Determination of Substantial Chemical Compounds of Agarwood Oil for Quality Grading

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Abstract - **Agarwood is a resin saturated heartwood producing its ownessential oil. This oil comprises of a complex mixture of chromone derivatives, oxygenated sesquiterpenes and sesquiterpene hydrocarbons. This mixture has a heavy woody scentand is one of the contributors to the Agarwood oil quality. In this paper, a study that focuses on the approach to select the substantial chemical compounds for Agarwood quality grading was carried out. GC-MS analysis was used to extract the chemical compounds from the Agarwood oil. The data were then pre-processed using techniques such as missing values ratio, natural logarithm and min. max. normalization. Next, synthetic data were generated using MUNGE to fulfil the passing condition of sampling adequacy test. To determine the substantial compounds, PCA and Pearson's correlation were used. This approach was successful in determining three substantial compounds namely β-agarofuran, α-agarofuran and 10-epi-γ-eudesmol. These substantial chemical compounds will be used later to predict the quality of Agarwood oil.**

Index Terms—**Correlation, Principle Components Analysis, Statistical Analysis, Statistical Learning**

I. INTRODUCTION

AGARWOOD is a fragrant wood and known by many names in different cultures such as Chen Xiang, Gaharu, Eaglewood, Jinkoh, Kanankoh, Kyara and Qi-Nan[1]. It is aresin-saturated heartwood and this resin is materialized by injuring the plant using physical cuts, insects, chemical stimulationor bacterial infections [2-5]. Agarwood comprises of many families such as Leguminosae, Euphorbiaceae and Thymelaeaceae. The Thymelaeaceae family consists of two genera: Aquilaria and Gyrinops [3, 6, 7]. In Southeast Asia, nineteen species has been recognized in the taxonomical classification of genus Thymelaeaceae [3, 4]. One of the essential species from this family is Aquilaria Malaccensis and it is common species in Malaysia [2, 5].

Agarwood tree is a beneficial tree because every part is valuable as example, tree trunks (stem) and branches can be changed into chips, flakes of uniform quality powder or essential oils (Agarwood oil) which is also known as concentrated volatile aromatic compounds [1, 3, 5, 7, 8]. The price of Agarwood oil depends on its quality. Their relationship is proportional to each other. The quality is defined based on colour, odour, high fixative properties and consumer perception [7, 9]. In terms of grades, some countries use high and low [3, 9-11] and some use A, B, C and D [3, 10, 12, 13]. In terms of application, Agarwood and its oil are used in perfume, medicine and religious ceremony [2, 3, 5, 7, 9].

The quality of Agarwood oil is decided by its resin content [3, 5-7]. It inhibits tree extractives with aromatic terpenes [1, 7] and carries a high complex mixture of volatile organic compound sand gives particular strong woody scent. The combination of these fragrant compounds produces a special characteristic odour to the plant and often used by human in a form of Agarwood essential oil[14].This oil consists of a complex mixture of sesquiterpene hydrocarbons, oxygenated sesquiterpenes and chromone derivatives which are significant and active compounds in Agarwood[1-3, 5, 9, 15]. These compounds are substantial in determining the quality of Agarwood oil. The names of these compounds are various guaienes exampleα-guaiene, β-agarofuran, α-agarofuran, 10-epi-ɤ-eudesmol and valerianol. In addition, they are the major compounds present in high quality oil [1, 3, 5, 9, 10, 15].There are many techniques to extract the essential oil from Agarwood such as supercritical fluid extraction, solvent extraction, hydro-distillation and etc. Before the extraction, a pre-treatment needs to be performed on Agarwood samples such as chemical treatment, soaking in water and sonication [16]. In some research, the extracted oil is further analysed using Gas Chromatography–Mass Spectrometer (GC-MS) [1, 3, 7, 9, 10, 15]and Solid-Phase Microextraction (SPME) [3, 10, 15].

Boxplot is one of the graphical technique used to display distributional shapes and to detect unusual observations[17]. It is made up of inter quartile range (IQR), sample median, outliers and whiskers. A box consisting of the first quartile (Q1) to the third quartile (Q3) represents the IQR. This box's area represents 50% of the distribution. A sample median is defined as a line at the height of second quartile (Q2). Outliers are defined as extreme points outside the observations. They are represented by points outside the interval (Q1 – 1.5 IQR; Q3 +

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1.5 IQR where IQR = Q3 – Q1). Whiskers are lines that reach the maximum or minimum points from the ends of the box. Box plot shows the location and distribution of data using median and inter quartile range. It also shows the skewness of data using the whiskers length and median position [7, 17-19].

In statistical analysis, missing values have a direct impact on the quality of the data. Within a dataset, if the missing values are less than 1% of its total data, they are considered negligible and manageable if they are between 1 and 5%. However, if the missing values are between 5 and 15%, a sophisticated method is required to handle them. Missing values can have severe impact on the interpretation of the data if they are greater than 15%.There are a number of approaches to manage missing values. The first approach is the case elimination. This approach consists of determination and elimination of the attributes with high level of missing values. Second is mean imputation. It replaces the missing values of an attribute using mean. Third is the imputation of median. It replaces the missing values of an attribute using median. Fourth is the imputation of k-NN. It replaces the missing values of an instance with the most similar instance using nearest neighbour [7, 20, 21].

