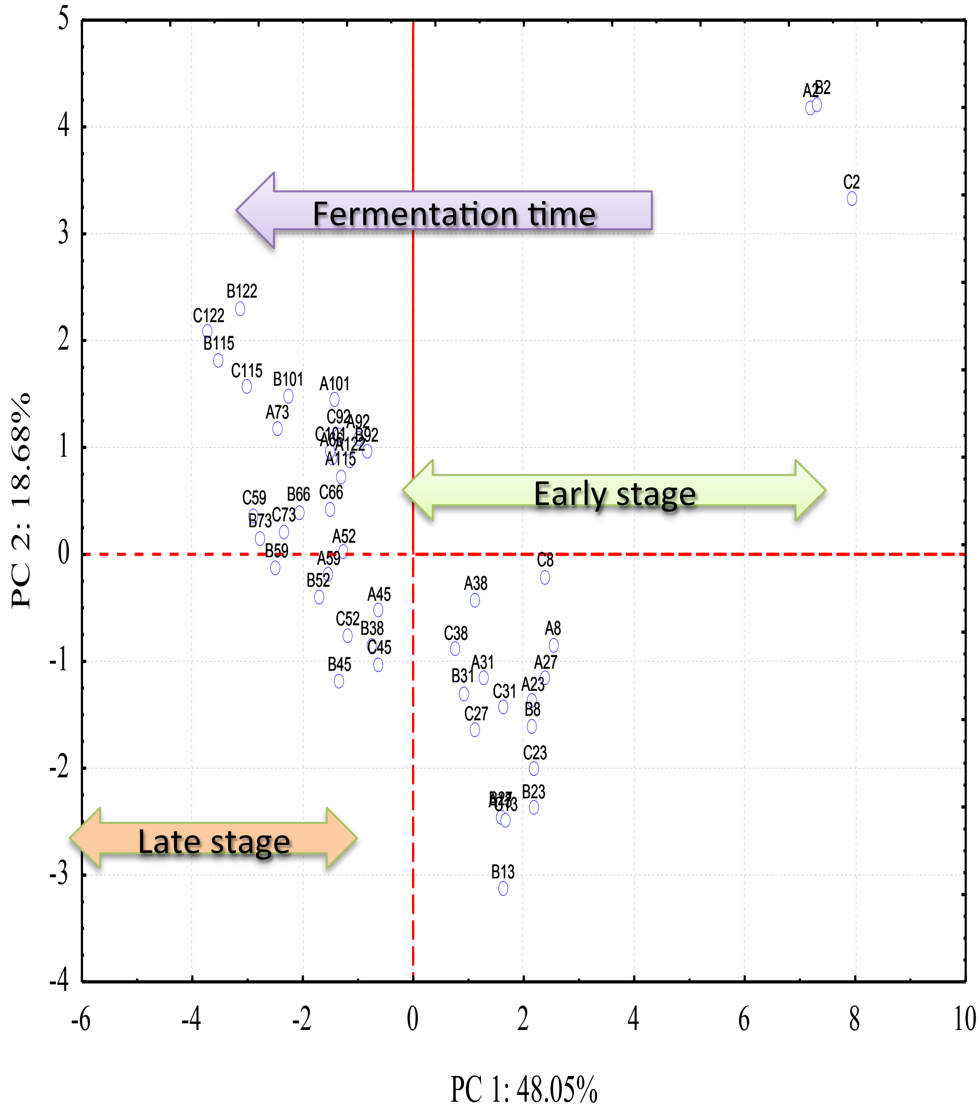
Investigate any underlying relationships among the heterogeneous variables measured

Discriminant Function Analysis (DFA)

Discriminate the three processes based on their holistic fingerprint of microbiological and biochemical data

