#### UNIVERSITI TEKNOLOGI MARA

# [PLEASE TYPE YOUR THESIS TITLE] CHEMOMETRICS METHOD WITH APPLICATIONS TO ENVIRONMENTAL AND QUANTITATIVE STRUCTUREACTIVITY RELATIONSHIP STUDIES [MAX 10 LINES]

#### MOHD ZULI BIN JAAFAR [MAX 2 LINES]

Choose an item

**July 2024** 

#### UNIVERSITI TEKNOLOGI MARA

# [PLEASE TYPE YOUR THESIS TITLE] CHEMOMETRICS METHOD WITH APPLICATIONS TO ENVIRONMENTAL AND QUANTITATIVE STRUCTUREACTIVITY RELATIONSHIP STUDIES [MAX 10 LINES]

#### MOHD ZULI BIN JAAFAR [MAX 2 LINES]

Choose an item submitted in Choose an item of the requirements for the degree of Master of Education

(Educational Management and Leadership)

**Faculty of Education** 

**July 2024** 

#### **CONFIRMATION BY PANEL OF EXAMINERS**

I certify that a Panel of Examiners has met on Enter viva date to conduct the final examination of Mohd Zuli Bin Jaafar on Choose an item Doctors of Philosophy thesis entitled "Chemometrics Method with Applications to Environmental and Quantitative Structure-Activity Relationship Studies" in accordance with Universiti Teknologi MARA Act 1976 (Akta 173). The Panel of Examiner recommends that the student be awarded the relevant degree. The Panel of Examiners was as follows:

Ahmad Sazali Hamzah, PhD Professor Faculty of Applied Sciences Universiti Teknologi MARA (Chairman)

Mohammad Nawawi Seroji, PhD Associate Professor College of Engineering Universiti Teknologi MARA (Internal Examiner)

Mohd Zuli Jaafar, PhD Senior Lecturer Faculty of Applied Sciences University of Bristol (External Examiner)

#### PROF IR DR ZUHAINA HAJI ZAKARIA

Dean Institute of Postgraduates Studies Universiti Teknologi MARA

Date: 17 July 2024

#### **AUTHOR'S DECLARATION**

I declare that the work in this Choose an item. was carried out in accordance with the regulations of Universiti Teknologi MARA. It is original and is the results of my own work, unless otherwise indicated or acknowledged as referenced work. This thesis has not been submitted to any other academic institution or non-academic institution for any degree or qualification.

I, hereby, acknowledge that I have been supplied with the Academic Rules and Regulations for Post Graduate, Universiti Teknologi MARA, regulating the conduct of my study and research.

Name of Student : Administrator DELL

Student ID. No. : 2014202020

Programme : Master of Science (Integrated Construction Project

Management) - AP780

Faculty : Applied Sciences

Thesis Title : Chemodmetrics with Applications to Environmental

and Quantitative Structure-Activity Relationship

**Studies** 

Signature of Student : .....

Date : July 2024

#### **ABSTRACT**

The lack of management data and not knowing what level of park quality local authorities are trying to deliver is becoming a growing concern. The problem of urban landscape cannot be solved simply by providing more parks and spending more money on development and management. There is an urgent need for innovation, for better understanding of the current and potential role of the park to meet the needs in modern urban life. Thus, the adoption of a strategic approach is needed to planning and managing that urban landscape to carry out its function and roles. This research aim is to study the factors of park attributes that influence the development, planning and management of successful urban park in Kuala Muda. It specifically studies on Taman Tasik Cini as the sole representative of urban park in the context of Kuala Muda Structure Plan 2020. This research is based on data obtained from survey questionnaire that polled public attitudes regarding the factors of park attributes based on visitor's perception and Harris's (2008), park success factors. The data was analysed to evaluate and determine the park attributes and its level of preferences that influence the strategic approach to the planning and management of successful urban park. The research suggested that successful urban park as are linked to the physical and functional qualities of the park; security and comfort; visitors' preferences and needs of the place. The results of the study also suggested that a holistic strategic approach is needed for the local authority to successfully managing the urban park. It is hope that the study can contribute to the improvement of urban park planning and management in Kuala Muda.

--please delete--

Note:

Master – minimum 200 words

PhD – minimum 250 words

Limit to one (1) page only

No Paragraph

Font: Times New Roman - 12

#### **ACKNOWLEDGEMENT**

Firstly, I wish to thank God for giving me the opportunity to embark on my PhD and for completing this long and challenging journey successfully. My gratitude and thanks go to my supervisor Assoc Prof Datuk.

My appreciation goes to the Captain and crewmembers of the MMC who provided the facilities and assistance during sampling. Special thanks to my colleagues and friends for helping me with this project.

Finally, this thesis is dedicated to the loving memory of my very dear late father and mother for the vision and determination to educate me. This piece of victory is dedicated to both of you. Alhamdulilah.

--please delete--

Must include all supervisors' names

Limit to one (1) page only

Font: Times New Roman - 12

#### TABLE OF CONTENTS

|                |   | Page            |
|----------------|---|-----------------|
| CON            | FIRMATION BY PANEL OF EXAMINERS         | ii              |
| AUT            | HOR'S DECLARATION                       | iii             |
| ABS            | ГКАСТ                                   | iv              |
| ACK            | NOWLEDGEMENT                            | v               |
| TAB            | LE OF CONTENTS                          | vi              |
| LIST           | OF TABLES                               | ix              |
| LIST           | OF FIGURES                              | X               |
| LIST           | OF PLATES                               | xi              |
| LIST           | OF SYMBOLS                              | xii             |
| LIST           | OF ABBREVIATIONS                        | xiii            |
| LIST           | OF NOMENCLATURE                         | xiv             |
| <b>CHA</b> 1.1 | PTER 1 INTRODUCTION Research Background | <b>1</b><br>1   |
| 1.2            | Motivation for This Work                | 1               |
| 1.3            | Problem Statement                       | 1               |
| 1.4            | Research Objectives                     | 4               |
| 1.5            | Research Question                       | 4               |
| 1.6            | Significance of Study                   | 5               |
|                | 1.6.1 Univariate Regression             | 10              |
|                | 1.6.2 Multivariate Regression           | 10              |
| 1.7            | Limitation                              | 11              |
| 1.8            | Assumption                              | 11              |
| 1.9            | Ethical Committee                       | 11              |
| 1.10           | Thesis Scope                            | 11              |
| 1.11           | Thesis Outline                          | 11              |
| <b>CHA</b> 2.1 | PTER 2 LITERATURE REVIEW Introduction   | <b>12</b><br>12 |

