UNIVERSITI TEKNOLOGI MARA

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

MOHD ZULI BIN JAAFAR
[MAX 2 LINES]

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May 2025

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MOHD ZULI BIN JAAFAR
[MAX 2 LINES]

Thesis submitted in partial fulfilment of the requirements for

Bachelor of Computer Science (Hons.)

College of Computing, Informatics and Mathematics

May 2025

SUPERVISOR APPROVAL

PROJECT TITLE

BY

STUDENT NAME
STUDENT ID

This thesis was prepared under the supervision of the project supervisor, **Supervisor's Name**. It was submitted to the College of Computing, Informatics and Mathematics and was accepted in partial fulfilment of the requirements for the degree of Choose an item..

Approved by

……………………………..

Supervisor's Name
Project Supervisor

JUNE 1, 2025

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.

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Note:

250-300 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.

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Must include all supervisors names

Limit to one (1) page only

Font: Times New Roman - 12

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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

C_g Covariance matrix for class g

LIST OF ABBREVIATIONS

Abbreviations

PCA   Principal Component Analysis

LIST OF NOMENCLATURE

13

Nomenclatures

      A   Amplitude Ratio, (No Units)

      C   Centroid of pipe, inches

CHAPTER 1

INTRODUCTION

This chapter provides the background and rationale for the study. It also gives details of the significance of privacy over the Internet, the issues and problems that led to this research.

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

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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

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Table 1.2
The Statistical Information of APM Dataset

Batch	No of samples	Average per month	Percentage of LoD (Coarse APM)	Percentage of LoD (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 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.

$$y = mx + 3 \qquad\qquad\qquad (1.1)$$

$$y = mx + 3 \qquad\qquad\qquad (1.2)$$

$$y = mx + 3 \qquad\qquad\qquad (1.3)$$

$$y = mx + 4 \qquad\qquad\qquad (1.4)$$

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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

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Th... ...you click Design an... ...s change to match... ...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 Descriptors	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	Topo	2D	119	Molecular descriptors obtained from the molecular graph (usually H-depleted), i.e 2D-descriptors conformationally independent.
3	Walk and path counts	Wap	2D	47	Molecular descriptors obtained from the molecular graph, counting paths, walk and self returning walks of different lengths.
4	Connectivity indices	Coni	2D	33	Topological Molecular descriptors calculated from the vertex degree of the atoms in the H-depleted molecular graph.
5	Information indices	Info	2D	47	Molecular descriptors calculated as information content of molecules, based on the calculation of equivalences classes from the molecular graph. Among them, the indices of neighbourhood degree and edge multiplicity.
6	2D autocorrelations	2D	2D	96	Molecular descriptors calculated from the molecular graph by summing 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 eigenvalues	Bur	2D	64	Molecular descriptors contained from the positive and negative eigenvalues of the adjacency matrix, weighting the diagonal element with atom weight.
9	Topological charge indices	Topoc	2D	21	First 10 eigenvalues (absolute values) obtained from a corrected adjacency matrix.

No	Molecular Descriptors	Abbreviation	Groups	Amount	Description
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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 descriptors	WHIM	3D	99	Molecular descriptors obtained as statistical indices of the atom projected onto the 3 principal components obtained from weighted covariance matrices of the atomic coordinates.

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Figure 1.1   The Spectra of Cooking Oil after One Hour Heating.
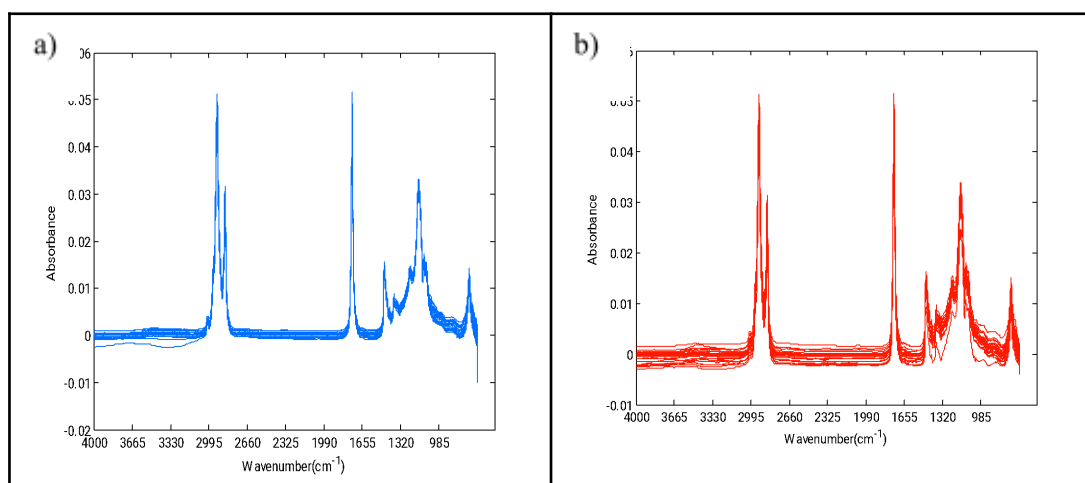
Figure 1.2   FTIR spectra for non-fried (a) and fried palm oils (b)

