

# Statistical Analysis of *Cymbopogon* Chemical Compounds for Oils Species

Khairul Anis Athirah Kamarulzaini, Nurlaila Ismail, Mailina Jamil, Nor Azah Mohd Ali, Sahrim Lias & Mohd Nasir Taib

**Abstract**—*Cymbopogon* essential oil is extracted from the *Cymbopogon* species which are citronella and lemongrass. This situation may cause confusion and mistake by the selection of the planters. This essential oil is commonly used as aromatherapy and pharmacological activities such as anti-bacterial. The compounds identified in this *Cymbopogon* oils are mainly geraniol, citronellal, citronellol, geranyl acetate, linalool, limonene and germacrene D. The paper aims to summarize the statistical analysis of *Cymbopogon* chemical compounds between citronella and lemongrass for oils species by using SPSS software. This study consists of data extraction for the oils species using GC-MS machine to identify their chemical compounds. Then, statistical analysis data was performed which consist of the values of abundances. Next, the descriptive statistics data was carried out by evaluating the minimum and maximum data, mean, standard deviation, variance and kurtosis. The result showed that geraniol compound achieved the highest value of abundances and descriptive statistics for both datasets compared to other compounds because it has a role as a fragrance, an allergen and a plant metabolite. This is proven that statistical analysis and descriptive statistics in this study were able to summarize the preliminary data of *Cymbopogon* oil compounds according to its species which are lemongrass and citronella.

**Index Terms**— *Cymbopogon* oil, citronella, lemongrass, gas chromatography-mass spectrometry (GC-MS), statistical analysis

## I. INTRODUCTION

*Cymbopogon* essential oils are the oil extracted from the different parts of *Cymbopogon* grass. *Cymbopogon*, a genus with belongs to the Poaceae family [1], in a major group of Angiosperms. *Cymbopogon*'s name is derived between "kymbe" (boat) and "pogon" (beard) from the Greek words that refer to the flower spike [2]. The genus of *Cymbopogon* has 55 species which are generally distributed in the tropical and subtropical regions of Africa, America, Asia and other tropical countries [3, 4]. Natural sources of essential oils can be extracts by several species of *Cymbopogon* such as *C.citratus* (lemongrass), *C.martini* (palmarosa), *C.winterianus* (citronella java) and *C.nardus* (jamarosa) [5-7].

This manuscript is submitted on 30th July 2019 and accepted on 10th March 2020. Khairul Anis Athirah Kamarulzaini, Nurlaila Ismail and Mohd Nasir Taib are with the Faculty of Electrical Engineering, Universiti Teknologi MARA, 40450 Shah Alam, Selangor (email: khairulanisathirah@yahoo.com.my)

Mailina Jamil, Nor Azah Mohd Ali and Sahrim Lias are with Department of Herbal Product Development Programme, Natural Product Division, Forest Research Institute Malaysia (FRIM), 52109 Kepong, Selangor.

Two main species of *Cymbopogon* for this study are lemongrass and citronella. This genus is outstanding for its high content of essential oils that is commercially valuable and used in the cosmetics, perfumery, foods and flavor industries. Additionally, the oils showed several biological activities including anticancer, antimicrobial, pesticides, anti-inflammatory, mosquito repellent, and hypoglycemic activity [4, 8]. The geraniol compounds present the results that has potent anti-inflammatory, anti-angiogenic, anti-cell proliferative, and apoptosis [9].

Table 1 shows the summarized uses of lemongrass oil for various purposes in various countries. For citronella oils, before the recorded history of mankind, these essential oils commonly used in religious ceremonies and embellishment, to therapy and personal use [10]. As active flavor and aromatic ingredients of perfumery and cosmetic mixtures, the demand for these oils is also speedily increasing in hygiene and health care formulations (e.g. oils in toothpastes, mouthwashes etc.) including aromatherapy in fringe medicines [10, 11]. Also, another dimension of their commercial importance to some specific oil components that used as chiral auxiliaries in synthetic organic chemistry and microbial transformations of common structures to allow highly functionalized substances to enlarge economic value [11]. The parts used are the leaves and the whole plant. Lemongrass is non-toxic grass while citronella can be toxic to pollinators [11].

