

**CHEMOMETRIC EVALUATION ON PROFILES OF LARD AND
SELECTED EDIBLE FATS AFTER HEATING-PROCESS USING
SPECTROSCOPY AND CHROMATOGRAPHY TECHNIQUES**

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AUTHOR DECLARATION

I hereby declare that the work in this thesis is my own except for quotations and summaries, which have been duly acknowledged.

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ABSTRAK

Tujuan penyelidikan ini adalah menilai profil lemak babi menggunakan kaedah kemometriks untuk mendiskriminasikan lemak babi daripada jenis lemak lain setelah proses pemanasan dan penentuan biomarker dalam lemak babi. Dalam penyelidikan ini, dua jenis persampelan dilakukan. Pertama, sejumlah 270 sampel lemak babi daripada lemak perut (BL), lemak belakang (BK) dan lemak bahu (SF) dikumpulkan dari wilayah utara, selatan dan tengah, Semenanjung Malaysia dan diuji menggunakan teknik FTIR. Penilaian secara kemometriks ke atas profil lemak babi dilakukan menggunakan PCA dan dilanjutkan dengan menggunakan teknik Hotelling T^2 . Persamaan vektor skor ditemui pada 3PC pertama (99.5% selang keyakinan) dan berjaya disahkan oleh projeksi PCA. Ini menunjukkan profil FTIR bagi lemak babi adalah serupa bagi semua wilayah dan bahagian badan. Kedua, untuk tujuan diskriminasi, sebanyak 60 sampel-sampel lemak dari babi, ayam, lembu, kambing dan tumbuhan telah disediakan menggunakan dua belas protokol proses pemanasan (pada suhu 120 °C, 180 °C, 240 °C selama 0.5, 1, 2 & 3 jam). Lemak-lemak haiwan dan tumbuhan tanpa pemanasan juga termasuk dalam tambahan kajian ini. Selepas proses pemanasan, sampel-sampel lemak dianalisis menggunakan FTIR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, GC-FID dan LC-MS/MS. Diskriminasi lemak-lemak dilakukan menggunakan teknik-teknik pengkelasan multivariasi (LDA, MDA, QDA & SVM) dan regresi multivariasi (OSC-PLSR, PCR & PLSR) pada FTIR dan $^1\text{H-NMR}$ data. Pengkelasan multivariasi mendapati MDA, QDA, dan SVM pada $^1\text{H-NMR}$ memberikan keputusan yang terbaik untuk pengelasan lemak babi daripada lemak-lemak lain. Bagi regresi multivariasi, keputusan OSC-PLSR pada FTIR (R^2 , $adj. R^2$, RMSEC, RMSEV & MSE; 0.985, 0.984, 0.049, 0.051 & 0.056) mengatasi prestasi keputusan OSC-PLSR pada $^1\text{H-NMR}$. Akhir sekali, pemprofilan lemak babi oleh $^{13}\text{C-NMR}$, GC-FID dan LC-MS/MS untuk menentukan biomarker lemak babi telah dilakukan menggunakan teknik PCA. Data $^{13}\text{C-NMR-PCA}$ menunjukkan lemak babi dapat dibezakan dengan lemak ayam pada C-2 oleh isomer TAG yang dikaitkan dengan resonan δ 34.21 dan δ 62.10. Manakala, data GC-FID-PCA mendapati bahawa lemak haiwan dan lemak tumbuhan boleh dibezakan selepas degradasi isomer asid lemak (FAs) *cis* kepada *trans*. Lemak babi yang dipanaskan pada 180 °C (pada 0.5, 1 & 2 jam) didapati berbeza lebih ketara oleh LC-MS/MS-PCA yang disumbangkan oleh asid lemak tepu (SFA) daripada kumpulan lipid diasilgliserol (DAG) dan asid fosfatidik (PA). Aplikasi kemometrik didapati berjaya mendiskriminasikan lemak babi dari lemak-lemak lain setelah proses pemanasan dan biomarker FAs yang dikenalpasti secara tentatif.