In order to have a normal distributed data, logarithmic transformation can be applied. One common alternative for logarithmic transformation is the natural logarithm, where the constant e (e≈2.7183) is used as the base. Mathematically, logarithm for any number less than zero is undefined, and between 0 and 1 and above than 1 need to be handled differently. Therefore, the data should be anchored at 1 [7, 22, 23]. To deal with zero values, a constant is often added, such as "ln(x + 1)" [24].

Shapiro Wilk test is applied for samples size less than 50. This test can distinguish the different in normality due to skewness, kurtosis or both. It has become a favourable test due to its good power properties [7, 25].

Synthetic data generation is a common practice in many research areas especially in situation where the real data may be difficult to obtain due to budget, time, etc. Synthetic data is a substitute for real data and can be employed to provide a controlled testing environment which meets specific condition. In terms of applications, the data can be used in the process of verification, simulation or proof of concepts [26].

Kaiser-Meyer-Olkin (KMO) and Bartlett's tests are the two test that need to be computed before running the Factor Analysis or Principle Components Analysis (PCA). KMO test measures the sampling adequacy of data. It produces KMO index which range from 0 to 1. To shows that the data are suitable for Factor Analysis or PCA, the minimum acceptable KMO index is 0.5 [27].

Principle Component Analysis (PCA) is a quantitative method to lower the dimension of data with a lot of variables to a new set of variable called Principle Component (PC) without losing much information. Each PC in PCA is a linear combination of the original variables and orthogonal to one another [8, 28, 29]. Basically, PCA is where principal components are obtained based on eigen value (value >1) and then rotated for orthogonal plotting[30]. The steps to do PCA are [28, 29]:

i. Compute covariance matrix, C.
ii. Calculate eigen values and eigenvectors of matrix C.
iii. Arrange the eigen values in descending order.
iv. Form a transformation matrix that consists of eigenvectors associated with eigen values.
v. Project the data onto transformation matrix.

To select significant principle components, Scree Plot has been applied. The Scree Plot is a heuristic graphic method that consists of: eigenvalues in y-axis against the principle components in x-axis. The method used in Scree Plot is by inspecting the shape of the resulting curve in order to detect the point at which the curve changes drastically (elbow). This point on the curve indicates the maximum number of components or factors to retain[31]. The original or unrotated factors are hard to interpret and not meaningful. To solve these problems, factor rotation techniques such as Varimax and Quartimax are used. Varimax is a rotation method used in statistical analysis. It rotates orthogonally by minimizing the number of variables with high loadings which can be either positive or negative and by maximizing the variance of each factor loading by making high loadings higher and low loadings lower. This method simplifies factor interpretation. Mathematically, it redistributes the total variance among variables between smaller numbers of factors with relatively equal variances. The amount of variations among the major unrotated factors will be redistributed among the other smaller factors[32]. To select the significant compounds, interpretation of correlation coefficient can be applied after factors rotation. Table I shows a few interpretation of Pearson's correlation coefficient.

TABLE I
INTERPRETATION OF PEARSON'S CORRELATION COEFFICIENTS

Correlation Coefficient		Dancey and Reidy[33]	Quinnipiac University[33]	Chan Y. H.[33]
1.00	-1.00	Perfect	Perfect	Perfect
0.90	-0.90	Strong	Very Strong	Very Strong
0.80	-0.80	Strong	Very Strong	Very Strong
0.70	-0.70	Strong	Very Strong	Moderate
0.60	-0.60	Moderate	Strong	Moderate
0.50	-0.50	Moderate	Strong	Fair
0.40	-0.40	Moderate	Strong	Fair
0.30	-0.30	Weak	Moderate	Fair
0.20	-0.20	Weak	Weak	Poor
0.10	-0.10	Weak	Negligible	Poor
0.00	0.00	None	None	None

This study focuses on determining the substantial chemical compounds of Agarwood oil and can be divided into 3 parts in general: pre-processing, generation of synthetic data and determination of substantial chemical compounds. It comprises of 4 sections namely introduction, method, results and discussion, and conclusion. Introduction represents the literature review of Agarwood oil, box plot, missing values ratio, natural logarithm transformation, normalization, MUNGE, PCA and Pearson's correlation. Method consists of two parts specifically data acquisition and data analysis. In data analysis, the method of pre-processing, generation of synthetic data and determination of substantial chemical compounds were explained. The findings of this study were shown and discussed in results and discussion. The accomplishment of this study was described in conclusion.

II. METHOD

Method consists of two subsections: Data Acquisition and Data Analysis. Data acquisition is the process of obtaining the chemical compounds of Agarwood oil. Data analysis involves all the techniques used in this analysis specifically missing values ratio, natural logarithm, min.max. normalization MUNGE, principal components analysis and correlation coefficient.

A. Data Acquisition

In this paper, all 22 Agarwood oil samples come from Aqualaria species. They are acquired from Forest Research Institute Malaysia (FRIM) and Universiti Malaysia Pahang (UMP). These chemical compounds were extracted and analysed using GC-MS. The temperature of GC-MS apparatus was initially set for 10 min. at 60º C. The temperature then was increased at3º C per minute and stopped at 230º C.The flow rate of the gas carrier namelyhelium was set at 1ml per min. The temperature of ion source was set at 280º C. By matching them with the mass spectral library (HPCH2205.L; Wiley7Nist05a.L; NIST05a.L), 104 chemical compounds were recognized with the aid of a chemist.