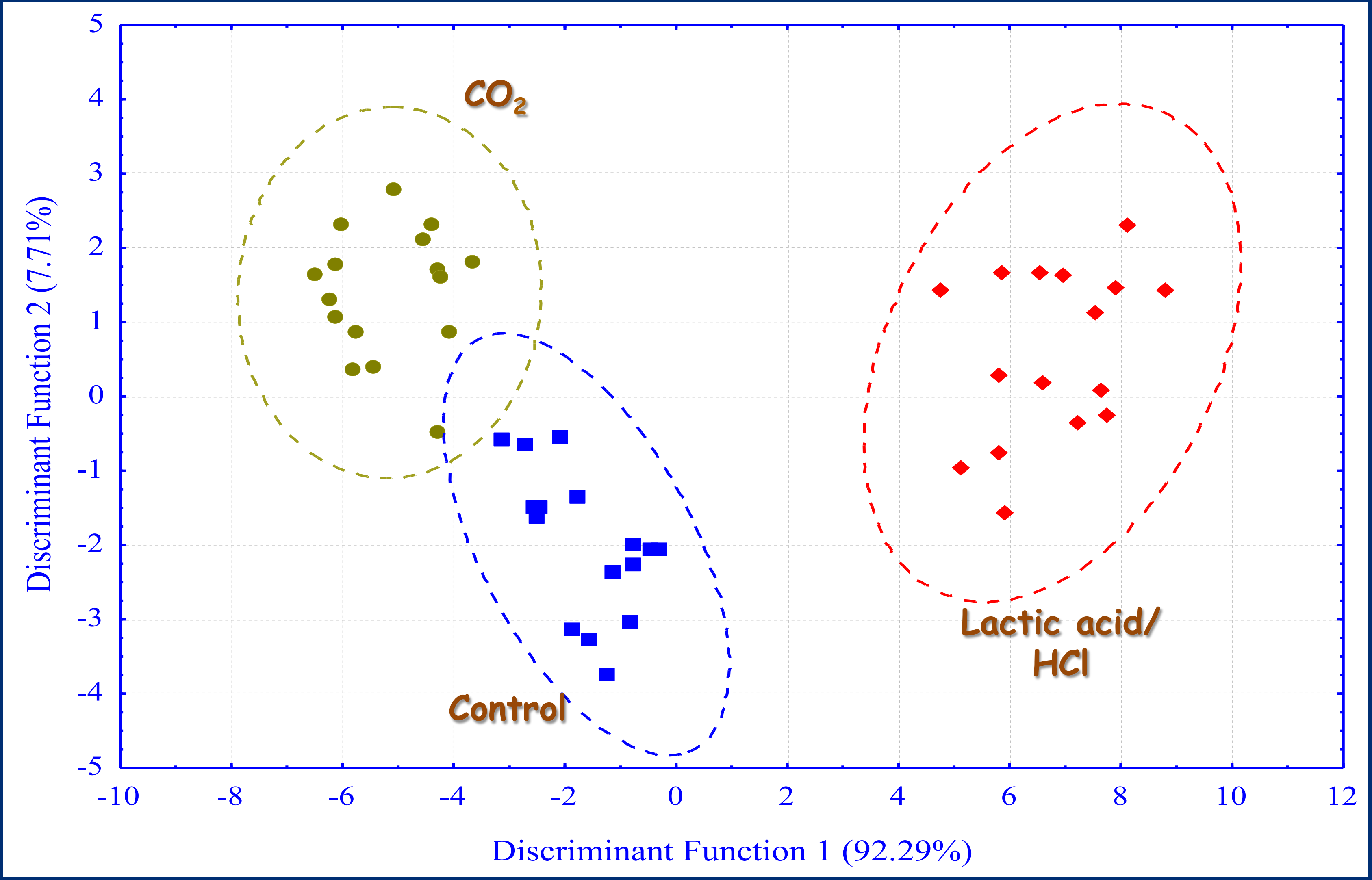
RESULTS; Principal Components Analysis (PCA)





Plot of loadings and scores

RESULTS – Discriminant Function Analysis (DFA)



DFA plot for the three fermentation processes

Conclusions

- PCA analysis could be used effectively, as an unsupervised method, to incorporate all the microbiological and physicochemical measurements throughout the fermentation and describe the evolution of the process in terms of time.

- DFA could effectively discriminate, as a supervised method, the different processed olives based their microbiological and physicochemical characteristics attained throughout fermentation.