ABSTRACT

This research aims to evaluate the profile of lard using the chemometric method to discriminate lard from other types of fat after the heating-process and determination of biomarkers in lard. In this research, two types of samples were conducted. First, a total of 270 lard were collected from belly fats (BL), back fats (BK), and shoulder fats (SF) from northern, southern, and central regions of Peninsular Malaysia, which were measured using FTIR. PCA utilised the chemometrics evaluation on lard profiles using PCA and extended Hotelling T^2 . The scores vectors were found inside Hotelling T^2 eclipses at first 3 PCs (99.5% confidence interval) and successfully validated by PCA projection. This indicates that the FTIR profile for lard is undifferentiated for all regions and body parts. Second, for discrimination purposes, a total of 60 fats, lard, chicken, beef, mutton, and plant have undergone twelve heating-process protocols (at 120 °C, 180 °C, 240 °C for 0.5, 1, 2 & 3 hrs). In addition, each species without any heating was included in this study. After the heating-process, fat samples were analysed using FTIR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, GC-FID, and LC-MS/MS. The classification was performed using multivariate classification (LDA, MDA, QDA & SVM) and multivariate regression (OSC-PLSR, PCR & PLSR) on FTIR and $^1\text{H-NMR}$. Multivariate classification found MDA, QDA, and SVM on $^1\text{H-NMR}$ provided the best results for classifying lard from other fats. In the multivariate regression, the result of OSC-PLSR on FTIR (R^2 , $adj. R^2$, RMSEC, RMSEV & MSEP; 0.985, 0.984, 0.049, 0.051 & 0.056) was found to outperform than the OSC-PLSR on $^1\text{H-NMR}$. Finally, profiling lard by $^{13}\text{C-NMR}$, GC-FID, and LC-MS/MS combined with the PCA were conducted to determine the biomarker of lard. The $^{13}\text{C-NMR-PCA}$ data found that the lard differed against the chicken fats at C-2 of the TAG isomer, denoted by δ 34.21 and δ 62.10 resonances. Meanwhile, the GC-FID-PCA data found that animal fats and plant fats can differ after fatty acids (FAs) degradation of the *cis* into *trans* isomers. The lard heated at 180 °C (at 0.5, 1 & 2 hrs.) was found to differ significantly from others by LC-MS/MS-PCA, contributed by saturated fatty acids (SFA) of the diacylglycerol (DAG) and phosphatidic acids (PA) lipid classes. The application of chemometrics was found to discriminate lard against other fats after the heating-process successfully, and FAs were tentatively identified as biomarkers.

TABLE OF CONTENTS

CONTENT	PAGE
AUTHOR DECLARATION	ii
ACKNOWLEDGEMENTS	iii
ABSTRAK	iv
ABSTRACT	v
الملخص	vi
TABLE OF CONTENTS	vii
LIST OF TABLES	xi
LIST OF FIGURES	xii
LIST OF APPENDICES	xiv
LIST OF UNITS OF MEASUREMENTS	xv
LIST OF SYMBOLS	xvi
LIST OF EQUATIONS	xvii
LIST OF ABBREVIATIONS	xviii
CHAPTER 1: INTRODUCTION	1
1.1 Background of the Study	1
1.2 Statement of the Problem	4
1.3 Research Question	5
1.4 Scope of the Study	5
1.5 Objectives of the Study	7
1.6 The Significance of the Study	7
CHAPTER 2: LITERATURE REVIEW	9
2.1 Chemometrics Technique	9
2.1.1 Principal Component Analysis (PCA)	10
2.1.1.1 Hotelling's T-Squared (T^2)	12
2.1.1.2 PCA Projection	12
2.1.2 Multivariate Classification	14
2.1.2.1 Linear Discriminant Analysis (LDA)	15
2.1.2.2 Support Vector Machines (SVM)	17
2.1.2.3 Evaluation of Multivariate Classification	18
2.1.3 Multivariate Regression	19
2.1.3.1 Principal Component Regression (PCR)	20
2.1.3.2 Partial Least Squares (PLS)	21
2.1.3.3 Orthogonal Signal Correction Partial Least Squares (OSC-PLS)	23
2.1.3.4 Multivariate Regression Coefficient as Important Features Assessment	23
2.1.3.5 Evaluation of Multivariate Regression Analysis	24
2.1.4 Data Pre-processing	27
2.2 Application of Chemometrics in Lard Profiles for <i>Halal</i> Authentication	29
2.2.1 FTIR spectroscopy in Authenticity Studies	31
2.2.2 NMR (^1H & ^{13}C)	39
2.2.3 Chromatography (GC-FID, GC-MS, & HPLC)	41