The chemical compounds of these *Cymbopogon* essential oils have been investigated, which have more than eighty compounds and the most important compounds are geraniol, citronellal and limonene. The other compound that present are citral (a mixture of geraniol and neral), citronellol, linalool, elemol, geranyl acetate, 1,8-cineole,  $\beta$ -caryophyllene, methyl heptenone, and geranyl formate [5, 7, 12, 13]. Thus, this study aims to summarize the statistical analysis of *Cymbopogon* chemical compounds for oils species using SPSS software. This study will also evaluate descriptive statistic of *Cymbopogon* oils species between lemongrass oils and citronella oils. For the planters and local herbal industries, this project is useful as *Cymbopogon* species are easily grown and have the potential for future brand development. And also this situation may help planters select the right species of *Cymbopogon*.

TABLE 1  
C.CITRATUS OIL'S ETHNO-PHARMACOLOGY

Country	Uses	References
Malaysia & Indonesia	As tea, soup, an emmenagogue	[2, 14, 15]
Thailand	As a fragrance, eaten as a flavoring, medicinal such as a stomachic and for diabetes	[2, 16-18]
India	To repel snakes, drops of essential oil for gastric troubles, drops of essential oil adding with lemon juice for cholera, used for bathing in cases of severe fever and headache, as a sedative for the central nervous system	[2, 19-21]
Middle East	For pharmacological activities such as a renal antispasmodic and diuretic	[2, 22]
South America	As a tea for sore throat, indigestion and an emetic cause vomiting	[2, 23]
North America	As a hypotensive for throat and rheumatism	[2, 24]
USA	Used externally healing wounds and bone fractures	[2, 25]
Brazil	Popularly used for pharmacological such as diuretic, antispasmodic, antipyretic, analgesic anti-inflammatory, and sedative	[2, 26]

II. GC-MS FOR CYMBOPOGON OILS

The lemongrass and citronella fresh samples used in this study were collected from Pahang and Melaka. These samples were dried in room temperature for 3 to 4 days before distilled to obtain the essential oils. After that, the essential oil was stored in the container screw-top clear vial and tightly closed for the safety data information. This study has been carried out by using gas chromatograph and mass spectroscopy (GC-MS). The chemical analysis of the *Cymbopogon* oils was performed by using the Agilent Technologies 7890A/5975C Series MSD with HP-5MS column (30m x 0.25mm ID x 0.25µm film thickness that showed in fig. 1. The oven temperature program was the following: initial temperature of 60 °C, increasing by 3 °C/min to 180 °C, and held for 10 min. The samples were dissolved in Dichloromethane (DCM) then helium was used as

the carrier gas with a 1.0mL/min injector volume. The injector and detector temperature were held at 280 °C. The resulting compounds are presented in terms of by comparing retention times, peak area (%) and mass spectra. The chemical compounds were identified by matching them to the mass spectral library such as HPCH2205.L; Wiley7Nist05a.L and NIST05a.L. The experiment parameter for GC-MS is tabulated in Table 2. This is a common technique to analyses the chemical compounds [27-30]. GC-MS was used to separate every compound individually [31, 32]. This technique has been proven by the previous researcher [30, 32], where the chemical composition was discriminated by herbal material while the abundances of the fruits were determined. Other than that, by using this technique, the colour can be analyzed. The best way that previous researcher [9, 33] used is focusing on the colour of oil because different colour shows the different chemical compounds. By using GC-MS, it has been found that fresh oil represents the best characters of *Cymbopogon* oils species.



Fig. 1. The Agilent Technologies 7890A/5975C Series MSD

TABLE 2  
ANALYSIS CONDITION OF GC-MS

GC-MS Analysis Condition	
Column	HP-5MS
Length (m)	30
Diameter (mm)	0.25
Film thickness (µm)	0.25
Temperature program	60°C for 10min then 3°C/min to 230°C for 1min
Carrier gas	Helium, Flow rate: 1.0mL/min
MS Condition	
EI	70eV
Source temperature	200°C
Scan range	20 - 500µ
Scan speed (s/spectrum)	1/sec

III. SPSS SOFTWARE FOR CYMBOPOGON OILS

SPSS software is a complete system which is used for statistical analysis [34]. This SPSS statistics data version 25 is used in this study to analyze all the data of *Cymbopogon* oils

in developing descriptive statistics. Fig. 2 showed the step to key in the data in SPSS software for the first time. Firstly, to launch the software, the software need to open. After a few second, the window for data editor will appears and then ready to enter the data. The data that used as input in this research are the abundance of chemical compounds of *Cymbopogon* oils. The variable view is used to change the variable named if needed. After run the data, the result box will prompt. The result or target of SPSS observation is the species of *Cymbopogon* either lemongrass or citronella.