|                 | 2.1.1 Data Pre-Processing and Data Drift: The Utility of Principal               | 1            |
|-----------------|--|--------------|
|                 | Component Analysis, Self-Organizing Maps and Class Separation                    | ı            |
|                 | Indices  | 12           |
|                 | 2.1.2 Multivariate Linear Regression   | 13           |
| 2.2             | Environmental Studies for Data Pre-Processing and Data Drift: The Utility        | <b>/</b>     |
|                 | of Principal Component Analysis, Self-Organizing Maps and Class                  | S            |
|                 | Separation Indices   | 13           |
|                 | 2.2.1 Data Pre-Processing and Data Drift: The Utility of Principal               | 1            |
|                 | Component Analysis, Self-Organizing Maps and Class Separation                    | ı            |
|                 | Indices  | 14           |
|                 | 2.2.2 Airborne Particulate Matter Datasets                                       | 15           |
|                 | 2.2.3 Meteorological Dataset   | 16           |
| 2.3             | Quantitative Structure Activity Relationships Studies on the Active and          | 1            |
|                 | Inactive Antimalarial Compounds  | 17           |
| <b>CHAF</b> 3.1 | PTER 3 RESEARCH METHODOLOGY Introduction   | <b>23</b> 23 |
| 3.2             | Data Pre-Processing for Classification   | 23           |
|                 | 3.2.1 Individual Transformation  | 24           |
|                 | 3.2.2 Row Scaling  | 25           |
|                 | 3.2.3 Column Scaling   | 26           |
| 3.3             | Exploratory Data Analysis Principal Component Analysis                           | 27           |
| 3.4             | Quantitative Structure Activity Relationships Studies on The Active and          | 1            |
|                 | Inactive Antibacterial Compounds   | 29           |
|                 | PTER 4 RESULTS ON EXPLORATORY METHOD FOR<br>ANTIBACTERIAL AND ANTIFUNGAL ACIVITY | 32           |
| 4.1             | Introduction   | 32           |
| 4.2             | Chemometrics   | 32           |
| 4.3             | PCA and PLS Work.  | 33           |
|                 | PTER 5 CONCLUSION  | 34           |
| 5.1             | Introduction   | 34           |
| 5.2             | Data cleaning  | 34           |
| 5.3             | Data Pre-Processing  | 34           |

| REFERENCES       | 35 |
|------------------|----|
| APPENDICES       | 36 |
| AUTHOR'S PROFILE | 39 |

#### LIST OF TABLES

| Tables    | Title  | Page |
|-----------|--|------|
| Table 1.1 | The Title for This Table is Here                             | 2    |
| Table 1.4 | The Statistical Information of APM Dataset                   | 2    |
| Table 1.5 | The Title for This Table is Here                             | 3    |
| Table 1.6 | The Sample of the Table with More Than One Page Items        | 7    |
| Table 2.1 | The Temperature Infomation                                   | 12   |
| Table 2.2 | The Environmental Dataset Infomation                         | 12   |
| Table 2.3 | Summary of the Meteorological Parameters                     | 14   |
| Table 2.4 | Title for Third Table in Chapter 2                           | 15   |
| Table 2.5 | The Statistical Information of APM Dataset                   | 16   |
| Table 2.6 | The Sample of the Table with More Than One Page Items        | 19   |
| Table 3.1 | The QSAR Dataset the Sources in This Thesis for Regression   |      |
|           | and Classification   | 31   |
| Table 3.2 | To change the overall look of your document, choose new      |      |
|           | Theme elements on the Page Layout tab. the look of your      |      |
|           | document to the original contained in your current template. | 31   |

#### LIST OF FIGURES

| Figures    | Title   | Page         |
|------------|---|--------------|
| Figure 1.1 | The Spectra of Cooking Oil after One Hour Heating.            | 9            |
| Figure 1.2 | FTIR spectra for non-fried (a) and fried palm oils (b)        | 9            |
| Figure 1.3 | FT-NIR spectra for non-fried (blue) and fried (red) palm oils | 11           |
| Figure 3.1 | Compressive Strength of Rice Husk Ash (RHA) Concrete o        | $\mathbf{f}$ |
|            | Grade 30  | 24           |
| Figure 3.2 | Typical Steps Involved in QSAR Methodology                    | 28           |
| Figure 3.3 | A Map Showing The Sampling Location in Islamabad, Pakistan    | n            |
|            |   | 28           |
| Figure 3.4 | A PCA Plots for Data Processing Strategy                      | 30           |

#### LIST OF PLATES

| Plates    | Title  | Page |
|-----------|--|------|
| Plate 1.1 | MZJ Formatting Logo  | 5    |
| Plate 1.2 | A Picture of Light   | 6    |
| Plate 2.1 | A Sample of Grass and Bamboo 2                             | 17   |
| Plate 2.2 | A Sample of Formatting Method                              | 22   |
| Plate 2.3 | The View of the Tuanku Syed Sirajuddin Building, UiTM from | m    |
|           | the Dataran Tengku Fauziah                                 | 22   |

#### LIST OF SYMBOLS

#### **Symbols**

A Number of PLS or PCA components in the model and the number of selected latent variable in the model

a Number of the PLS or PCA component

b PLS regression coefficient

b Number of blocks (b=1,2,3....,K)

C Coarse APM block  $C_p$  Pooled covariance matrix for the two classes

Covariance matrix for class g

#### LIST OF ABBREVIATIONS

#### Abbreviations

PCA Principal Component Analysis

#### LIST OF NOMENCLATURE

#### Nomenclatures

- A Amplitude Ratio, (No Units)
- C Centroid of pipe, inches

#### CHAPTER 1

#### INTRODUCTION

#### 1.1 Research Background

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected.

Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

#### 1.2 Motivation for This Work

Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme. Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme.

#### 1.3 Problem Statement

Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document as shown in Table 1.1.

To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other. For example, you can add a matching cover page, header, and sidebar. Click Insert and then choose the

elements you want from the different galleries.

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look You can easily change the formatting of selected

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages,

Table 1.1
The Title for This Table is Here

| Title                                       | Title                                       | Title                                       |
|---|---|---|
| To change the overall look of your document | To change the overall look of your document | To change the overall look of your document |
| To change the overall look of your document | To change the overall look of your document | To change the overall look of your document |

Source: World Bank report 2016

Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document.

To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other. For example, you can add a matching cover page, header, and sidebar. Click Insert and then choose the elements you want from the different galleries as shown in Table 1.2.

Table 1.2
The Statistical Information of APM Dataset

| Batch | No of samples | Average per month | Percentage of LoD<br>(Coarse APM) | Percentage of LoD<br>(Fine APM) |
|-------|---------------|-------------------|-----------------------------------|---------------------------------|
| 1     | 100           | 8 samples         | 1.70%                             | 6.48%                           |
| 2     | 102           | 9 samples         | 9.29%                             | 9.09%                           |
| 3     | 176           | 9 samples         | 2.65%                             | 4.34%                           |

Table 1.3
The Title for This Table is Here

| Chemical C<br>Composition | Surface Area (m2g-1)   | Porosity (cm3g-1)      |
|---------------------------|------------------------|------------------------|
| Neutral clay 0.68 0.68    | Neutral clay 0.68 0.68 | Neutral clay 0.68 0.68 |
| Bleaching clay            | Bleaching clay         | Bleaching clay         |
|                           |                        |                        |
| 0.80                      | 0.89                   | 0.99                   |

Note: Influence of the physical chemistry properties of an acid activated bentonite in the bleaching of olive oil. (Pradas et.al., 1993, p. 23)

Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme as shown in (1.3). Equation (1.4) gives example on the use of word "Equation" in front of the equation numbering whenever a sentence starts with an equation.

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab.

$$y = mx + 3 \tag{1.1}$$

$$y = mx + 3 \tag{1.2}$$

$$y = mx + 3 \tag{1.3}$$

$$y = mx + 4 \tag{1.4}$$

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab.

#### 1.4 Research Objectives

To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other. For example, you can add a matching cover page, header, and sidebar. Click Insert and then choose the elements you want from the different galleries.

- a) To perform data pre-processing and exploratory analysis by using PCA, SOMs and Class Separation Indices.
- b) To analysis analysis Multiblock methods and regression analysis of environmental dataset.
- c) To find the trend using pattern recognition in method QSAR with the application of SOMs and PLSDA.
- d) To test model validity using data Splitting Methods for Regressions and Classifications.

#### 1.5 Research Question

- i) Video provides a powerful way to help you prove your point.
- ii) When you click Online Video, you can paste in the embed code for the video you want to add.
- iii) You can also type a keyword to search online for the video that best fits your

document.

- iv) To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other.
- v) For example, you can add a matching cover page, header, and sidebar.

#### 1.6 Significance of Study

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly. The sample of plates shown in Plate 1.2



Plate 1.1 MZJ Formatting Logo



Plate 1.2 A Picture of Light

Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document.

To make your document look professionally produced, Word provides header, footer, cover page, and text box designs that complement each other. For example, you can add a matching cover page, header, and sidebar. Click Insert and then choose the elements you want from the different galleries.

Themes and styles also help keep your document coordinated. When you click Design and choose a new Theme, the pictures, charts, and SmartArt graphics change to match your new theme. When you apply styles, your headings change to match the new theme.

Save time in Word with new buttons that show up where you need them. To change the way a picture fits in your document, click it and a button for layout options appears next to it. When you work on a table, click where you want to add a row or a column, and then click the plus sign.

Reading is easier, too, in the new Reading view. You can collapse parts of the document and focus on the text you want. If you need to stop reading before you reach the end, Word remembers where you left off - even on another device.