B. Data Analysis

This subsection includes dimension reduction, data transformation, data rescaling, normality test, generation of synthetic data and determination of substantial chemical compounds. The general process flow of data analysis is represented by Fig. 1.

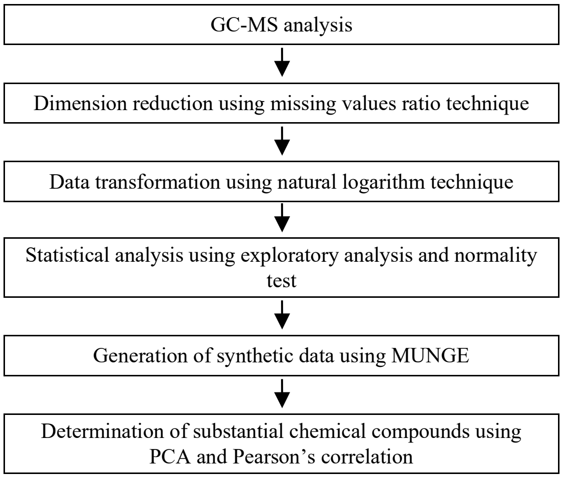


Fig. 1: General process flow of data analysis

Figure 2 shows the flow diagram of dimension reduction, data transformation and data rescaling. GC-MS data consists of 22 samples of Agarwood oil with 104 chemical compounds. First, the number of chemical compounds was reduced using missing values ratio technique. In order to select competent data, the eigen values of correlation matrix were calculated with a decrease of 1% missing values and it stops when the correlation matrix has no negative eigen values. Samples with equal or more than 72% of missing values were removed at the end. Only 20 were left out of 106 chemical compounds.

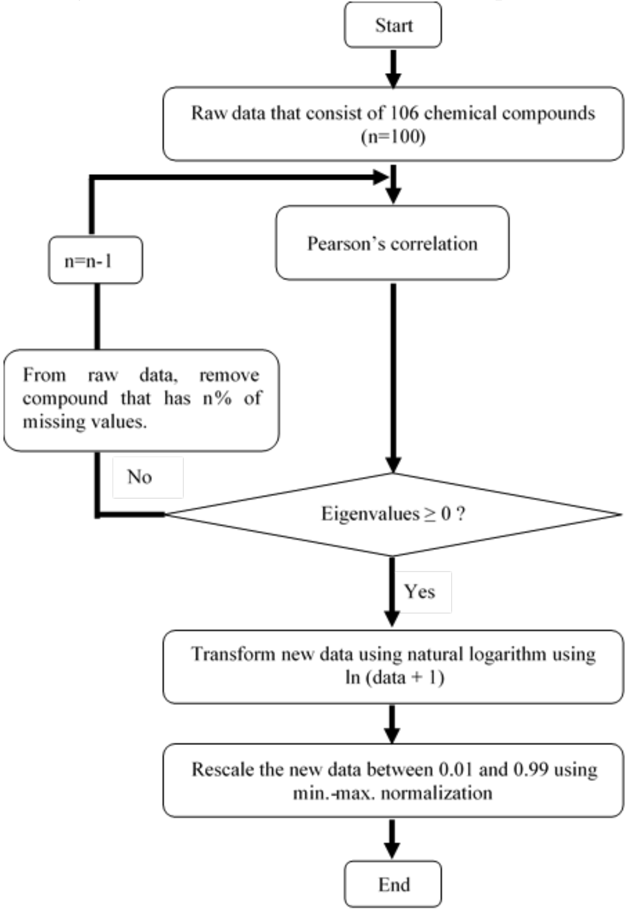


Fig. 2: Flow diagram of dimension reduction, data transformation and data rescaling

The data with20 compounds were then transformed using natural logarithm. The formula used is expressed by (1) [24]. This technique is useful for data with positive skewness [7, 22, 23].

$$a' = ln(a + 1) \tag{1}$$

Each attribute was subsequently rescaled using min. max. normalization from 0.01 to 0.99 as indicated in (2) [34]. This rescaling was applied to raw data, data after missing values ratio and data after natural logarithm for comparison.

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}} * (x_{newmax} - x_{newmin}) + x_{newmin} \tag{2}$$

Then using the box plot and the normality test, the rescaled data were analysed. Box plot provides relevant information such as quartiles, maximum and minimum value, median and outliers. It has certain advantages such as simplicity of design, quick expression of critical information of dataset and data distribution[35]. Due to its ability to detect non-normality for a wide variety of statistical, Shapiro Wilk was selected for normality test. It is an efficient omnibus test of normality, regardless of sample size and distribution [36, 37]. If the p-value is less than the level of significance chosen, the null hypothesis can be rejected and thus, it supports the non-Gaussian distribution[38]. Shapiro's Wilk test is defined by (3) and (4)[36].

$$w = \frac{(\sum_{i=1}^{N} a_i y_i)}{\sum_{i=1}^{N} y_i - m_1} \tag{3}$$

where

$$w = \frac{(\sum_{i=1}^{N} a_i y_i)}{\sum_{i=1}^{N} y_i - m_1} \tag{4}$$

It is necessary to generate synthetic data before selecting the significant compounds using PCA. A technique called MUNGE was applied here. This technique is based on closest neighbour. First, the closest neighbours for each element were determined from the original dataset. Here, Euclidean distance was used to calculate the distance. Next, the element e from original dataset was exchanged with its nearest neighbour e' with probability p and remains unchanged with probability 1-p [39, 40].The synthetic data that were generated should pass the test of KMO and Bartlett. The value of KMO and p-value of Bartlett should be greater than or equal to 0.5 and smaller than 0.05 respectively [27].