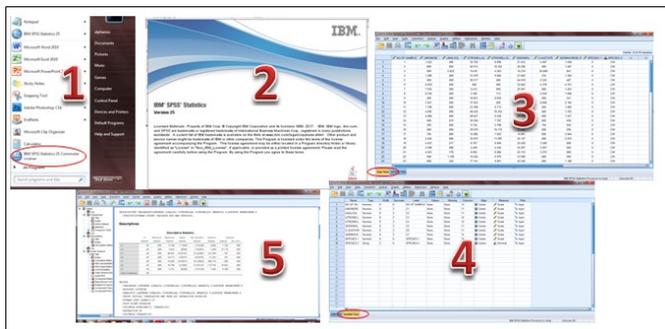


Fig. 2. Guideline in using SPSS software

#### IV. RESULTS AND DISCUSSION

##### A. *Cymbopogon* Oil Statistical Analysis

The graph in fig.3 shows the abundances pattern from GC and GC-MS data analysis of the *Cymbopogon* oils using seven selected types of chemical compounds such as C1 = limonene, C2 = linalool, C3 = citronellal, C4 = citronellol, C5 = geraniol, C6 = geranyl acetate, C7 = germacrene D. There are 45 samples of *Cymbopogon* oils includes lemongrass and citronella. From the general observations for seven types of chemical compounds, it is found that the various peak appeared where it proves that each type of chemical compounds has different pattern of abundances.