Table 1.4
The Sample of the Table with More Than One Page Items

| No | Molecular<br>Descriptors | Abbreviation | Groups | Amount | Description   |
|----|--------------------------|--------------|--------|--------|---|
| 1  | Constitutional           | Con          | 0D     | 48     | 0D-descriptors, independent from molecular connectivity and conformations. Atom and bonds         |
|    | descriptors              |              |        |        | counts, molecular weight, sum of atomic properties, etc   |
| 2  | Topological              | Торо         | 2D     | 119    | Molecular descriptors obtained from the molecular graph (usually H-depleted), i.e 2D-descriptors  |
|    | descriptors              |              |        |        | conformationally independent.   |
| 3  | Walk and path            | Wap          | 2D     | 47     | Molecular descriptors obtained from the molecular graph, counting paths, walk and self returning  |
|    | counts                   |              |        |        | walks of different lengths.   |
| 4  | Connectivity             | Coni         | 2D     | 33     | Topological Molecular descriptors calculated from the vertex degree of the atoms in the H-        |
|    | indices                  |              |        |        | depleted molecular graph.   |
| 5  | Information              | Info         | 2D     | 47     | Molecular descriptors calculated as information content of molecules, based on the calculation of |
|    | indices                  |              |        |        | equivalences classes from the molecular graph. Among them, the indices of neighbourhood           |
|    |                          |              |        |        | degree and edge multiplicity.   |
| 6  | 2D                       | 2D           | 2D     | 96     | Molecular descriptors calculated from the molecular graph by summing the products of atom         |
|    | autocorrelations         |              |        |        | weights of the terminal atoms of all the paths of the considered path length (the lag)            |
| 7  | Edge adjacency           | Edge         | 2D     | 107    | Topological Molecular descriptors derived from the edge adjacency matrix which encodes the        |
|    | indices                  |              |        |        | connectivity between graph edges.   |
| 8  | Burden                   | Bur          | 2D     | 64     | Molecular descriptors contained from the positive and negative eigenvalues of the adjacency       |
|    | eigenvalues              |              |        |        | matrix, weighting the diagonal element with atom weight.  |
| 9  | Topological              | Торос        | 2D     | 21     | First 10 eigenvalues (absolute values) obtained from a corrected adjacency matrix.                |
| -  | charge indices           |              |        |        |   |

| No | Molecular<br>Descriptors | Abbreviation | Groups | Amount | Description   |
|----|--------------------------|--------------|--------|--------|---|
| 10 | Eigenvalue-based         | EiG          | 2D     | 44     | Topological descriptors calculated by the eigenvalues of the square(usually symmetric) matrix       |
|    | indices                  |              |        |        | representing a molecular graph.   |
| 11 | Randic molecular         | Ran          | 3D     | 41     | Molecular descriptors derived from the distance distribution moments of the geometry matrix,        |
|    | profiles                 |              |        |        | defined as the average row sum of its entries raised at the k-th power, normalized by the factor k. |
| 12 | Geometrical              | Geo          | 3D     | 74     | Different kinds of conformationally dependent descriptors based on the molecular geometry.          |
|    | descriptors              |              |        |        | Reliable values are obtained if reliable conformations were previously calculated.                  |
| 13 | RDF descriptors          | RDF          | 3D     | 150    | Molecular descriptors obtained by radial basis functions centred on different interatomic distances |
|    |                          |              |        |        | (from 0.5A to 15.5A)  |
| 14 | 3D-MoRSE                 | 3D           | 3D     | 160    | Molecular descriptors calculated by summing atom weights by different angular scattering            |
|    | descriptors              |              |        |        | function.   |
| 15 | WHIM                     | WHIM         | 3D     | 99     | Molecular descriptors obtained as statistical indices of the atom projected onto the 3 principal    |
|    | descriptors              |              |        |        | components obtained from weighted covariance matrices of the atomic coordinates.                    |

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

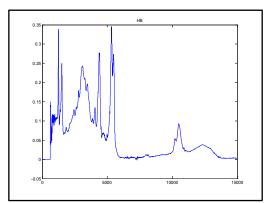


Figure 1.1 The Spectra of Cooking Oil after One Hour Heating.

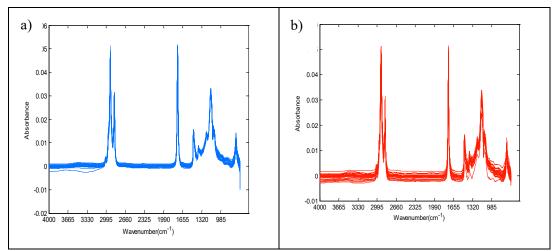


Figure 1.2 FTIR spectra for non-fried (a) and fried palm oils (b)

#### 1.6.1 Univariate Regression

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

#### 1.6.2 Multivariate Regression

#### 1.6.2.1 Principal Components Regression

When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab.

#### 1.6.2.2 Multivariate Regressions using PLS Method

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

- a) On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document.
- b) You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly. To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template. On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document.

#### 1.7 Limitation

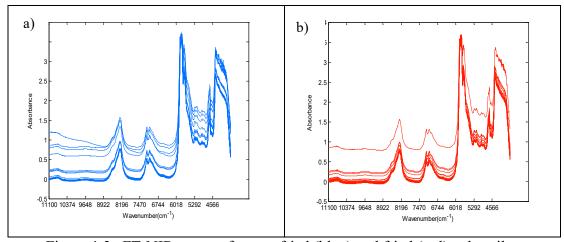


Figure 1.3 FT-NIR spectra for non-fried (blue) and fried (red) palm oils

#### 1.8 Assumption

#### 1.9 Ethical Committee

#### 1.10 Thesis Scope

#### 1.11 Thesis Outline

# CHAPTER 2 LITERATURE REVIEW

#### 2.1 Introduction

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly. As shown in Table 2.1 and Table 2.2

Table 2.1 The Temperature Infomation

| Variable  | Minimum | Maximum | Average | Standard<br>deviation |
|---|---------|---------|---------|-----------------------|
| Minimum temperature over 24 hours preceding 0300 GMT (0C) | 0.0     | 30.0    | 15.33   | 7.06                  |
| Maximum temperature over 24 hours preceding 1200 GMT (0C) | 12.5    | 44.7    | 29.85   | 6.93                  |

Table 2.2
The Environmental Dataset Infomation

| Variable                      | Minimum | Maximum | Average | Standard deviation |
|-------------------------------|---------|---------|---------|--------------------|
| Average relative humidity (%) | 31.0    | 97.0    | 63.70   | 14.80              |
| Average pressure (hPa)        | 994.37  | 1022.43 | 1009.04 | 6.48               |
| Average wind speed (Knot)     | 0.0     | 9.0     | 0.79    | 1.43               |
| Average rainfall (mm)         | 0.0     | 140.0   | 3.82    | 14.05              |

## 2.1.1 Data Pre-Processing and Data Drift: The Utility of Principal Component Analysis, Self-Organizing Maps and Class Separation Indices

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. The sample of equation is given in (2.1). On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look as shown in (2.2).

$$y = mx + 3 \tag{2.1}$$

$$y = mx + dx + 5 \tag{2.2}$$

#### 2.1.2 Multivariate Linear Regression

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

# 2.2 Environmental Studies for Data Pre-Processing and Data Drift: The Utility of Principal Component Analysis, Self-Organizing Maps and Class Separation Indices

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab.