CHAPTER 3: METHODOLOGY	45
3.1 Experimental Design	45
3.2 Profiling of Lard from Collected Pig Samples at Northern, Central, and Southern Malaysia	47
3.2.1 Chemicals and Materials	47
3.2.1.1 Chemicals	47
3.2.1.2 Lard Samples	47
3.2.2 Instruments	48
3.2.3 Samples Preparation	48
3.2.3.1 Preparation of Lard Samples	48
3.2.3.2 Extraction of Lard Samples	49
3.2.3.3 Samples Preparation for FTIR Analysis	49
3.3 Profiling on Pork (Lard), Chicken, Beef, Mutton, and Plant Fats after Heating-Process	51
3.3.1 Chemicals and Materials	51
3.3.1.1 Chemicals	51
3.3.1.2 FAMEs Standard	51
3.3.2 Samples of Lard and Selected Fats	52
3.3.3 Apparatus and Instruments	52
3.3.4 Sample Preparation of Animals Fats	54
3.3.4.1 Heating-Process Protocols	54
3.3.4.2 Extraction of Fats after Heating-Process	55
3.3.4.3 Sample Preparation of FTIR Analysis	55
3.3.4.4 Sample Preparation of ¹ H-NMR Analysis	56
3.3.4.5 Sample Preparation of ¹³ C-NMR Analysis	56
3.3.4.6 Sample Preparation of GC-FID Analysis (FAs Methylation)	56
3.3.4.7 Sample Preparation of LC-MS/MS Analysis	57
3.3.5 Fats Analysis	58
3.3.5.1 FTIR Analysis	58
3.3.5.2 NMR (¹ H & ¹³ C) Analysis	58
3.3.5.3 GC-FID Analysis	58
3.3.5.4 LC-MS/MS Analysis	59
3.4 Data Analysis	60
3.4.1 Data Pre-processing	60
3.4.1.1 Data of FTIR	61
3.4.1.2 Data of ¹ H-NMR.	61
3.4.1.3 Data of ¹³ C-NMR	61
3.4.1.4 Data of GC-FID	62
3.4.1.5 Data of LC-MS/MS	62
3.4.2 Chemometrics Techniques	62
3.4.2.1 Kennard-Stone (K-S) Algorithm Selection	64
3.4.2.2 Flowchart of Chemometrics Evaluation	65
CHAPTER 4: RESULTS AND DISCUSSION	62
4.1 Profiling of Lard from Collected Pig Samples at Northern, Central, and Southern Malaysia using FTIR combined with Principal Component Analysis (PCA)	62
4.1.1 Introduction	62