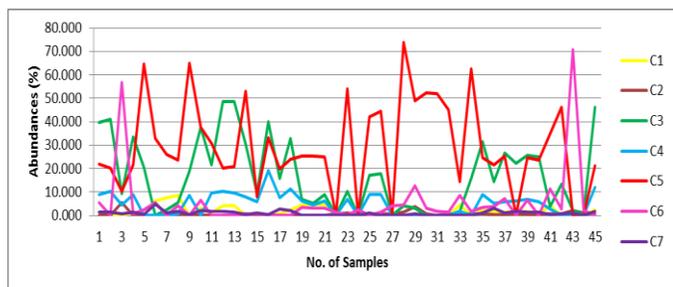


Fig. 3. Abundances of *Cymbopogon* oils

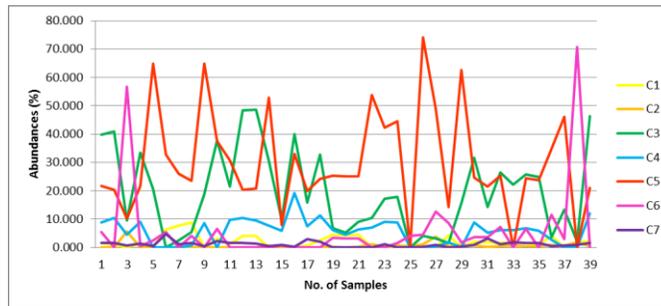


Fig. 4. Abundances of citronella oils

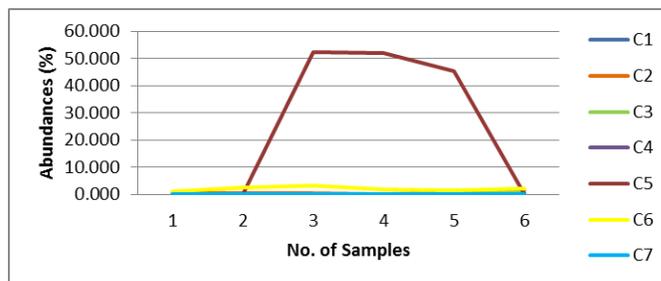


Fig. 5. Abundances of lemongrass oils

Compound 1 which is limonene, has the highest peak is 8.749% belongs to the number sample eight, follow by the number sample seven which is the abundances are 7.632%. The minimum abundances of this sample are 0.000% in the range of samples which are from sample twenty-two until sample twenty-seven. For the samples 19, 20 and 21, the value of abundances are in the range 4.398% - 4.523%. Second is compound 2 which is linalool. The ranges of the peak abundances of linalool compound are between 0.000% until 5.623%. From the overall data set, it can be seen that the maximum value of abundances is 5.623% at the sample three. The lowest peak among all the value of abundances belongs to the number of samples from samples 4 until samples 18 which are 0.000%. Third, compound 3 which is citronellal. Number sample twelve and number sample thirteen shows the highest peak compare to other with the value of abundances are 48.424% and 48.647%, followed by samples 39 which is 46.362%. From overall dataset, the minimum value of abundances which is 0.000% belongs to the peak of 6 and 25. In addition, there are three samples with the value of abundances between 0.001% until 5.000%, which are 2.415%, 4.049%, 3.419%, 1.629%, 3.642% and 2.133% for the samples 7, 26, 27, 28, 36 and 38. Next, for compound 4 which is citronellol, it clearly shows the highest peak value of abundances for this compound is 19.172% belongs to the sample 16. After reviewing the whole dataset, it can be conclude that most of the citronellol compound is in the range 5.000% to 10.000% and below 5.000% belong to the sample 3, 5, 6, 7, 8, 10, 20, 25, 26, 27, 28, 29, 36, 37 and 38.

Compound 5 which is geraniol. The first peak is 64.818% belongs to number samples five. The second peak is 64.874% belongs to the number samples of nine. The third peak is

52.926% which is the sample number fourteen. Lastly, the highest peak among others is 74.054% which is the sample number twenty-eight. The minimum value of abundances is 0.000% for the samples 25, 33 and 38. Geranyl acetate shows the pattern of abundances as a compound 6. It can be seen that the highest peak is 70.784% belong to the number sample thirty-eight. Sample three clearly show the second highest peak which is the value of abundances is 56.809%, followed by sample number twenty-seven which is 12.7225. From overall dataset, the most abundances value is ranged between 0.000% until 5.000%. Lastly, the abundances pattern in compound 7 which is germacrene D. The first peak is 4.721% belongs to number samples six. The second highest peak is 2.944% belongs to the number samples of seventeen. The next peak is 3.223% which is the sample number thirty-one. The next highest peak is 2.944% belongs to the number samples seventeen. Most the value of abundances is in the range of 0.500% to 1.000%. It can be concluded that the minimum value of abundances is 0.000% and the maximum value of abundances is 4.721% after reviewing the whole dataset.

From all the chemical compounds that found in lemongrass oils that shows in fig.5, compound 5 which is geraniol have the highest value of abundances compares to other which is 52.270% belongs to number samples three. The second peak is quite high as sample three which is 52.097% belongs to the number samples of four. The next peak is 45.274% which is

the sample number five. Lastly, it clearly seen that the minimum value of abundances is 0.000% for the samples 1, 2 and 6. Next is compound 6 (geranyl acetate) which is 3.212% and compound 2 which is linalool that have the value of abundances is 1.082%. The maximum value of abundances for the compound 3 which is citronellal is 0.843%, quite high compare to compound 1 (limonene) which is 0.124%. Lastly, for the lowest maximum value abundances are 0.000% belongs for both compound 4 (linalool) and compound 7 (germacrene D). In addition, the total number samples of lemongrass oils species are 6.

### B. Descriptive Analysis

The aim do the preliminary analysis is to inspect and to explore the nature of variables. Table 3 and table 4 shows the summary statistic of the compound of *Cymbopogon* oils for citronella oils and lemongrass oils that includes the minimum and the maximum number of the data, the means, standard deviation, variance and kurtosis. The function of descriptive statistics is to check the data to describe their characteristics and to check the variable for any violation of the assumptions made by the tests. The kurtosis value provides information about the flatness of the frequency distribution. Positive kurtosis shows the more peaked while negative kurtosis showed less peaked compared to the normal distribution.

TABLE 3  
DESCRIPTIVE STATISTICS OF CITRONELLA OILS

	N	Minimum	Maximum	Mean		Std. Deviation	Variance	Kurtosis	
	Statistic	Statistic	Statistic	Statistic	Std. Error	Statistic	Statistic	Statistic	Std. Error
C1 (LIMONENE)	39	0.0000	8.749	1.998	0.362	2.263	5.121	1.252	0.741
C2 (LINALOOL)	39	0.0000	5.623	0.585	0.175	1.092	1.191	13.385	0.741
C3 (CITRONELLAL)	39	0.0000	48.647	19.430	2.365	14.769	218.121	-0.894	0.741
C4 (CITRONELLOL)	39	0.0000	19.172	5.662	0.722	4.510	20.336	0.407	0.741
C5 (GERANIOL)	39	0.0000	74.054	30.040	2.890	18.043	325.555	0.135	0.741
C6 (GERANYL ACETATE)	39	0.0000	70.784	5.951	2.259	14.107	198.995	15.725	0.741
C7 (GERMACRENE.D)	39	0.0000	4.721	5.951	0.162	1.001	1.020	3.193	0.741