You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

### 2.2.1 Data Pre-Processing and Data Drift: The Utility of Principal Component Analysis, Self-Organizing Maps and Class Separation Indices

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. The sample of equation is given in (2.3). On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look as shown in (2.4).

$$y = mx + 3 \tag{2.3}$$

$$y = mx + dx + 5 \tag{2.4}$$

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

Table 2.3 Summary of the Meteorological Parameters

| Variable                      | Minimum | Maximum | Average | Standard deviation |
|-------------------------------|---------|---------|---------|--------------------|
| Minimum temperature over 24   | 0.0     | 30.0    | 15.33   | 7.06               |
| hours preceding 0300 GMT (0C) |         |         |         | ,                  |
| Maximum temperature over 24   | 12.5    | 44.7    | 29.85   | 6.93               |
| hours preceding 1200 GMT (0C) | 12.0    |         | 23.00   | 0.50               |
| Average relative humidity (%) | 31.0    | 97.0    | 63.70   | 14.80              |

| Average pressure (hPa)    | 994.37 | 1022.43 | 1009.04 | 6.48  |
|---------------------------|--------|---------|---------|-------|
| Average wind speed (Knot) | 0.0    | 9.0     | 0.79    | 1.43  |
| Average rainfall (mm)     | 0.0    | 140.0   | 3.82    | 14.05 |

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab.

#### 2.2.2 Airborne Particulate Matter Datasets

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

Table 2.4
Title for Third Table in Chapter 2

| Title                                       | Title                                       | Title                                       |
|---|---|---|
| To change the overall look of your document | To change the overall look of your document | To change the overall look of your document |
| To change the overall look of               | To change the overall look of               | To change the overall look of               |

| your document | your document | your document |  |
|---------------|---------------|---------------|--|
|               |               |               |  |

Source: World Bank report 2016

Table 2.5
The Statistical Information of APM Dataset

| Batch | No of samples | Average per month | Percentage of LoD<br>(Coarse APM) | Percentage of LoD<br>(Fine APM) |
|-------|---------------|-------------------|-----------------------------------|---------------------------------|
| 1     | 100           | 8 samples         | 1.70%                             | 6.48%                           |
| 2     | 102           | 9 samples         | 9.29%                             | 9.09%                           |
| 3     | 176           | 9 samples         | 2.65%                             | 4.34%                           |

#### 2.2.3 Meteorological Dataset

#### 2.2.3.1 Data Pre-Processing and Data Drift

- a) You Can Use These Galleries To Insert Tables, Headers, Footers, Lists, Cover Pages, And Other Document Building Blocks. When You Create Pictures, Charts, Or Diagrams, They Also Coordinate With Your Current Document Look.
- b) You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab.

You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

### 2.3 Quantitative Structure Activity Relationships Studies on the Active and Inactive Antimalarial Compounds

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.



Plate 2.1 A Sample of Grass and Bamboo 2

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

Table 2.6
The Sample of the Table with More Than One Page Items

| No | <b>Molecular Descriptors</b> | Abbreviation | Groups | Amount | Description  |
|----|------------------------------|--------------|--------|--------|--|
| 1  | Constitutional descriptors   | Con          | 0D     | 48     | 0D-descriptors, independent from molecular connectivity and                |
|    |                              |              |        |        | conformations. Atom and bonds counts, molecular weight, sum of atomic      |
|    |                              |              |        |        | properties, etc  |
| 2  | Topological descriptors      | Торо         | 2D     | 119    | Molecular descriptors obtained from the molecular graph (usually H-        |
|    |                              |              |        |        | depleted), i.e 2D-descriptors conformationally independent.                |
| 3  | Walk and path                | Wap          | 2D     | 47     | Molecular descriptors obtained from the molecular graph, counting paths,   |
|    | counts                       |              |        |        | walk and self returning walks of different lengths.                        |
| 4  | Connectivity                 | Coni         | 2D     | 33     | Topological Molecular descriptors calculated from the vertex degree of     |
|    | indices                      |              |        |        | the atoms in the H-depleted molecular graph.                               |
| 5  | Information                  | Info         | 2D     | 47     | Molecular descriptors calculated as information content of molecules,      |
|    | indices                      |              |        |        | based on the calculation of equivalences classes from the molecular        |
|    |                              |              |        |        | graph. Among them, the indices of neighbourhood degree and edge            |
|    |                              |              |        |        | multiplicity.  |
| 6  | 2D                           | 2D           | 2D     | 96     | Molecular descriptors calculated from the molecular graph by summing       |
|    | autocorrelations             |              |        |        | the products of atom weights of the terminal atoms of all the paths of the |
|    |                              |              |        |        | considered path length (the lag)   |
| 7  | Edge adjacency indices       | Edge         | 2D     | 107    | Topological Molecular descriptors derived from the edge adjacency          |
|    |                              |              |        |        | matrix which encodes the connectivity between graph edges.                 |
| 8  | Burden                       | Bur          | 2D     | 64     | Molecular descriptors contained from the positive and negative             |
|    | eigenvalues                  |              |        |        | eigenvalues of the adjacency matrix, weighting the diagonal element with   |

