EXTRACTION OF ESSENTIAL OIL OF *AQUILARIA MALACCENSIS* (GAHARU) USING HYDRO-DISTILLATION AND SOLVENT EXTRACTION METHODS

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ASHWIN CHARLES BENEDICT

Thesis submitted to the Faculty of Chemical and Natural Resources Engineering in Partial Fulfillment of the Requirement for the
Degree of Bachelor Engineering in Chemical Engineering

Faculty of Chemical & Natural Resources Engineering
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APRIL, 2009

I declare that this thesis entitled “Extraction of the Essential Oil of *Aquilaria Malaccensis* (Gaharu) Using Hydro-distillation and Solvent Extraction Methods” is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any degree.

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I dedicate this thesis to my family, without whom none of this would have been worth the challenge…

Supportive parents;
Benedict Charles and Hazel Mirandah

Not-so-little sisters;
Evelyn Charles and Jocelyn Charles

This is for the four of you.

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ABSTRACT

Agarwood oil is regarded as one of the most expensive natural products in the world due to the fragrance inducing compounds it contains. However, current studies on the chemical composition of agarwood essential oil are woefully lacking and this poses a threat to the agarwood industry. This research aims to identify the best extraction method for isolating gaharu essential oil and to create a list of compounds contained in a sample of grade C agarwood. In the present work, the composition of agarwood essential oil obtained through hydro-distillation and solvent extraction with acetone, dichloromethane and hexane as the solvents were analyzed for marker compound identification using gas chromatography-mass spectrometry (GC-MS). Studying another parameter of this experiment, the sample hydro-distillated in the lab was compared with industrial grade hydro-distillation to determine the difference in quality between industrial and lab scale hydro-distillation. Of the three solvents used, acetone eluted the highest number of compounds. The lab scale hydro-distillated sample eluted 34 compounds at a quality of 50% and above whereas the solvent extraction sample eluted 25 compounds. There was no significant difference found between lab scale and industrial scale hydro-distillation.

ABSTRAK

Minyak gaharu dianggap antara produk asli yang paling mahal di dunia kerana komposisi kimianya yang menghasilkan bau yang sangat harum. Namun demikian, kajian-kajian yang dijalankan sebelum ini tidak menyeluruh dan informasi yang tidak mencukupi mengenai komposisi kimia minyak gaharu menjadi punca ancaman terhadap industry gaharu. Kajian ini bertujuan untuk memutuskan kaedah penyulingan minyak gaharu yang paling efektif dan juga untuk menghasilkan satu senarai kompaun dalam sampel gaharu gred C. Komposisi kimia minyak gaharu yang diperolehi dari kaedah 'hydro-distillation' dan 'solvent extraction' dianalisa menggunakan GC-MS. Satu lagi aspek yang dikaji dalam experimen ini adalah perbandingan antara 'hydro-distillation' pada skala berbeza yakni skala makmal dan skala industri. Perbandingan antara tiga pelarut yang digunakan menunjukkan acetone sebagai pelarut yang terbaik. 34 kompaun dikenal pasti dari sampel 'hydrodistillation' manakala 25 didapati dari sampel 'solvent extraction' menggunakan acetone apabila dianalisa pada kualiti 50%. Perbandingan antara sampel-sampel 'hydro-distillation' menunjukkan bahawa tiada perbezaan ketara dari segi kualiti antara prosedur makmal dan prosedur pada skala industri.

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LIST OF ABBREVIATIONS

CAS	Chemical Abstracts Service
CITES	Convention on International Trade in Endangered Species and Wild Fauna and Flora
D	Debye
Dbh	Diameter Breast Height (for bark of trees)
D, d	Diameter
GCMS	Gas Chromatography Mass Spectrometry
Ha	Hectare
ID	Identification
MAHA	Malaysian Agriculture and Horticulture Agrotourism
MF	Molecular Formula
RT	Retention Time
VDW	Van der Waal's

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Aquilaria Malaccensis is a species of plant in the Thymelaeaceae family found primarily in Bangladesh, Bhutan, India, Indonesia, Iran, Laos, Malaysia, Myanmar, the Philippines, Singapore, and Thailand. The Aquilaria genus is more broadly recognized as Agar wood, Jin Koh, Aloes wood, Gaharu, Eagle wood, Jinkoh and Oud. Among the other species of agarwood besides the Malaccensis include agallocha, gradiflora, ophispermum, sinesis, crassna, pentandra and yunnanensis. The term agarwood, although widely used to refer to the members of the Aquilaria genus, more specifically refers to the resinous heartwood from the Aquilaria trees.