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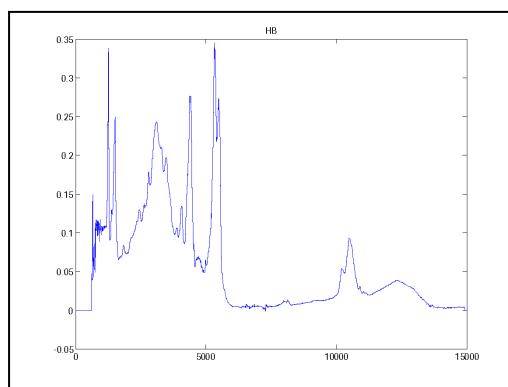iginal contained in your current template. On the Insert tab, the galleries include items that are designed to coordinate with the overall look of your document.

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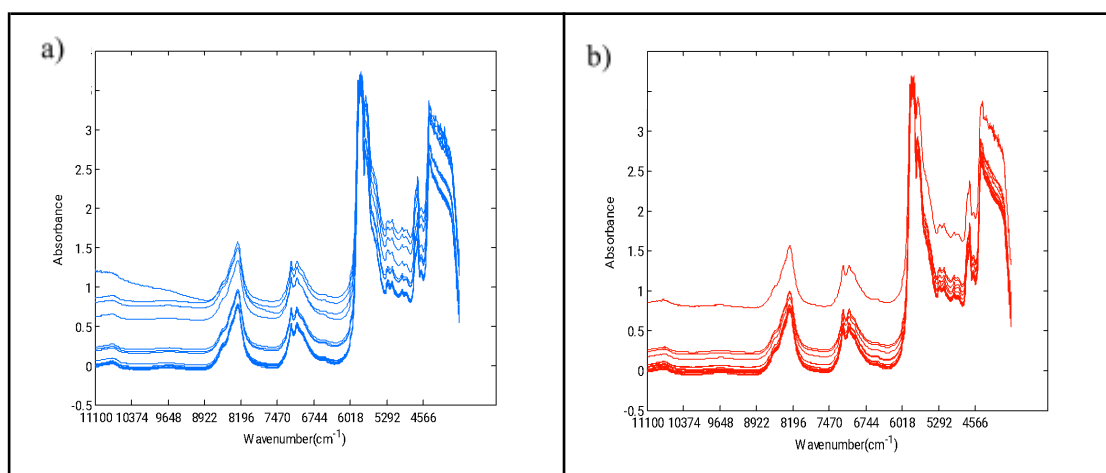
Figure 1.3   FT-NIR spectra for non-fried (blue) and fried (red) palm oils

1.8   **Assumption**

1.9   **Ethical Committee**

1.10   **Thesis Scope**

1.11   **Thesis Outline**

CHAPTER 2

LITERATURE REVIEW

This chapter provides the background and rationale for the study. It also gives details of the significance of privacy over the Internet, the issues and problems that led to this research.

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 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.

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

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

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

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

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 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
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

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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.

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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 your document	To change the overall look of your document	To change the overall look of 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 (Coarse APM)	Percentage of LoD (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.

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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.