| No | Molecular Descriptors     | Abbreviation | Groups | Amount | Description   |
|----|---------------------------|--------------|--------|--------|---|
|    |                           |              |        |        | atom weight.  |
| 9  | Topological               | Торос        | 2D     | 21     | First 10 eigenvalues (absolute values) obtained from a corrected            |
|    | charge indices            |              |        |        | adjacency matrix.   |
| 10 | Eigenvalue-based indices  | EiG          | 2D     | 44     | Topological descriptors calculated by the eigenvalues of the                |
|    |                           |              |        |        | square(usually symmetric) matrix representing a molecular graph.            |
| 11 | Randic molecular profiles | Ran          | 3D     | 41     | Molecular descriptors derived from the distance distribution moments of     |
|    |                           |              |        |        | the geometry matrix, defined as the average row sum of its entries raised   |
|    |                           |              |        |        | at the k-th power, normalized by the factor k.                              |
| 12 | Geometrical descriptors   | Geo          | 3D     | 74     | Different kinds of conformationally dependent descriptors based on the      |
|    |                           |              |        |        | molecular geometry. Reliable values are obtained if reliable                |
|    |                           |              |        |        | conformations were previously calculated.                                   |
| 13 | RDF descriptors           | RDF          | 3D     | 150    | Molecular descriptors obtained by radial basis functions centred on         |
|    |                           |              |        |        | different interatomic distances (from 0.5A to 15.5A)                        |
| 14 | 3D-MoRSE descriptors      | 3D           | 3D     | 160    | Molecular descriptors calculated by summing atom weights by different       |
|    |                           |              |        |        | angular scattering function.  |
| 15 | WHIM                      | WHIM         | 3D     | 99     | Molecular descriptors obtained as statistical indices of the atom projected |
|    | descriptors               |              |        |        | onto the 3 principal components obtained from weighted covariance           |
|    |                           |              |        |        | matrices of the atomic coordinates.   |
| 16 | GETAWAY descriptors       | GATE         | 3D     | 197    | Descriptors calculated from the leverage matrix obtained by the centred     |
|    |                           |              |        |        | atoic coordinates (molecular influences matrix, MIM). The first four        |
|    |                           |              |        |        | descriptors are calculated as information content and connectivity          |
|    |                           |              |        |        | indices. HATA and H descriptors are 3D-autocorrelation descriptors          |

| No | <b>Molecular Descriptors</b> | Abbreviation | Groups | Amount | Description  |
|----|------------------------------|--------------|--------|--------|--|
|    |                              |              |        |        | obtained from MIM; R and R+ descriptors obtained from the leverage.  |
|    |                              |              |        |        | Geometry matrix.   |
| 17 | Functional group counts      | Funct        | Others | 152    | Molecular descriptors based on the counting of chemical functional   |
|    |                              |              |        |        | groups. They are calculated by knowing the molecular composition and |
|    |                              |              |        |        | atom connectivities.   |
| 18 | Atom-centred fragments       | Atom         | Others | 120    | Molecular descriptors, based on the counting of 120 atom-centered    |
|    |                              |              |        |        | fragments, as defined by Ghose-Crippen. Some fragments are undefined |
|    |                              |              |        |        | by the authors. They are calculated by knowing the molecular         |
|    |                              |              |        |        | composition and atom connectivities.                                 |
| 19 | Charged descriptors          | charged      | Others | 14     | Fourteen charge descriptors which are reliable only when charge are  |
|    |                              |              |        |        | estimated by quantum molecular methods                               |

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

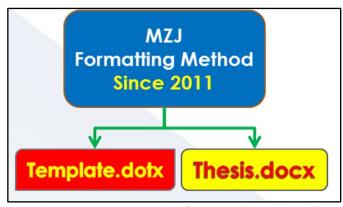


Plate 2.2 A Sample of Formatting Method



Plate 2.3 The View of the Tuanku Syed Sirajuddin Building, UiTM from the Dataran Tengku Fauziah

## **CHAPTER 3**

## RESEARCH METHODOLOGY

#### 3.1 Introduction

(UiTM Paragraph 1a) Example of Paragraph 1a Style On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

## 3.2 Data Pre-Processing for Classification

(UiTM Paragraph 1) On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert table. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

(UiTM Paragraph 1a) To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

(UiTM Paragraph 1) On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab.

(UiTM Paragraph 1b) Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you

want to add. You can also type a keyword to search online for the video that best fits your document.

(UiTM Paragraph 1) Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document.

(UiTM Paragraph 1c) Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document.

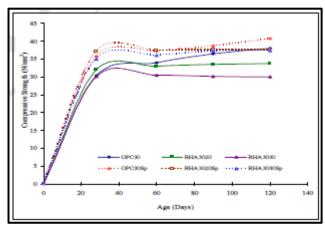


Figure 3.1 Compressive Strength of Rice Husk Ash (RHA) Concrete of Grade 30

## 3.2.1 Individual Transformation

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. The sample for writing an equation are shown at (3.1) and (3.2);

$$^{sq}x_{ii} = \sqrt[q]{x_{ii}} \tag{3.1}$$

$$x_{ii} = \log_{10} x_{ii} \tag{3.2}$$

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template. On The Insert Tab, The Galleries Include Items That Are Designed To Coordinate With The Overall Look Of Your Document.

Save time in Word with new buttons that show up where you need them. To change the way a picture fits in your document, click it and a button for layout options appears next to it. When you work on a table, click where you want to add a row or a column, and then click the plus sign.

Reading is easier, too, in the new Reading view. You can collapse parts of the document and focus on the text you want. If you need to stop reading before you reach the end, Word remembers where you left off - even on another device.