TABLE 4  
DESCRIPTIVE STATISTICS OF LEMONGRASS OILS

	N	Minimum	Maximum	Mean		Std. Deviation	Variance	Kurtosis	
	Statistic	Statistic	Statistic	Statistic	Std. Error	Statistic	Statistic	Statistic	Std. Error
C1 (LIMONENE)	6	0.0000	0.124	0.021	0.021	0.051	0.003	2.449	0.845
C2 (LINALOOL)	6	0.0000	1.082	0.621	0.124	0.304	0.093	-0.100	0.845
C3 (CITRONELLAL)	6	0.0000	0.843	0.141	0.141	0.344	0.118	2.449	0.845
C4 (CITRONELLOL)	6	0.0000	0.000	0.000	0.000	0.000	0.000		
C5 (GERANIOL)	6	0.0000	52.270	24.940	11.201	27.437	752.783	0.034	0.845
C6 (GERANYL ACETATE)	6	0.0000	3.212	2.019	0.293	0.717	0.514	0.915	0.845
C7 (GERMACRENE.D)	6	0.0000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

The average is probably the most commonly used method of describing the middle of data. The means of this species is determined by summing all the data for each compound and dividing by the number of samples which are 39 and the formula is expressed in (4.1) [35]. The highest mean are geraniol compounds with 30.040, followed by citronellal compound which is 19.430. The others mean compound is limonene with 1.998, linalool which is 0.585, citronellol which is 5.662, geranyl acetate which is 5.951 and 5.951 for germacrene D compound. The standard error means determines how significantly the samples of the data to be from the true population mean. The lowest standard error mean is germacrene D which is 0.162 and secondly is linalool which is 0.175. Third is the limonene compound which is 0.362, followed by citronellol which is 0.722 and geranyl acetate which is 2.259. Lastly for the standard error mean are citronellal compound which is 2.365 and geraniol compound which is 2.890.

Table 3 also shows the standard deviation statistic which is the number of variability is measure for a set of data from the mean statistic. The formulae for the standard deviation is expressed in (4.2) [35]. It can be seen that the highest standard deviation is the geraniol compound which is 18.043. The second highest is the citronellal compound which is 14.769. Next is geranyl acetate and citronellol which are 14.107 and 4.510. For the limonene compound, the standard deviation statistic is 2.263, followed by linalool which is 1.092 and germacrene D which is 1.001. By using SPSS software, it also shows the result of the variance and the formula is expressed as (4.3) [35]. The result from the standard deviation is the square root of variance statistic. From the table, it can be noticed that geraniol has a larger amount of variance which is 325.555 compared to others like citronellal which is 218.121, geranyl acetate which is 198.995 and citronellol which is 20.336. The variance of limonene compound is 5.121 continue with the linalool compound which is 1.191 and germacrene D compound which is 1.020.

Last but not least are the values of kurtosis for citronellal chemical compounds. It can be divided into three groups which are normal distribution, positive kurtosis and negative kurtosis. Higher kurtosis means more of the variance in the result. A standard normal distribution has a kurtosis of 3 which is excess kurtosis exactly 0. A negative kurtosis called platykurtic has a distribution with kurtosis less than 3 which is excess kurtosis <0 and a positive kurtosis called leptokurtic has a distribution with kurtosis >3 which is excess kurtosis >0. There is 4 chemical compounds exist in positive kurtosis such as citronellal compound which is -0.894, geraniol compound which is 0.135, citronellol which is 0.407 and limonene which is 1.252. For negative kurtosis, there are linalool which is 13.385, geranyl acetate which is 15.725 and germacrene D which is 3.193.

Table 4 shows the descriptive statistic for lemongrass oils. The lowest mean for lemongrass oils species are citronellol and germacrene D which are 0.000. While for the highest means are geraniol compounds with 24.940, followed by geranyl acetate compound which is 2.019. The others mean compound is limonene with 0.021, linalool which is 0.621 and citronellal which is 0.141. The lowest standard error mean are

germacrene D and citronellol which are 0.000 and secondly is limonene which is 0.021. Third is the linalool compound which is 0.124, followed by citronellal which is 0.141 and geranyl acetate which is 0.293. Lastly the highest standard error mean are geraniol compound which is 11.201.

