

UNIVERSITI TEKNOLOGI MARA

**SYSTEMATIC CLASSIFICATION
OF PINEAPPLE VARIETIES BY
CHEMOMETRIC APPROACHES
USING SENSORY ANALYSIS,
VOLATILE COMPOUNDS AND
PHENOLIC COMPOSITIONS**

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Thesis submitted in fulfillment
of the requirements for the degree of
Master of Science
(Chemistry)

Faculty of Applied Sciences

May 2022

ABSTRACT

Classification and quality control of fruits in Malaysia is based on the morphological traits manual done by the agricultural officer. Thus, this approach could be biased and inconsistent due to solely dependent on human perception and judgment. The main objective of this study was to systematically classify four pineapple varieties (Josephine, MD2, Morris, and Sarawak) using sensory attributes, phenolic and volatile organic compounds (VOCs). The aroma of pineapple is made up of a wide range of volatile and non-volatile compounds depending on the varieties can be valuable factors in classifying the fruits. Initially, phytochemical assays including antioxidant activity, total phenolic content (TPC), and total flavonoid content (TFC) were carried out to assess its ability in differentiating pineapple varieties. Chromatographic profiles of VOCs were obtained by extracting pineapples of different varieties using solid phase microextraction and gas chromatography mass spectrometry (SPME-GCMS). Optimisation of SPME operating parameters was conducted using three-factor, Box–Behnken response surface experimental design to evaluate the interactive effects of temperature, extraction time and salting effect on the amount of selected VOCs. Based on the maximum amount of these VOCs, the optimum operating extraction conditions for SPME were set up at a temperature of 30 °C, a time of 29 min, and salt addition of 1g. Phenolic compounds from pineapple pulp were extracted using pressurised liquid extraction prior to separation using a 2-dimensional-liquid chromatography–diode array detector (2D-LC-DAD). Sensory profiles conducted using quantitative descriptive analysis (QDA) revealed the fruity aroma of pineapple was insignificant to differentiate between the pineapple varieties with a scale of 4.13 ± 2.07 , 5.33 ± 2.58 , 3.87 ± 2.07 , and 3.00 ± 0.00 for Morris, Josephine, MD2, and Sarawak, respectively. It can be concluded sensory analysis alone could be biased and unreliable in discriminating pineapple varieties. By combining chemometric analysis using the sensory data, volatile and phenolic compounds more significant finding was observed. Principal component analysis (PCA) supported the hierarchical cluster analysis (HCA) whereby four distinct groups were obtained representing different varieties of pineapple. Partial least square discriminant analysis (PLS-DA) was applied to correlate between phenolic, volatile, and sensory attributes which allowed clear identification of potential marker compounds responsible for varietal discrimination of each pineapple variety. Artificial neural network (ANN) models were developed using phenolic (P-ANN1) and volatile (P-ANN2) data sets as input variables. Results showed the classification model P-ANN2 using input VOCs gave better discriminating between pineapple varieties with correct classifications rates of 97.1% in the prediction model, 92.3% in the testing phase, and 92.0% for the validation phase. A comprehensive and systematic classification of the four pineapple varieties was established by combining the 13 sensory attributes, 10 selected phenolic compounds, and 35 VOCs.

ACKNOWLEDGEMENT

In the name of Allah, the Most Merciful and The Most Gracious. All praise to Allah for His blessing that gives air to breathe and all His bounty because with gracious and merciful I manage to complete this project and theses. I am truly thankful to Him as I had completed this thesis. Upon completing this project, I would like to express my gratitude to many parties due to many people have influenced the direction and outcome of this project.

I would like to express my special thanks to Associate Professor Dr. Rozita Osman for her supervision at various stages of this research, taking part in useful decisions, and giving necessary advice and precious guidance which were valuable for my study both theoretically and practically. I would like to thank the Ministry of Higher Education (MOHE) for the financial support for this study (600-IRMI/FRGS 5/3 (009/2019)). My gratitude goes to the staff of the Centre for Postgraduate Studies, Faculty of Applied Sciences for their help towards my postgraduate affairs. My appreciation goes to the staff of the Analytical Laboratory of Applied Sciences Faculty; Pn. Roslizawati Ishak and Pn. Noor Haida Kamalul Khudzi at the UiTM Shah Alam for the provision of facilities and their warm hospitality during the progression of the experimental work in the laboratory.