## 3.2.2 Row Scaling

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.nYou Can Use These Galleries To Insert Tables, Headers, Footers, Lists, Cover Pages, And Other Document Building Blocks.

When you create pictures, charts, or diagrams, they also coordinate with your current document look. You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab.

You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

#### 3.2.3 Column Scaling

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

"You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly."

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to

the original contained in your current template. On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document.

## 3.3 Exploratory Data Analysis Principal Component Analysis

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.

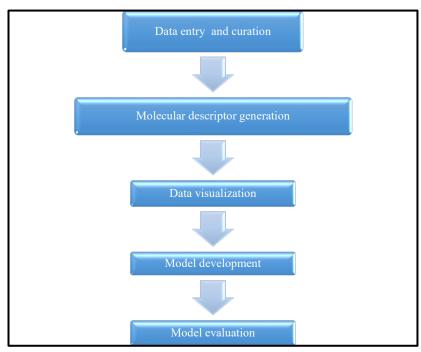


Figure 3.2 Typical Steps Involved in QSAR Methodology



Figure 3.3 A Map Showing The Sampling Location in Islamabad, Pakistan

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template.

# 3.4 Quantitative Structure Activity Relationships Studies on The Active and Inactive Antibacterial Compounds

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look.

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly. To change the overall look of your document, choose new Theme elements on the Page Layout tab. the look of your document to the original contained in your current template.

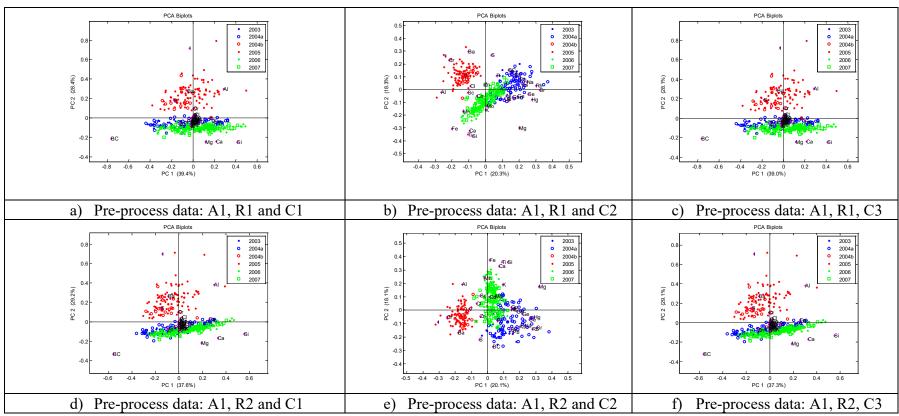


Figure 3.4 A PCA Plots for Data Processing Strategy

Table 3.1
The QSAR Dataset the Sources in This Thesis for Regression and Classification

| No | Name         | Dimension | Classes/ Types                            | Reference |
|----|--------------|-----------|---|-----------|
| 1  | Blood Brain  | 406 × 926 | Non-penetrating (class 1), 136            |           |
|    | Barrier      |           | compounds                                 |           |
|    |              |           | Penetrating (class 2), 270 compounds      |           |
| 2  | Antimalarial | 57 × 1661 | Regression                                |           |
| 3  | Skin         | 131 × 926 | Strong skin sensitizers (Class 1), 67     |           |
|    |              |           | compounds                                 |           |
|    |              |           | Non- strong skin sensitizers(class 2), 64 |           |
|    |              |           | compounds                                 |           |

Table 3.2 To change the overall look of your document, choose new Theme elements on the Page Layout tab. the look of your document to the original contained in your current template.

#### **CHAPTER 4**

# RESULTS ON EXPLORATORY METHOD FOR ANTIBACTERIAL AND ANTIFUNGAL ACIVITY

#### 4.1 Introduction

On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document. You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks. When you create pictures, charts, or diagrams, they also coordinate with your current document look. (Abbas et al., 2011)

- a) On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document.
- b) You can use these galleries to insert tables, headers, footers, lists, cover pages, and other document building blocks.
- c) When you create pictures, charts, or diagrams, they also coordinate with your current document look.
- d) You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab.
- e) You can also format text directly by using the other controls on the Home tab.

## 4.2 Chemometrics

You can easily change the formatting of selected text in the document text by choosing a look for the selected text from the Quick Styles gallery on the Home tab. You can also format text directly by using the other controls on the Home tab. Most controls offer a choice of using the look from the current theme or using a format that you specify directly.(2010a; 2010b; 2013)

## 4.3 PCA and PLS Work.

To change the overall look of your document, choose new Theme elements on the Page Layout tab. To change the looks available in the Quick Style gallery, use the Change Current Quick Style Set command. Both the Themes gallery and the Quick Styles gallery provide reset commands so that you can always restore the look of your document to the original contained in your current template. (Mohd Zuli Jaafar et al., 2006; Mohd Z Jaafar et al., 2011; Lazim et al., 2013; Sim et al., 2015)

## **CHAPTER 5**

## **CONCLUSION**

Video provides a powerful way to help you prove your point. When you click Online Video, you can paste in the embed code for the video you want to add. You can also type a keyword to search online for the video that best fits your document.