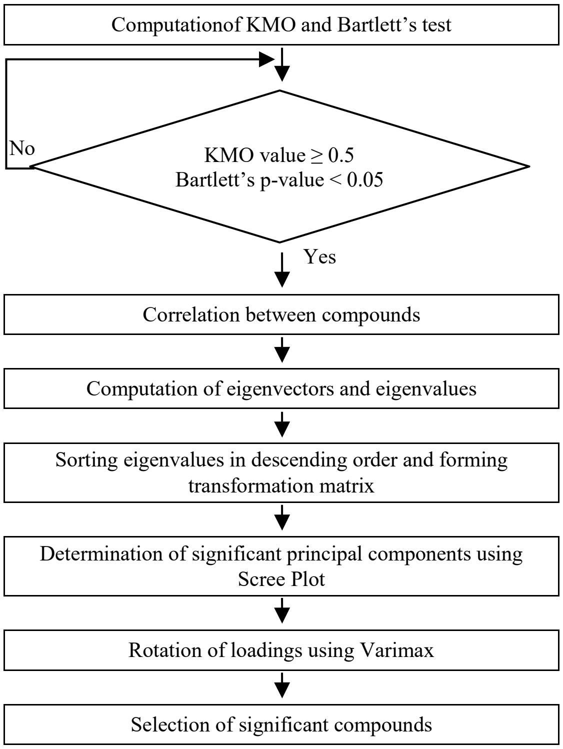


Fig. 3: Flow chart of KMO and Bartlett's test, and PCA

PCA and Pearson's correlation were then used to identify substantial chemical compounds. The data with 19 chemical compounds were first computed using Pearson's Correlation. These correlated data were used as PCA input. Figure 3 displays the flow chart of KMO and Bartlett's test, and PCA. Then from the correlation matrix, the eigen values and eigenvectors were determined. Next in descending order, the eigen values were sorted. After that, a transformation matrix was computed which consists of eigenvectors associated with eigenvalues. Significant principal components were then determined using Scree Plot. Y-axis represents the eigen values and x-axis principle components. The first elbow and the large gap of the Scree Plot were observed and the principal components until the first elbow and before the gap are known as the significant principal components [31]. Finally, the principal components were rotated using Varimax and significant chemical compounds were extracted by selecting a chemical compound with a correlation coefficient greater than or equal to 0.60[33].

The significant chemical compounds obtained from PCA were again reduced by Pearson's correlation. The substantial chemical compounds were determined by selecting a chemical compound with correlation coefficients greater than or equal to 0.60. The Pearson's correlation coefficient is calculated using (5)[41].

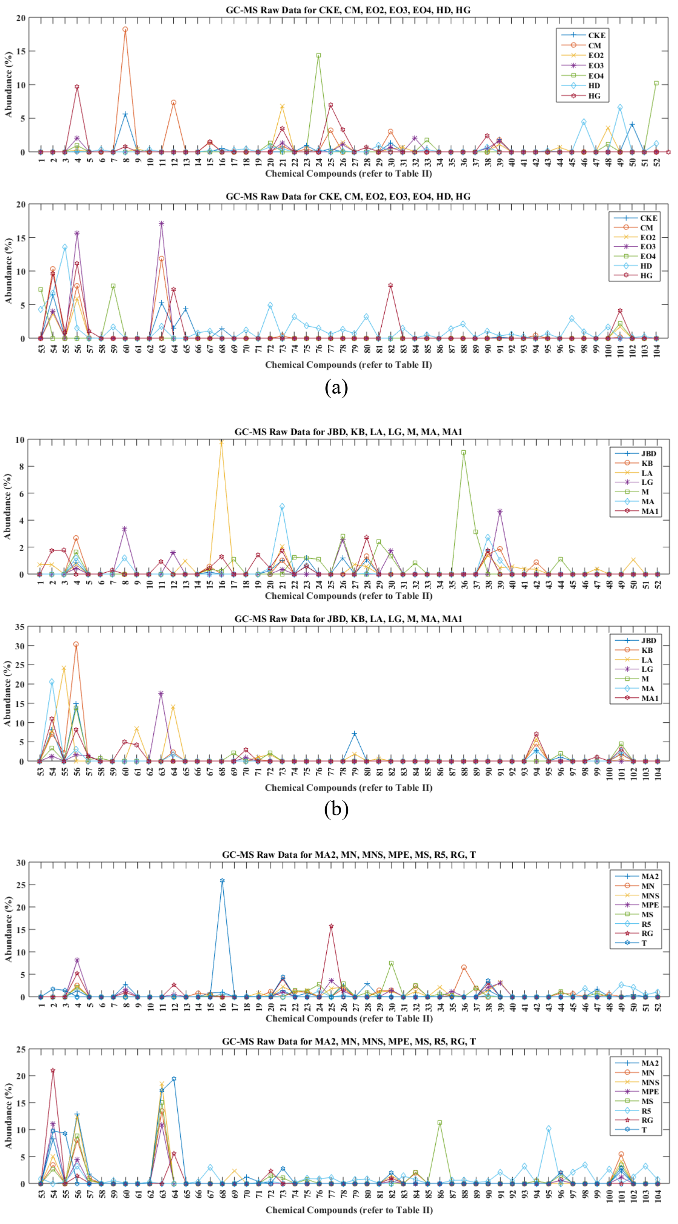
$$r = \frac{(\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}))}{\sqrt{(\sum_{i=1}^{n}(x_i - \bar{x})^2)}\sqrt{(\sum_{i=1}^{n}(y_i - \bar{y})^2)}} \tag{5}$$

III. RESULTS AND DISCUSSION

This section is divided into two sub-sections: pre-processing and determination of substantial compounds. Pre-processing consists of results and discussion after missing values ratio technique, natural logarithm technique and Shapiro-Wilks test. Meanwhile, under the determination of substantial compounds, the results of PCA and Pearson's correlation were shown and discussed.