4.1.2	Data Pre-processing	69
4.1.3	Principal Component Analysis (PCA)	72
4.1.4	Hotelling T ² Similarity Assessment of MSC-PCA Models	76
4.1.5	Prediction of Lard by MSC-PCA Projection	78
4.2	Discrimination of Pigs (Lard), Chicken, Beef, Mutton, and Plant Fats After Heating-Process using FTIR, ¹ H-NMR, and ¹³ C-NMR with Chemometrics Techniques	84
4.2.1	Introduction	84
4.2.2	Profiling of Lard and Selected Edible Fats After the Heating-Process.	85
4.2.2.1	FTIR	85
4.2.2.2	¹ H-NMR	87
4.2.3	Data Pre-processing	89
4.2.3.1	FTIR	89
4.2.3.2	¹ H-NMR	91
4.2.4	PCA	92
4.2.4.1	PCA of FTIR data	92
4.2.4.2	PCA of ¹ H-NMR data	97
4.2.5	Multivariate Classification (MVC)	99
4.2.5.1	Class Sensitivity	101
4.2.5.2	Class Specificity	102
4.2.5.3	Classification Measures of the MCC.	104
4.2.6	Multivariate Regression (MVR)	105
4.2.6.1	FTIR	105
4.2.6.2	¹ H-NMR	107
4.2.6.3	Comparison between FTIR and ¹ H-NMR Multivariate Regression	108
4.2.7	Correlation Chemical Features of Lard after Heating-Process by OSC-PLSR	110
4.2.7.1	FTIR	110
4.2.7.2	¹ H-NMR	111
4.2.8	Profiling of ¹³ C-NMR Lard vs Chicken fats	114
4.2.9	Data Pre-processing of ¹³ C-NMR Spectra	115
4.2.10	PCA of ¹³ C-NMR Lard vs Chicken fats	117
4.3	Evaluation on Fatty Acids (FAs) of Lard and Selected Fats after Heating-Process using GC-FID and LC-MS/MS combined with Principal Component Analysis (PCA)	121
4.3.1	Gas Chromatography with Flame Ionization Detection (GC-FID)	121
4.3.1.1	Introduction	121
4.3.1.2	Fatty Acids (FAs) Profiling	121
4.3.1.3	PCA of GC-FID	123
4.3.2	Liquid Chromatography with Tandem Mass Spectrometry (LC-MS/MS)	128
4.3.2.1	Introduction	128
4.3.2.2	Profiling of Lard and Selected Fats by LC-MS/MS	128
4.3.2.3	Glycerolipids of the PCA by LC-MS/MS (LC-MS/MS-GL-PCA)	129

4.3.2.4	Glycerophospholipids of the PCA by LC-MS/MS (LC-MS/MS-GPPL-PCA)	133
CHAPTER 5: CONCLUSION AND RECOMMENDATION		137
5.1	Profiling of Lard from Collected Pig Samples at Northern, Central, and Southern in Malaysia using FTIR combined with Principal Component Analysis (PCA)	137
5.2	Discrimination of Pigs (Lard), Chicken, Beef, Mutton, and Plant Fats after Heating-Process using FTIR, ¹ H-NMR, and ¹³ C-NMR with Chemometrics Techniques	138
5.3	Evaluation on Fatty Acids (FAs) of Lard and Selected Fats after Heating-Process using GC-FID and LC-MS/MS combined with Principal Component Analysis (PCA)	140
REFERENCES		142
APPENDICES		163

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LIST OF TABLES

Tables	Page
Table 2.1: Application Chemometrics and FTIR on Profiles Lard.	38
Table 3.1: Chemicals.	47
Table 3.2: Total Pigs Fat of the Body Parts and Regions.	48
Table 3.3: Chemicals.	51
Table 3.4: Heating-Process Protocols.	55
Table 4.1: Comparison between Four Different Significance Levels (α).	77
Table 4.2: Multivariate Classification on FTIR and $^1\text{H-NMR}$.	100
Table 4.3: Statistics for Multivariate Regression.	108
Table 4.4: Wavenumbers Contributed to the Lard.	111
Table 4.5: Summary of the δ by $^1\text{H-NMR-OCR-PLS}$.	113
Table 4.6: <i>X</i> -correlation Loadings Plot of the GC-FID-PCA.	125
Table 4.7: <i>X</i> -correlation Loadings Plot of All Fats (LC-MS/MS-GL-PCA).	130
Table 4.8: <i>X</i> -correlation Loadings Plot (LC-MS/MS-GL-PCA).	132
Table 4.9: <i>X</i> -correlation Loadings Plot (LC-MS/MS-GPPL-PCA).	134