- 5.1 Introduction
- 5.2 Data cleaning
- 5.3 Data Pre-Processing

## **REFERENCES**

- Abbas, M., Shehab, A. A.-M., Hassan, N., & Al-Samuraee, A. (2011). Effect of temperature and deposition time on the optical properties of chemically deposited nanostructure PbS thin films. Thin Solid Films, 519(15), 4917-4922.
- Abdulgafour, H., Hassan, Z., Al-Hardan, N., & Yam, F. (2010a). Growth of high-quality ZnO nanowires without a catalyst. Physica B: Condensed Matter, 405(19), 4216-4218.
- Abdulgafour, H., Hassan, Z., Al-Hardan, N., & Yam, F. (2010b). Growth of zinc oxide nanoflowers by thermal evaporation method. Physica B: Condensed Matter, 405(11), 2570-2572.
- Abdulgafour, H., Hassan, Z., Yam, F., & Chin, C. (2013). Sensing devices based on ZnO hexagonal tube-like nanostructures grown on p-GaN heterojunction by wet thermal evaporation. Thin Solid Films, 540, 212-220.
- Jaafar, M. Z., Hasan, M. N., & Wong, T. W. (2006). Quantitative structure-activity relationships of peroxisome proliferator activated receptor Y agonist.

## **APPENDICES**

## **APPENDIX 1**

## **Example of the Codes in PLS Algorithms**

```
function Results = AnovaMLRegresion(X,Y)

## This is the finction to calculate the stat parameters for MLR or Anova for Regression
## clear all
## load('G:\dataset\Handbook of Regression and Modeling158.mat')

## LS Reg
[m,p] = size(X);
Xnew = [ones(m,1) X];
b=inv(Xnew'*Xnew)*Xnew'*Y;

## pred
Ypred=Xnew*b;
## DOF
DoFReg = p;
DoFRes = m - p - 1;

## residual error
e = (Y - Ypred);

## SS
SSRes = e'*e;
```

## **APPENDIX 2**

# Table of Parameters Used in Data Processing for PLS Testing Precuders on the Classification of Biological Activity

| Туре | Formula  | Description     |
|------|--|-----------------|
| C1   | $x_{ij} = x_{ij} - \overline{x}_j$   | Mean centring   |
| C2   | $x_{ij} = \frac{x_{ij} - \bar{x}_{j}}{\sqrt{\frac{1}{I} \sum_{i=1}^{I} (x_{ij} - \bar{x}_{j})^{2}}}$ | Standardisation |
| C3   | $x_{ij} = \frac{x_{ij} - \min(x_i)}{\max(x_i) - \min(x_i)}$  | Range scaling   |

## **AUTHOR'S PROFILE**



Mohd Zuli Jaafar obtained Bachelor of Science in Chemistry (Hons.) in 1996 from University Malaya, Kuala Lumpur, MSc in Chemistry (2002) from Universiti Teknologi Malaysia and PhD in Chemometrics (2011) from the University of Bristol, United Kingdom. His PhD thesis involves several methods in Chemometrics and Pattern Recognition includes Data Preprocessing, Regression, Classification and Variable Selection. Currently he is working on several scientific dataset i.e. Fourier Transform Infrared Spectroscopy, Near Infrared, Particle-Induced X-Ray Emission and Quantitative Structure-Activity Relationship.

#### **List of Publication:**

- Sim, S.F., T.Y. Ling, S. Lau, and M.Z. Jaafar, A novel computer-aided multivariate water quality index. Environ Monit Assess, 2015. 187(4): p. 181.
- Yatim, N.N.M., Z.M. Zain, M.Z. Jaafar, Z. Md Yusof, A.R. Laili, M.H. Laili, and M.H. Hisham. Noninvasive glucose level determination using diffuse reflectance near infrared spectroscopy and chemometrics analysis based on in vitro sample and human skin. in Systems, Process and Control (ICSPC), 2014 IEEE Conference on. 2014.
- Rasaruddin, N.F., M.E.N.M. Ruah, M.N. Hasan, and M.Z. Jaafar, Determination of Iodine Value of Palm Oils Using Partial Least Squares Regression-Fourier Transform Infrared Data. Jurnal Teknologi, 2014. 70(5).
- Rasaruddin, N.F., M.N. Hasan, M.E.N.M. Ruah, S.S. Fong, and M.Z. Jaafar. Signal processing strategies in FT-NIR and FTIR spectra of palm oils. in Signal

- Processing & its Applications (CSPA), 2014 IEEE 10th International Colloquium on Signal Processing and its Application 2014. IEEE.
- Waheed, S., M.Z. Jaafar, N. Siddique, A. Markwitz, and R.G. Brereton, PIXE analysis of PM2. 5 and PM2. 5–10 for air quality assessment of Islamabad, Pakistan: Application of chemometrics for source identification. Journal of Environmental Science and Health, Part A, 2012. 47(13): p. 2016-2027.
- Ridzuan, M.S.M., M.Z. Jaafar, and M.M. Zain. Quantitative structure-activity relationship (QSAR) modelling of N-aryl derivatives as cholinesterase inhibitors. in Humanities, Science and Engineering Research (SHUSER), 2012 IEEE Symposium on. 2012. IEEE.
- Jaafar, M.Z., A.H. Khan, S. Adnan, A. Markwitz, N. Siddique, S. Waheed, and R.G. Brereton, Multiblock analysis of environmental measurements: A case study of using Proton Induced X-ray Emission and meteorology dataset obtained from Islamabad Pakistan. Chemometrics and Intelligent Laboratory Systems, 2011. 107(1): p. 31-43.
- Saim, N., R. Osman, D.R.S.A. Spian, M.Z. Jaafar, H. Juahir, M.P. Abdullah, and F. Ab Ghani, Chemometric approach to validating faecal sterols as source tracer for faecal contamination in water. Water research, 2009. 43(20): p. 5023-5030.
- Jaafar, M.Z., S.A.I.S.M. Ghazali, and M. Musa, Basic Chemistry 1 Objective Questions for Pre Sciences Students. 2008: Pusat Penerbitan Universiti, Universiti Teknologi MARA.
- Brereton, R.G., G. Lloyd, S. Fong, K. Wongravee, and M. Jaafar. Application of Modern Supervised Pattern Recognition Methods in Chemometrics. in Multivariate Analysis and Chemometry Applied to Environment and Cultural Heritage. 2008.