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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	Molecular Descriptors	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
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3	Walk and path counts	Wap	2D	47	Molecular descriptors obtained from the molecular graph, counting paths, walk and self returning walks of different lengths.
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8	Burden eigenvalues	Bur	2D	64	Molecular descriptors contained from the positive and negative eigenvalues of the adjacency matrix, weighting the diagonal element with

No	Molecular Descriptors	Abbreviation	Groups	Amount	Description
					atom weight.
9	Topological charge indices	Topoc	2D	21	First 10 eigenvalues (absolute values) obtained from a corrected 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.
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14	3D-MoRSE descriptors	3D	3D	160	Molecular descriptors calculated by summing atom weights by different angular scattering function.
15	WHIM descriptors	WHIM	3D	99	Molecular descriptors obtained as statistical indices of the atom projected 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	Molecular Descriptors	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.
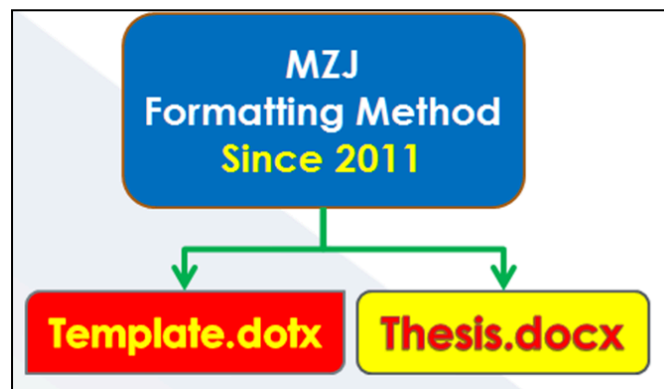

Plate 2.2   A Sample of Formatting Method

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

CHAPTER 3
RESEARCH METHODOLOG

This chapter provides the background and rationale for the study. It also gives details of the significance of privacy over the Internet, the issues and problems that led to this research.

3.1   Introduction

(Normal UiTM Paragraph 1a) 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 Classifcation

(Normal 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.

(Normal UiTM Paragraph 2b) 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.
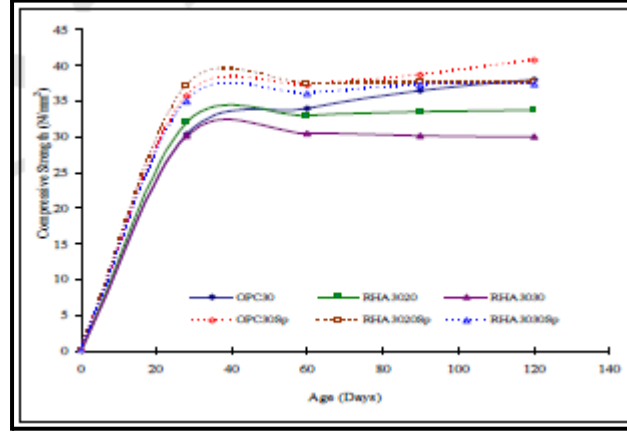
Figure 3.1   Compressive Strength of Rice Husk Ash (RHA) Concrete of Grade 30

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 (3.1and (3.2);

$$^{sq}x_{ij} = \sqrt[n]{x_{ij}} \qquad (3.1)$$

$$x_{ij} = \log_{10} x_{ij} \qquad (3.2)$$

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.

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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.

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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.
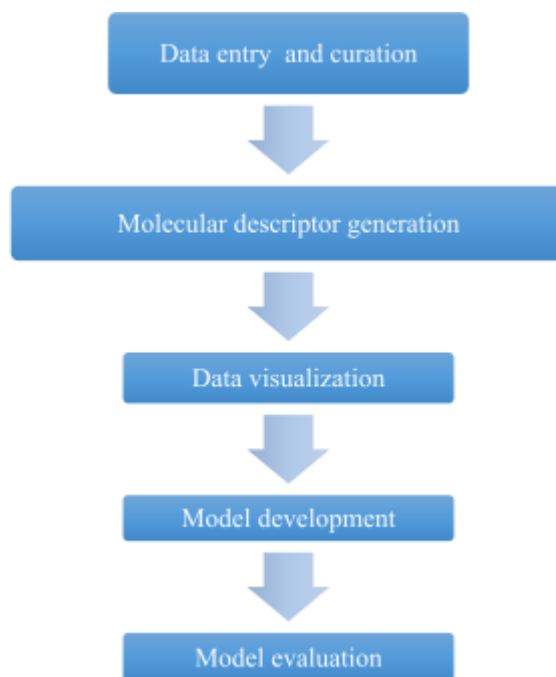
Figure 3.2   Typical Steps Involved in QSAR Methodology

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.