LIST OF FIGURES

Figures	Page
Figure 2.1: Illustration of Boundaries LDA (left) vs QDA (right).	16
Figure 2.2: Basic Idea of the Kernel Function in SVM.	17
Figure 3.1: Framework of Lard Profiling.	46
Figure 3.2: Chemometrics Technique for Lard Profiles.	66
Figure 3.3: Chemometrics Technique for the Heated Lard Profiles.	67
Figure 4.1: Comparison of the Untreated and Pre-processing FTIR Spectra.	69
Figure 4.2: Comparison of the FTIR-PCA Before and After Pre-processing.	72
Figure 4.3: Determination of Outliers by MSC-PCA.	76
Figure 4.4: Projection of the Test Set into MSC-PCA.	79
Figure 4.5: Influence Graph Plots F-Residual vs Hotelling T^2 .	80
Figure 4.6: Total Residual Variance of MSC-PCA.	81
Figure 4.7: Comparison of FTIR Spectra.	85
Figure 4.8: The Basic Structure of TAG.	87
Figure 4.9: ^1H -NMR Spectra.	88
Figure 4.10: Comparison of Normalised vs 2 nd DSG FTIR Spectra.	89
Figure 4.11: ^1H -NMR Spectra After Pre-processing.	91
Figure 4.12: The Normalised-PCA Overview of the FTIR Data.	93
Figure 4.13: The 2 nd DSG-PCA Overview of the FTIR Data.	94
Figure 4.14: The ^1H -NMR-PCA of Untreated and After Pre-processing.	97
Figure 4.15: Multivariate Regression on FTIR data.	105
Figure 4.16: Multivariate Regression on ^1H -NMR.	107
Figure 4.17: Variables Selection by p -Correlation.	112
Figure 4.18: Stacked individual ^{13}C -NMR Spectra of Lard vs Chicken Fats.	115
Figure 4.19: ^{13}C -NMR Spectra of the Lard & Chicken Fats.	116

Figure 4.20: ^{13}C -NMR Spectra After Baseline Pre-Processing.	117
Figure 4.21: ^{13}C -NMR-PCA of the Lard vs Chicken Fats.	118
Figure 4.22: Heatmap of ^{13}C -NMR-PCA.	119
Figure 4.23: TAG Isomers.	120
Figure 4.24: Box Plot of FAs	121
Figure 4.25: GC-FID-PCA.	124
Figure 4.26: Bar Plot Sum of Heat Values.	126
Figure 4.27: The Profiles of Fats by LC-MS/MS.	129
Figure 4.28: GL-PCA on LC-MS/MS Data of All Fats.	129
Figure 4.29: GL-PCA on LC-MS/MS of Lard vs Chicken.	131
Figure 4.30: GPPL-PCA on LC-MS/MS Data of All Fats.	133

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LIST OF APPENDICES

Appendices	Page
Appendix 1: PCA Overview of Untreated FTIR.	163
Appendix 2: Loading Plots of FTIR-PCA on Fats.	164
Appendix 3: Important Variables Selection of FTIR-OSC-PLSR.	165
Appendix 4: Assignment of the Main Resonances in the ^1H -NMR.	166
Appendix 5: Important Variables Selection of ^1H -NMR OSC-PLSR.	167
Appendix 6: Assignment of the Main Resonances in the ^{13}C -NMR.	168
Appendix 7: Estimation of the ^{13}C -NMR.	169
Appendix 8: Standard of FAME Integration.	170
Appendix 9: Typical Chromatogram of Lard.	171
Appendix 10: Most Prominent FAs GC-FID.	172
Appendix 11: Scores Plot of GC-FID-PCA and Clusters.	173
Appendix 12: Lipid Classes of the LC-MS/MS.	174
Appendix 13: Typical Spectra of Glycerolipids (GL).	176
Appendix 14: Typical Spectra of Glycerophospholipids (GPPL).	177
Appendix 15: List of Publications.	179

LIST OF UNITS OF MEASUREMENTS

°C	degree Celsius
g	gram
Hertz	Hz
kg	kilogram
L	litre
mg	milligram
mL	millilitre
M	molar
mol	mole
ppm	parts per million
µL	microlitre