A. Pre-Processing

The raw data were obtained from GC-MS analysis. 22 samples of Agarwood oil were analysed and each sample consists of 104 chemical compounds. The compound were measured as percentage of compound abundance. The abundance patterns of chemical compounds for each sample are displayed in Fig. 4(a), 4(b) and 4(c). The names of 104 chemical compounds can be found in Table II. It can be observed that a number of chemical compounds have a value of 0% abundance for nearly every sample as examples 2-phenyl propanal, nonanoic acid, decanoic acid, α-funebrene, β-maaliene, β-copaene and etc. The value of 0% indicates that the compound does not exist in a sample. These missing values need to be managed by a certain approach such as missing values ratio technique. Other chemical compounds such as 4-phenyl-2-butanone, β-agarofuran, α-agarofuran, 10-epi-γ-eudesmol, ɤ-eudesmol and dihydrocollumellarin are present in nearly all samples.



(a)

(b)

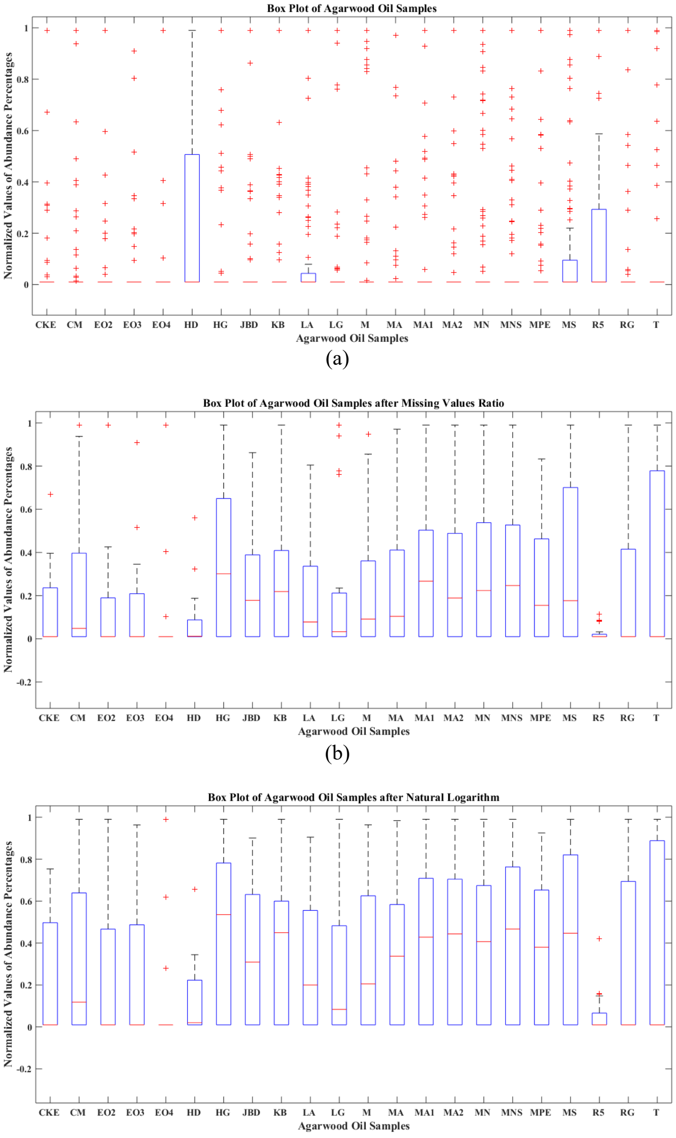
(c)

Fig. 4: (a) GC-MS raw data for CKE, CM, EO2, EO3, EO4, HD and HG; (b) GC-MS raw data for JBD, KB, LA, LG, M, MA and MA1; (c) GC-MS raw data for MA2, MN, MNS, MPE, MS, R5, RG and T

TABLE II
NAMES OF CHEMICAL COMPOUNDS OF AGARWOOD OIL ACQUIRED FROM THE GC-MS ANALYSIS.