3rd CASE STUDY ;

Pasteurized vanilla cream

Purpose: **To define spoilage indices during storage at different temperatures using GC/MS**

METHODS & TOOLS

Product : pasteurized vanilla cream

Storage temperature : 4, 8, 12, and 15°C

Microbiological analysis : Total viable counts (TVCs)

pH monitoring

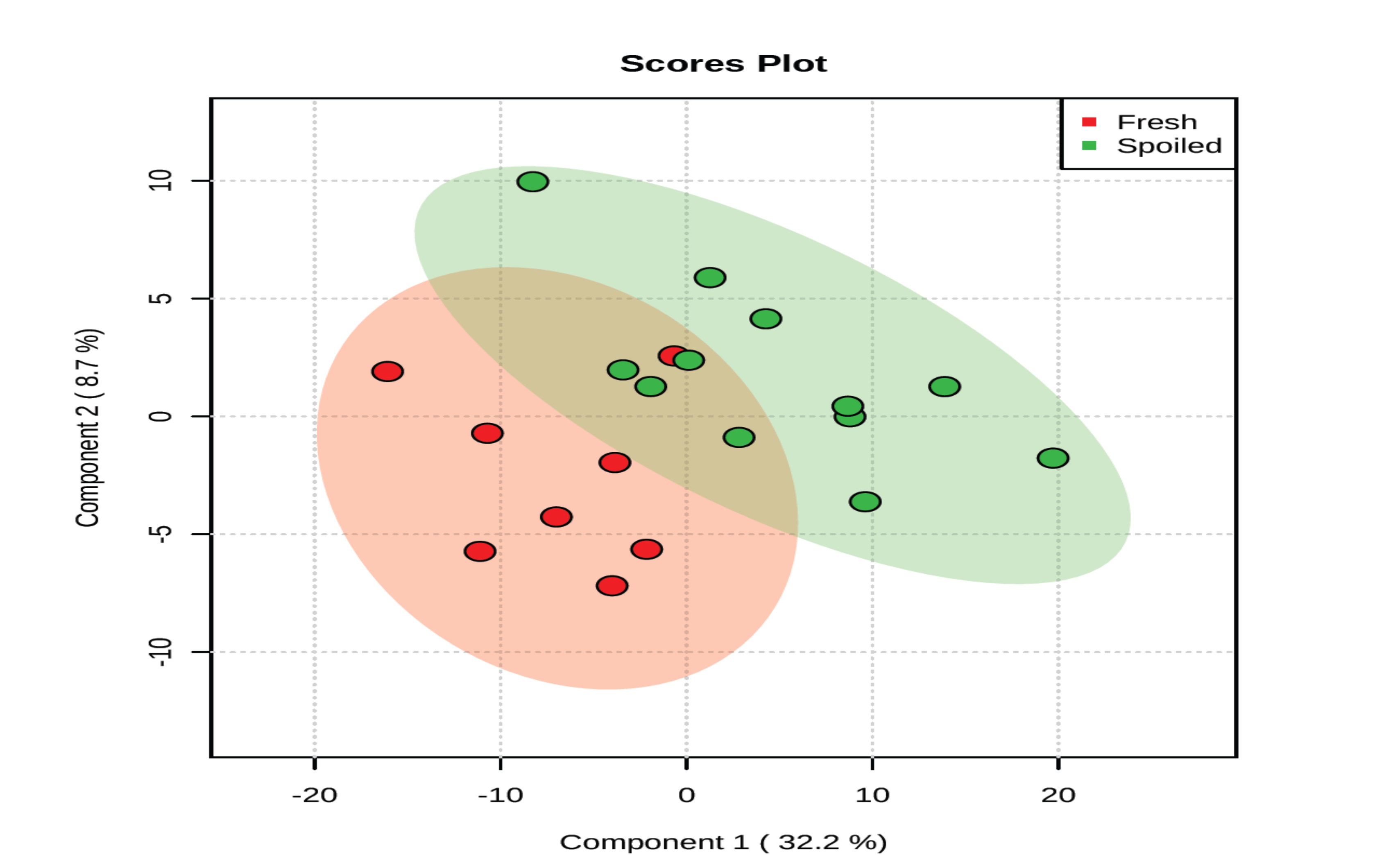
Organoleptic assessment : Spoilage detection based on changes in colour, odour and taste

Score range 1-3; 1=Fresh (TVC<4.5 log CFU/g), 2-3=Spoiled (TVC>4.5 log CFU/g)