Table 4 also shows that the highest standard deviation is the geraniol compound which is 27.437. The second highest is the geranyl acetate compound which is 0.717. Next is citronellal and linalool which are 0.344 and 0.304. For the limonene compound, the standard deviation statistic is 0.051, followed by citronellol and germacrene D which is both are 0.000. From the table above, it can be clearly seen that geraniol has a larger amount of variance which is 752.783 compared to others like geranyl acetate which is 0.514, citronellal which is 0.118 and linalool which is 0.093. The variance of limonene compound is 0.003 continue with the citronellol and germacrene D compound which is 0.000.

Last but not least are the values of kurtosis for lemongrass chemical compounds. All the compounds for lemongrass oil are exist in positive kurtosis such as limonene and citronellal compound which are 2.449, geranyl acetate compound with 0.915, geraniol compound which is 0.034, and linalool which is -0.100.

The formula for the mean is expressed as follows:

$$\text{Mean} = \frac{\sum x_i}{n} \quad (4.1)$$

The formula for the standard deviation is expressed as follows:

$$\text{Standard Deviation} = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n-1}} \quad (4.2)$$

The formula for the variance is expressed as follows:

$$\text{Variance} = \frac{\sum (x_i - \mu)^2}{n-1} \quad (4.3)$$

## V. CONCLUSION

This paper showed that the statistical analysis of data for *Cymbopogon* chemical compounds oil species and successfully determined the pattern of abundances in seven types of significant compounds by using 45 samples of *Cymbopogon* oils sample. All these chemical compounds are very significant to classify the species of *Cymbopogon* oils by setting the values of abundances (%) as input. This study also includes the minimum and the maximum number of the data, the means, standard deviation, variance and kurtosis. From statistical information, it can be seen that geraniol has the highest values compared to other features. It can be concluded that the significant compound for the *Cymbopogon* oils species must have geraniol. This technique successfully identified seven significant chemical compounds from many chemical compounds as extracted by GC-MS. The finding showed that the technique proposed is reliable and useful for the *Cymbopogon* oils classification system.

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**Khairul Anis Athirah Kamarulzaini** graduated with a B.Eng with Honors in Electrical Engineering majoring in System at Universiti Teknologi Mara (UiTM), Malaysia. Currently, she is a Research Assistant and a master student at Faculty of Electrical Engineering (Universiti Teknologi Mara (UiTM), Malaysia). She is taking Msc.Sc in Electrical Engineering and her research concentrate in modelling of *Cymbopogon* oils species.

**Nurlaila Ismail** received the B.Sc. in Electrical Engineering with Honors in 2005. She finished the M.Sc. degree in Electrical Engineering in 2011 and got the Ph.D in Electrical Engineering in 2014 at Universiti Teknologi MARA (UiTM), Shah Alam. Currently she teaches at Universiti Teknologi Mara, Malaysia, as a Senior Lecturer.

**Mohd Nasir Taib** is a senior lecturer at Faculty of Electrical Engineering at Universiti Teknologi MARA (UiTM), Shah Alam, Selangor. He received the B.Sc. in electrical engineering at University of Tasmania, Australia. He finished the M.Sc. degree in Control System with Distinction at University of Sheffiled, United Kingdom and got the Ph.D in Control & Instrumentation at UMIST, United Kingdom. The

main research area focuses on advanced signal processing with applications in intelligent control system, biomedical and pharmaceutical systems, process control & biotechnology, optical fiber sensors and microwave sensors.

**Mailina Jamil** is a research officer at Herbal Product Development Programme, Natural Product Division, Forest Research Institute Malaysia (FRIM), 52109 Kepong, Selangor.

**Nor Azah Mohd Ali** is a senior research officer at Herbal Product Development Programme, Natural Product Division, Forest Research Institute Malaysia (FRIM), 52109 Kepong, Selangor. She received her degree in bachelor of science at universiti of waterloo, canada in 1985. She finished her master of science at universiti kebangsaan malaysia in 1996 and got philosophy of science at universiti putra malaysia in 2004. Her specialized are chemistry (natural product chemistry) essential oil analysis and processing cosmetic formulation and product Development.

**Sahrim Lias** is a research officer at Herbal Product Development Programme, Natural Product Division, Forest Research Institute Malaysia (FRIM), 52109 Kepong, Selangor.