No.	Chemical Compounds	No.	Chemical Compounds
1	2-phenyl propanal	53	1,5-epoxy-nor-ketoguaiene
2	Benzaldehyde	54	10-epi-ɤ-eudesmol
3	Benzeneacetonitrile	55	Agarospirol
4	4-phenyl-2-butanone	56	ɤ-eudesmol
5	nonanoic acid	57	alloaromadendrene epoxide
6	decanoic acid	58	selina 3,11-dien-6α-ol
7	α-funebrene	59	jinkoh-eremol
8	α-gurjunene	60	guaia-3,9-dien-11-ol
9	a-cedrene	61	β-eudesmol
10	β-maaliene	62	Kusunol
11	β-copaene	63	α-eudesmol
12	β-Gurjunene	64	Valerianol
13	ϒ-elemene	65	selina 11-en-4α-ol
14	β-humulene	66	Bulnesol
15	α-guaiene	67	dehydrojinkoh-eremol
16	aromadendrane	68	β-bisabolol
17	amorpha-4,11-diene	69	Cadalene
18	drima-7,9(11)-diene	70	α-bisabolol
19	valencene	71	Selina-3,11-dien-9-one
20	ϒ-gurjunene	72	Cyperotundone
21	β-agarofuran	73	10-nor-calamenen-10-one
22	ϒ-muurolene	74	Rotundone
23	ar-curcumene	75	Longifolol
24	β-selinene	76	selina-4,11-dien-14-oic acid
25	cis-β-guaiene	77	selina-3,11-dien-14-al
26	α-muurolene	78	9,11-eremophiladiene
27	ϒ-guaiene	79	selina-3,11-dien-14-ol
28	β-dihydro agarofuran	80	selina-4,11-dien-14-al
29	α-bulnesene	81	Aristolone
30	ϒ-cadinene	82	β-costol
31	δ-cadinene	83	guaia-1(10),11-dien-15-ol
32	cis-calamenene	84	selina-3,11-dien-14-oic acid
33	α-elemol	85	Sinenofuranol
34	(Z)-nerolidol	86	14-hydroxy-α-muurolene
35	α-cadinene	87	2-hexadecanone
36	selina-3, 7(11)-diene	88	Dihyrokaranone
37	hedycaryol	89	guaia-1(10),11-dien-15-al
38	α-agarofuran	90	Karanone
39	elemol	91	oxo-agarospirol
40	dodecanoic acid	92	pentadecanoic acid
41	β-vetivene	93	Hexadecanol
42	ϒ-vetivenene	94	hexadecanoic acid
43	nor-keto-agarofuran	95	Eudesmol
44	β-calacorene	96	Thujopsenal
45	dodecanoic acid	97	palmitic acid
46	epoxy-bulnesene	98	2-hydroxyquaia-1(10),11,15-oic acid
47	spathulenol	99	Cyclohexadecanolide
48	viridiflorol	100	9-hydroxyselina-4,11-dien-14-oic acid
49	tetradecanal	101	Dihydrocollumellarin
50	β-Gurjunene	102	1,5-diphenyl-2-pentene
51	guaiol	103	guaia-1(10),11-dien-15,2-olide
52	hinesol	104	oleic acid

Figure 5(a), 5(b) and 5(c) display the box plots of raw GC-MS data, GC-MS data after missing values ratio and after natural logarithm technique respectively. Figure 5(a) shows that only 4 samples (HD, LA, MS and R5) had third and fourth quartile. Therefore, HD, LA, MS and R5 have50% of their data points between 0.01 and 0.99, 0.05, 0.1 and 0.3 respectively. In other samples, their data points were shown as outliers. All samples had a median of 0.01. Figure 5(b) reveals that only EO4 had no inter quartile range (IQR) after eliminating the compounds that have missing values equal to or greater than 72%.The medians of CKE, EO2, EO3, HD, R5, RG and T were equivalent to 0.01. Therefore, about 50% of the data points are above 0.01. The medians of other samples ranged from 0.05 to 0.3. It means that between this range lie 50% of the data points. The samples with outliers were CKE, CM, EO2, EO3, EO4, HD, LG, M and R5. Compared to the raw GC-MS data, the number of outliers decreases significantly. The range of second and third quartile, and the maximum value increased after the computing of the natural logarithm technique. In comparison to the Fig. 5(c) (data after the missing values ratio), only EO4, HD and R5 had outliers and the samples with a median of approximately 0.01 were still the same. All samples, except EO4, are right skewed. EO4 is the only sample that has not greatly improved in term of normal distribution.



(a)

(b)

(c)

Fig. 5: (d) Box plot of GC-MS raw data; (e) Box plot after the missing values ratio technique; (f) Box plot after natural logarithm transformation

Table III displays the p-values of Shapiro-Wilk normality test for each samples of Agarwood oil from raw GC-MS data, data after missing values ratio and after natural logarithm. The p-values of all samples were smaller than the selected alpha level (0.05) for raw GC-MS data. Therefore with 95% confidence, these data are not normally distributed. There was some improvement in p-values for HG, JBD, KB, MA, MA1, MA2, MN, MNS, MPE and MS after missing values ratio. JBD was the sample with the highest p-value (0.008). Even with some improvement in p-values, data are still not normal distributed. After natural logarithm transformation, the p-values increased for all samples except CKE, EO2, EO4, HD, LG, R5, RG and T. MN had the highest p-value which is 0.015. The p-values of JBD, MA, MA2, MN and MNS were between 0.012 and 0.015. Even with the improvement of p-value, the data are still not normal distributed. It was found that using the technique of z-score and the Artificial Neural Network, JBD and MA1 belong to high quality oil and CKE, HD and R5 belong to low quality oil[10, 42]. In this study, CKE, HD and R5 have smaller p-value than JBD and MA1.