I would never have been able to finish this journey without enormous support, continuous encouragement and understanding from my life partner, Rezza Burhanudin and my darling daughter, Ilhan Leah. Millions of thanks go to my beloved mom, Pn. Wan Sepiah Wan Awang and dad, En. Zainuddin Izharulhaq for the prayer they made from day one I started this journey. Special thanks to my friends for lending their hands during lab work, the ideas they shared and for all the ups and downs throughout this journey. I wish to extend our heartfelt and profound gratitude to all who in one or another way have contributed effort endless support and to make this endeavor a reality. All guidance and encouragement are greatly appreciated upon completing this project and thesis.

Thank you.

Syaidatul Faraha Zainuddin

May 2022

TABLE OF CONTENTS

	Page
CONFIRMATION BY PANEL OF EXAMINERS	ii
AUTHOR'S DECLARATION	iii
ABSTRACT	iv
ACKNOWLEDGEMENT	v
TABLE OF CONTENTS	vi
LIST OF TABLES	x
LIST OF FIGURES	xii
LIST OF PLATES	xv
LIST OF SYMBOLS	xvi
LIST OF ABBREVIATIONS	xvii
CHAPTER ONE: INTRODUCTION	1
1.1 Research Background	1
1.2 Problem Statement	3
1.3 Objectives of Study	5
1.4 Significance of study	5
1.5 Scope of study	6
CHAPTER TWO: LITERATURE REVIEW	8
2.1 Chapter Overview	8
2.2 Pineapple Morphology and Features	8
2.2.1 Compositional Changes during Maturation and Ripening	10
2.3 Malaysian Pineapple Varieties	11
2.3.1 Economic Importance of Pineapple Production	13
2.4 Phytochemicals Constituent and Antioxidant Properties	13
2.4.1 Phenolic compounds	14
2.4.2 Antioxidants	16
2.4.3 Volatile Compositions	17

2.5	Sample Extraction Methods	18
2.5.1	Extraction Methods for Phenolic Compounds	18
2.5.2	Extraction Methods for Volatile Organic Compounds (VOCs)	19
2.5.3	Optimisation of the HS-SPME	21
2.6	Sample Analysis	22
2.6.1	Determination of Antioxidant Activity, Phenolic and Flavonoid Content	23
2.6.2	Sensory Analysis by Quantitative Descriptive Analysis (QDA)	25
2.6.3	Chromatographic Fingerprint Analysis	26
2.7	Chemometrics Analysis	28
2.7.1	Hierarchical cluster analysis (HCA)	32
2.7.2	Principal Component Analysis (PCA)	32
2.7.3	Discriminant Analysis (DA)	33
2.7.4	Partial Least Square Discriminant Analysis (PLS-DA)	33
2.7.5	Artificial Neural Networks (ANN)	34
	CHAPTER THREE: RESEARCH METHODOLOGY	37
3.1	Chapter Overview	37
3.2	Chemical and Reagents	37
3.3	Instrumentations and Equipment	38
3.4	Samples Collection	38
3.5	Sample Analysis	39
3.5.1	DPPH Assay	39
3.5.2	Determination of Total Phenolic Content (TPC) by Folin-Ciocalteu Method	39
3.5.3	Determination of Total Flavanoid Content (TFC)	40
3.5.4	Analysis of Phenolic Compositions by PLE-2D-LC	41
3.5.5	Sensory Analysis by Quantitative Descriptive Analysis (QDA)	41
3.5.5.1	<i>Training of the panelists</i>	41
3.5.6	Analysis of Volatile Compositions by Gas Chromatography-Mass Spectrometry (GC-MS)	43
3.5.6.1	<i>Headspace Solid Phase Microextraction (HS-SPME) Procedure</i>	43