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LIST OF SYMBOLS

C	hyperplane SVM parameter
df	degree of freedom
hr	hour
hrs	hours
min	minutes
sec	second
vs	versus
α	significance level
δ	chemical shift
ϵ	epsilon
ν	Nu

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LIST OF EQUATIONS

Equations	Page
2.1	10
2.2	13
2.3	14
2.4	16
2.5	17
2.6	18
2.7	18
2.8	19
2.9	19
2.10	20
2.11	21
2.12	21
2.13	21
2.14	22
2.15	22
2.16	22
2.17	23
2.18	24
2.19	24
2.20	25
3.1	64
3.2	64

LIST OF ABBREVIATIONS

1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional
ANN	Artificial Neural Network.
ANOVA	Analysis of Variance
ATR	Attenuated Total Reflectance
CI	Confidence Interval
COW	Correlation Optimized Warping
CRM	Certified Reference Material
DA	Discriminant Analysis
DAG	Diacylglycerol
DSG	Derivatives Savitzky-Golay
EA/IRMS	Elemental Analyzer/Isotope Ratio Mass Spectrometry
EVCO	Extra Virgin Coconut Oil
FAME	Fatty Acid Methyl Ester
FAMEs	Fatty Acid Methyl Esters (<i>plural</i>)
FA	Fatty Acid
FAs	Fatty Acids (<i>plural</i>)
FTIR	Fourier Transform Infrared
GC	Gas Chromatography
GC × GC-TOF-MS	Dimensional Gas Chromatography Coupled with Time-Of-Flight Mass Spectrometry
GC-FID	Gas Chromatography with Flame Ionization Detection
GC-MS	Gas Chromatography-Mass Spectrometry
GL	Glycerolipid
GLC	Gas Liquid Chromatography
GPPL	Glycerophospholipid
HCA	Hierarchical Cluster Analysis
HPLC	High-Performance Liquid Chromatography
IPA	Isopropyl Alcohol
IR	Infrared
<i>k</i> -NN	<i>k</i> -Nearest Neighbours
K-S	Kennard-Stone
LC-MS/MS	Liquid Chromatography with Tandem Mass Spectrometry
LDA	Linear Discriminant Analysis
MAG	Monoacylglycerol
MDA	Mahalanobis Discriminant Analysis
MSC	Multiplicative Scatter Correction
MSEP	Mean Standard Error Prediction
MUFA	Monounsaturated Fatty Acids

MVR	Multivariate Regression
NIR	Near-Infrared Spectroscopic
NMR	Nucleus Magnetic Resonance
OPLS	Orthogonal Partial Least Squares
OPLS-DA	Orthogonal Partial Least Squares Discriminant Analysis
OPLSR	Orthogonal Partial Least Squares Regression
OSC-PLSR	Orthogonal Signal Correction Partial Least Squares Regression
PA	Phosphatidic Acids
PC	Principal Component
PCs	Principal Components (<i>plural</i>)
PCA	Principal Component Analysis
PCh	Phosphatidylcholines
PCR	Principal Component Regression
PG	Phosphatidyl-Glycerol
PI	Phosphatidylinositol
PLS	Partial Least Squares
PLSR	Partial Least Squares Regression
PUFA	Polyunsaturated Fatty Acids
QDA	Quadratic Discriminant Analysis
R^2	Coefficient of Determination
RBF	Radial Basis Function
RF	Random Forest
RMSEC	Root Mean Square Error of Calibration
RMSEV	Root Mean Square Error of Validation
SFA	Saturated Fatty Acids
SVM	Support Vector Machines
SVMDA	Support Vector Machines Discriminant Analysis
SVMR	Support Vector Machines Regression
TAG	Triacylglycerol
TAGs	Triacylglycerols (<i>plural</i>)
TLC	Thin Layer Chromatography
TMS	Tetramethylsilane
VCO	Virgin Coconut Oil