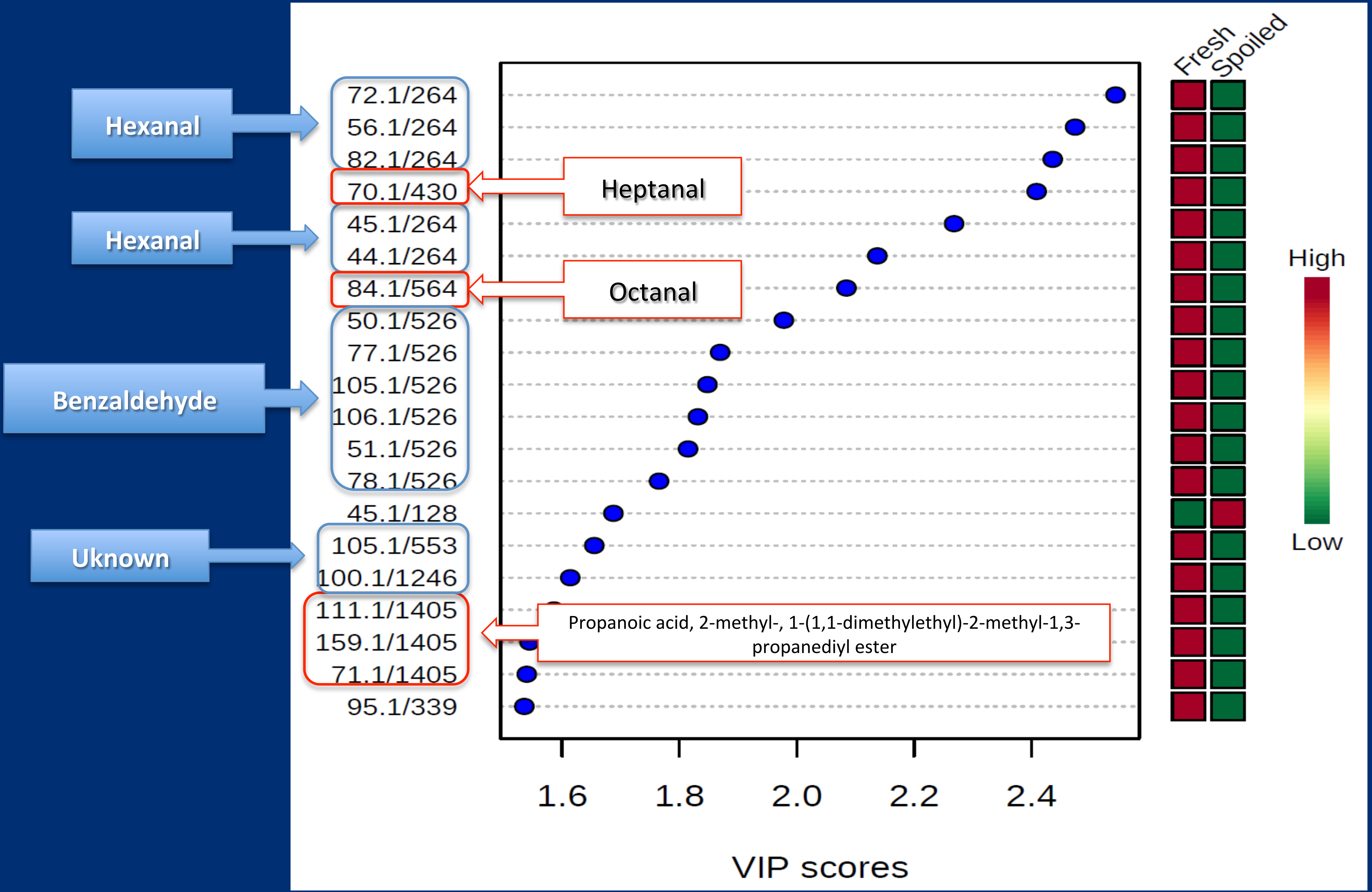
GC/MS analysis : Collection of data from GC/MS to monitor biochemical changes in vanilla cream during storage. Analysis undertaken by MetaboloAnalyst 3.0 (www.metaboanalyst.ca)

Xia, J., Mandal, R., Sinelnikov, I., Broadhurst, D., Wishart, D.S., 2012. MetaboAnalyst 2.0 - a comprehensive server for metabolomic data analysis. Nucleic Acids Research 40, W127-W133.