TABLE III
P-VALUES OF SHAPIRO-WILK NORMALITY TEST FOR AGARWOOD OIL SAMPLES

Sample	p-Value		
	Raw GC-MS Data	Data after Missing Values Ratio	Data after Natural Logarithm Transformation
CKE	0.000	0.000	0.000
CM	0.000	0.000	0.001
EO2	0.000	0.000	0.000
EO3	0.000	0.000	0.001
EO4	0.000	0.000	0.000
HD	0.000	0.000	0.000
HG	0.000	0.002	0.001
JBD	0.000	0.008	0.012
KB	0.000	0.003	0.005
LA	0.000	0.000	0.001
LG	0.000	0.000	0.000
M	0.000	0.000	0.001
MA	0.000	0.001	0.012
MA1	0.000	0.004	0.006
MA2	0.000	0.004	0.012
MN	0.000	0.004	0.015
MNS	0.000	0.006	0.013
MPE	0.000	0.002	0.006
MS	0.000	0.002	0.008
R5	0.000	0.000	0.000
RG	0.000	0.000	0.000
T	0.000	0.000	0.000

B. Determination of Substantial Compounds

Table IV shows the values of KMO and Bartlett's test before performing the PCA. The KMO value for original samples (22 samples) was only 0.248. The KMO value increased to 0.358 with 220 samples (original + synthetic) but was still below the accepted value (0.50). With 440 samples (original + synthetic), the KMO value increased to 0.442 but was still below the accepted value. The KMO value was greater than 0.50 (accepted value) when the total number of original and synthetic samples was 660. The 660 samples are therefore sufficient to run the PCA. In Bartlett's Test, the p-value for all numbers of samples is less than 0.05 and thus, suggests that PCA may be useful with this data.

TABLE IV
INDEX OF KMO AND SIGNIFICANT VALUE OF BARTLETT'S TEST

KMO and Bartlett's Test for 22 Samples (Original Samples)	
KMO Test (Measure of Sampling Adequacy)	0.248
Bartlett's Test (Significant Value)	0.000
KMO and Bartlett's Test for 220 Samples	
KMO Test (Measure of Sampling Adequacy)	0.358
Bartlett's Test (Significant Value)	0.000
KMO and Bartlett's Test for 440 Samples	
KMO Test (Measure of Sampling Adequacy)	0.442
Bartlett's Test (Significant Value)	0.000
KMO and Bartlett's Test for 660 Samples	
KMO Test (Measure of Sampling Adequacy)	0.510
Bartlett's Test (Significant Value)	0.000

Table V shows the eigen values of 20 principle components. PC1 until PC6 has eigen values greater than 1. In term of proportion, Both PC1 and PC2 have proportion of variance greater than 20%. These 2 PCs account for almost 42% of the variance explained.

TABLE V
EIGENVALUES OF PRINCIPLE COMPONENTS

PC	Eigenvalues	Variance (%)	Cumulative of Variance (%)
1	4.10	21.59	21.59
2	3.81	20.06	41.65
3	2.55	13.43	55.08
4	1.57	8.27	63.35
5	1.49	7.86	71.21
6	1.39	7.34	78.55
7	0.87	4.59	83.14
8	0.65	3.43	86.57
9	0.55	2.88	89.45
10	0.50	2.63	92.08
11	0.37	1.94	94.02
12	0.26	1.34	95.36
13	0.23	1.19	96.56
14	0.20	1.06	97.62
15	0.17	0.92	98.54
16	0.12	0.61	99.14
17	0.07	0.36	99.51
18	0.05	0.29	99.79
19	0.04	0.21	100.00
20	4.10	21.59	21.59

Figure 6 shows the Scree plot. There is a sharp decline (see first elbow) and a large gap between PC2 and PC3in eigen values [31]. Because of this, only two main components (PC1 and PC2) are considered to be significant.

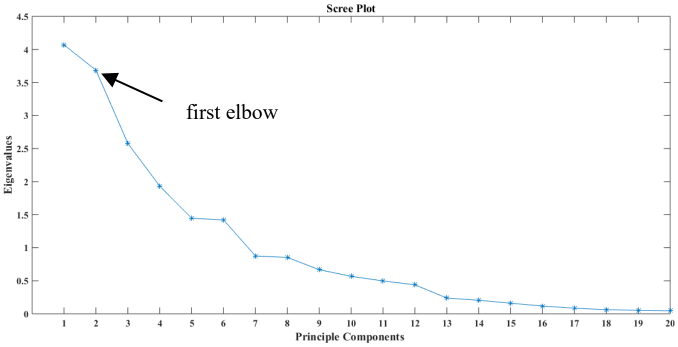


Fig. 6: Scree Plot using Eigenvalues

Table VI shows the correlation coefficients of chemical compounds for PC1 and PC2. There are 11 out of 20 chemical compounds listed in either PC1 or PC2 that have a moderate and very strong correlation (r ≥ 0.6)[33]. Their correlation coefficient varies from 0.61 to 0.81. The names of the 11 compounds are α-guaiene, β-agarofuran, ar-curcumene, β-dihydroagarofuran, φ-cadinene, α-agarofuran, 10-epi-φ-eudesmol, φ-eudesmol, alloaromadendrene epoxide, valerianol and dihydrocollumellarin.