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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 Barrier	406×926	Non-penetrating (class 1), 136 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.
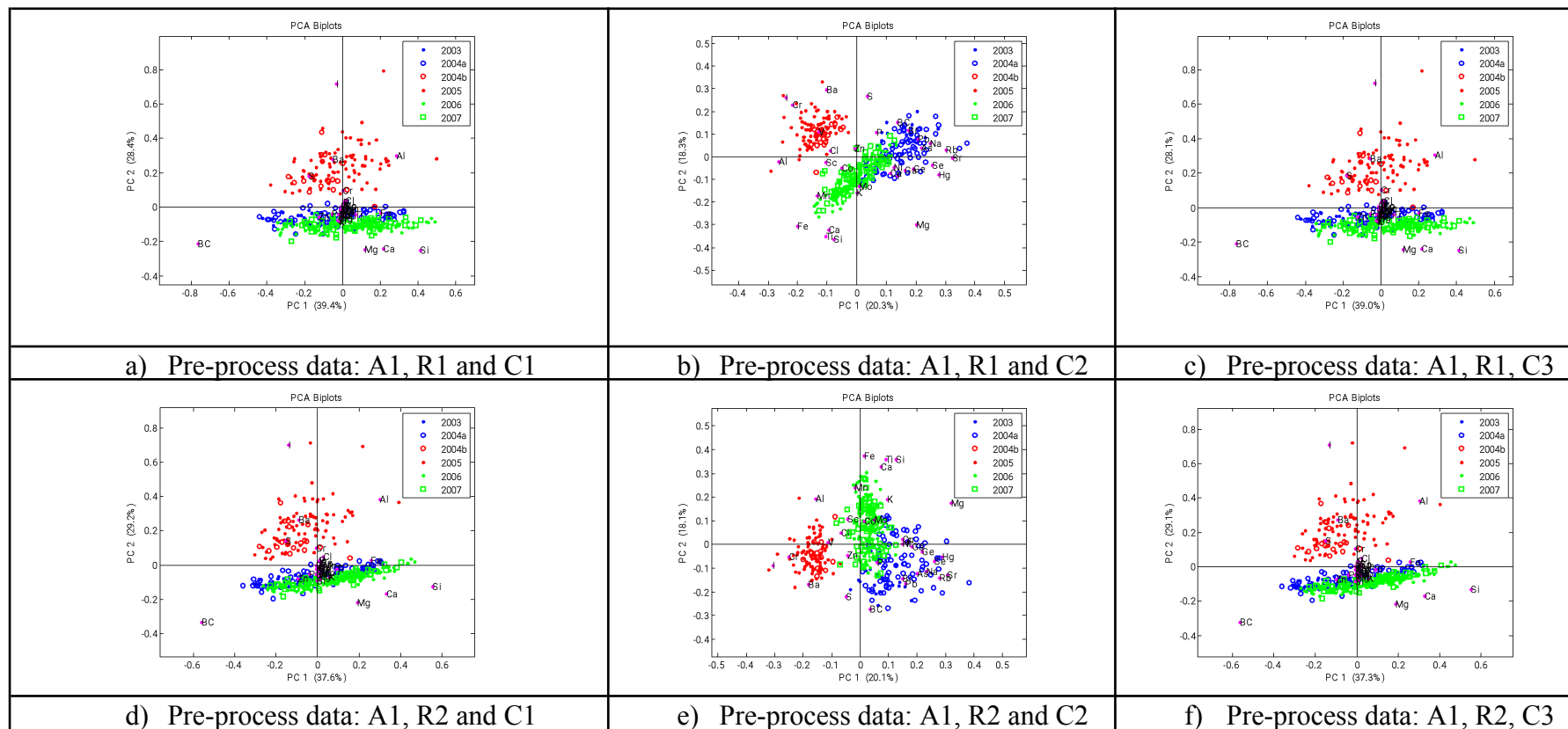
CHAPTER 4

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

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APPENDICES

APPENDIX 1

Example of the Codes in PLS Algorithms

```matlab
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

Type	Formula	Description
C1	$x_{ij} = x_{ij} - \bar{x}_j$	Mean centring
C2	$x_{ij} = \dfrac{x_{ij} - \bar{x}_j}{\sqrt{\dfrac{1}{I}\sum\limits_{i=1}^{I}(x_{ij} - \bar{x}_j)^2}}$	Standardisation
C3	$x_{ij} = \dfrac{x_{ij} - \min(x_i)}{\max(x_i) - \min(x_i)}$	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.

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