PLS analysis for discrimination (QUALITATIVE APPROACH) between fresh and spoiled samples at 12 and 15°C

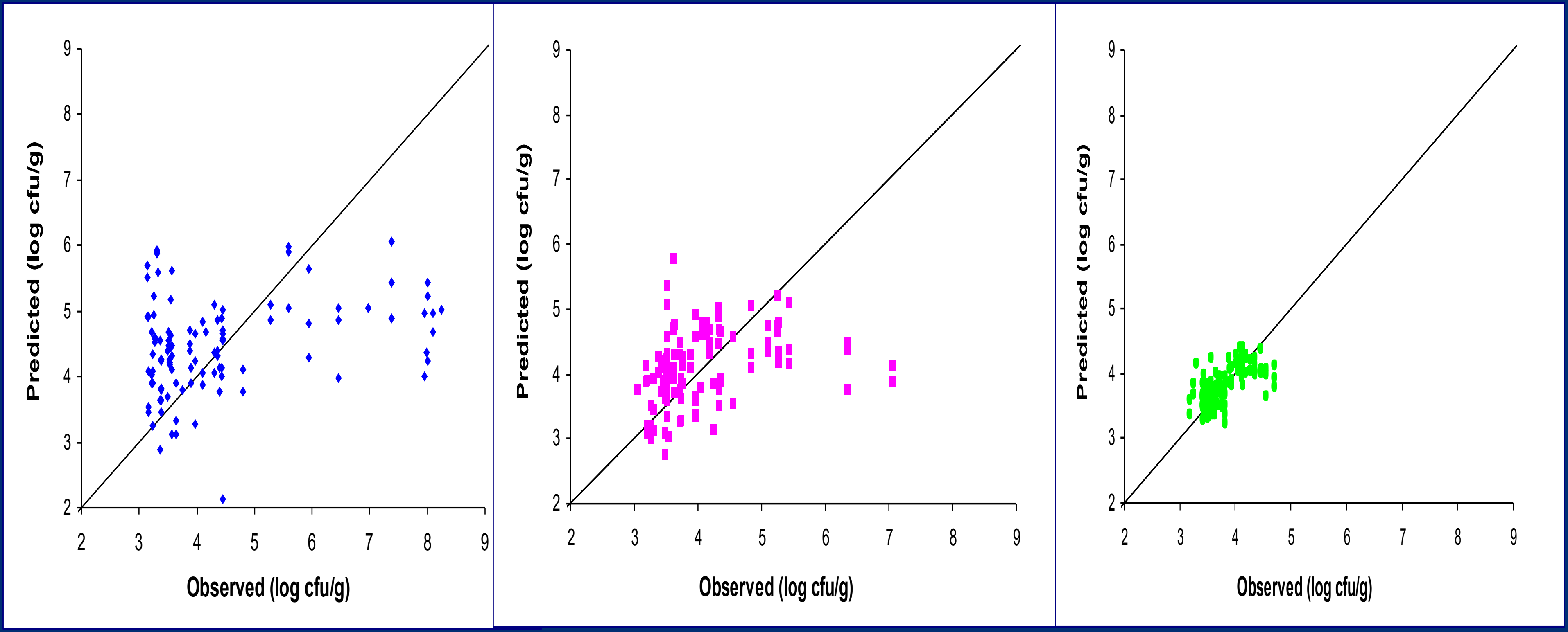


PLS analysis for discrimination between fresh and spoiled samples



Estimating Safety with FTIR (Fingerprints as Metabolomics)

Observed vs. predicted counts of *Salm*. Enteritidis as estimated from the validated values of the k- PLS models for the aerobic (a), MAP (b) and MAP/ OEO (c) packaging conditions



Data mining in food science

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Review

Data mining derived from food analyses using non-invasive/non-destructive analytical techniques; determination of food authenticity, quality & safety in tandem with computer science disciplines

CrossMark

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GENERAL CONCLUSIONS

Metabolomics have a great potential to be used for the benefit of:

(i) The consumer
(ii) Inspection authorities and
(iii) Food industries

Future Challenges

- Build intensive databases that will incorporate as much variability of the foodmatrix as possible.
- Apply other data analysis techniques (except PLS) to take into account the non linear nature of data.
- Extensive validation of models with independent experiments.

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Thank You for Your attention