TABLE VI
CORRELATION COEFFICIENT OF CHEMICAL COMPOUNDS IN PC1 AND PC2 AFTER ROTATION USING VARIMAX

Compounds	r-PC1	r-PC2
4-phenyl-2-butanone	-0.0667	-0.4514
α-gurjunene	0.2045	0.2059
α -guaiene	-0.0586	-0.6130
aromadendrane	-0.3897	0.1299
φ -gurjunene	-0.0107	-0.0444
β-agarofuran	-0.6725	-0.0295
ar-curcumene	0.3074	-0.6180
α -muurolene	0.5167	-0.5856
β -dihydro agarofuran	-0.3028	-0.6708
φ -cadinene	0.7981	-0.0880
α –agarofuran	-0.8137	-0.1860
Elemol	0.3899	0.2867
10-epi- φ –eudesmol	-0.6667	-0.1581
φ –eudesmol	0.2144	-0.7562
alloaromadendrene epoxide	0.2465	-0.6406

α –eudesmol	0.5776	0.1675
Valerianol	-0.7311	0.1317
hexadecanoic acid	-0.2335	-0.3337
Thujopsenal	-0.0634	-0.1809
Dihydrocollumellarin	-0.0534	-0.7604

Table VII shows the Pearson's correlation coefficients for the 11 significant chemical compounds after PCA. There were 3 pairs of compounds with a correlation coefficient greater than or equal to 0.60 and the pairs are β-agarofuran and α-agarofuran, β-agarofuran and 10-epi-γ-eudesmol, andα-agarofuran and 10-epi-γ-eudesmol. All of these pairs had apositive correlation and are therefore proportional to each other. These compounds are consistent with the significant compounds mentionedin the literature [1, 3, 5, 9, 10, 15].Some pairs such as α-guaiene and γ-cadinene, α-guaiene and valerianol, γ-cadinene and dihydrocollumellarin, and valerianol and dihydrocollumellarin have a correlation coefficient less than 0.1. It indicates that they are not correlated to each other. From these pairs, only valerianol and dihydrocollumellarin have a negative correlation. These two compounds are inversely proportional to each other.

TABLE VII
PEARSON'S CORRELATION COEFFICIENTS OF SIGNIFICANT CHEMICAL COMPOUNDS

	α-guaiene	β-agarofuran	ar-curcumene
α-guaiene	1.0000	0.0041	0.2520
β-agarofuran	0.0041	1.0000	-0.3000
ar-curcumene	0.2520	-0.3000	1.0000
β -dihydro agarofuran	0.4705	0.0527	0.3261
γ-cadinene	0.0613	-0.4262	0.3769
α –agarofuran	0.0445	0.6767	-0.1474
10-epi- φ –eudesmol	0.2319	0.6263	0.0380
φ –eudesmol	0.4921	0.0095	0.4743
alloaromadendrene epoxide	0.4442	-0.1230	0.3100
Valerianol	0.0740	0.5088	-0.3213
Dihydrocollumellarin	0.2972	0.1177	0.5155

	β -dihydro agarofuran	γ-cadinene	α –agarofuran
α-guaiene	0.4705	0.0613	0.044
β-agarofuran	0.0527	-0.4262	0.677
ar-curcumene	0.3261	0.3769	-0.147
β -dihydro agarofuran	1.0000	-0.2215	0.290
γ-cadinene	-0.2215	1.0000	-0.573
α –agarofuran	0.2899	-0.5725	1.000
10-epi- φ –eudesmol	0.2042	-0.2661	0.741
φ –eudesmol	0.4326	0.1720	0.017
alloaromadendrene epoxide	0.4604	0.1807	-0.062
Valerianol	0.0350	-0.4130	0.592
Dihydrocollumellarin	0.3287	0.0248	0.172

	10-epi- φ -eudesmol	φ -eudesmol	alloaromadendrene epoxide
α-guaiene	0.232	0.492	0.444
β-agarofuran	0.626	0.009	-0.123
ar-curcumene	0.038	0.474	0.310
β -dihydro agarofuran	0.204	0.433	0.460
γ-cadinene	-0.266	0.172	0.181
α -agarofuran	0.741	0.017	-0.062
10-epi- φ -eudesmol	1.000	0.052	-0.128
φ -eudesmol	0.052	1.000	0.339
alloaromadendrene epoxide	-0.128	0.339	1.000
Valerianol	0.484	-0.395	-0.206
dihydrocollumellarin	0.039	0.389	0.435

	valerianol	dihydrocollumellarin
α-guaiene	0.074	0.297
β-agarofuran	0.509	0.118
ar-curcumene	-0.321	0.515
β -dihydro agarofuran	0.035	0.329
γ-cadinene	-0.413	0.025
α -agarofuran	0.592	0.172
10-epi- φ -eudesmol	0.484	0.039
φ -eudesmol	-0.395	0.389
alloaromadendrene epoxide	-0.206	0.435
valerianol	1.000	-0.021
dihydrocollumellarin	-0.021	1.000

IV. CONCLUSION

In conclusion, the approach combining missing values ratio, PCA and Pearson's correlation is capable of determining the substantial chemical compounds. Three moderate and strong correlated compounds have been identified from 104 compounds and they are β-agarofuran, α-agarofuran and 10-epi-γ-eudesmol. These compounds are consistent with the list of major compounds described in the literature [1, 3, 5, 9, 10, 15]. They are substantial in determining the quality of Agarwood oil [1, 3, 5, 9, 10, 15]. For future work, these compounds can be used in identifying the grades of Agarwood oil using artificial intelligence technique due to the facts that β-agarofuran, α-agarofuran and 10-epi-γ-eudesmol can be found in high quality oil [1, 3, 5, 9, 10, 15]. In the case of none correlated compounds, a further analysis should be carried out to determine if they can be significant in the determination of Agarwood oil grades.

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