Occasionally the heartwood gets infected by a parasitc ascomycetous mold, *Phaeoacremonium parasitica*. As a response, the tree produces a resin high in volatile organic compounds that aids in suppressing or retarding the fungal growth (Wikipedia, 2008). This resin and its oil are valuable for their use in medicine, perfumery and other aromatic products.

There are many grades of agarwood, and the highest quality wood is extremely expensive. In fact, the first-grade wood is one of the most expensive natural products in the world, with prices of up to $13,000 per pound (Eden Botanicals, 2007). However the finest grade of agarwood is produced from naturally occurring fungal infection which happens slowly and very infrequently.

Because of its immense value and rarity, indiscriminate cutting of trees and over harvesting in hope of finding the treasured resin has lead to depletion of wild trees. The Convention on International Trade in Endangered Species of Wild Fauna and Flora (CITES) has listed Aquilaria Malaccensis as an endangered species. Efforts to protect the species involve inoculation of grown agarwood with the fungus as well as intentional injuring of the tree to encourage fungal infection to produce the required resin. However resin produced in this manner is deemed to be of secondary quality and has inferior market value compared to naturally harvested agarwood resin.

Essential oils from agarwood can be extracted by several methods which include distillation (typically using water or steam), solvent extraction, carbon dioxide extraction, cold pressing as well as florasol/phytol extraction. These extraction methods will be further discussed in the literature review.

1.2 Objectives

The main objectives of this preliminary study are:

1. To extract the Gaharu essential oil using the hydro-distillation and solvent extraction methods.
2. To analyze the chemical compounds present in the essential oil using Gas Chromatography – Mass Spectrometer (GCMS)
3. To compare the results of analysis between different extraction methods.
4. To compare the results of analysis between different sources of essential oil for the hydro-distillation method.
5. To compare the results of analysis between different solvents used for the solvent extraction method.

1.3 Scope of Study

The scope of this study is essentially to compare between the methods of hydro-distillation and solvent extraction. For hydrodistillation, the lab grade sample of agarwood distilled to obtain essential oil will be compared with previously procured samples from MAHA and Kelantan to examine differences in composition. In the solvent extraction procedure, three solvents used – hexane, dichloromethyl and acetone to extract three samples of essential oil. These three samples are then compared to the sample procured from hydro-distillation of the same lab grade agarwood to determine significant differences and similarities. The GCMS is used to perform analysis to determine the composition of each of the six samples.

1.4 Problem Statement

The main problem which needs to be addressed revolves around the issue of creating a standard by which to evaluate and assess the quality of essential oil produced from agarwood. Currently no applicable standard exists and prices as well as the quality of oil are arbitrarily determined by traders and clients.

Another problem which is highly correlated to the problem of quality is the reproduction of a successful formula. Current methods of producing perfumes and aromatic products from agarwood essential oil depend greatly on experience and lack scientific backing and suitably rigid procedures to ensure that a successful formula can be replicated.

This also brings to light the problems faced by law enforcement agencies and nature preservation groups that are trying to stop indiscriminate felling of Aquilaria trees. The woeful lack of information on agarwood and its essential oil has lead to exports being approved with little information on the species and not knowing whether exploitation is within sustainable levels.

1.5 Rationale and significance

The issue of finding a solvent or an extraction method that can be used to conveniently determine the quality of a sample, a majority of its components as well as the species from which the essential oil was obtained is a crucial part of this study. The discovery of such a solvent or any research leading to that discovery would pave the first steps towards solving the problems stated above.

CHAPTER 2

LITERATURE REVIEW

2.1 Background of Gaharu

Valued mainly for its aromatic, fumigatory, and medicinal properties, *gaharu* is the fragrant, resin-impregnated wood found in approximately 17 species of sub-canopy trees of the genus *Aquilaria* (Thymelaeaceae) commonly found in mixed hardwood hill forests across tropical Southeast Asia (Chung and Purwaningsih, 1999). Generally agreed to be the result of a pathological condition, this aromatic resin is produced as the tree sap thickens in response to injury and fungal infection. The degree to which the resin saturates the heartwood determines the market value of this product. In lesser quality specimens, the resin creates a mottled or speckled appearance in the naturally pale wood, but higher quality specimens are nearly solid in color—glossy and black. Through distillation, the most valuable specimens can yield an essential oil that is a key perfume ingredient; distillation residues and lesser quality material are commonly processed for incense. The species that produce high quality resin include *A. agallocha, A. crassna, A. bailloni*, and *A. grandiflora* (Burkill 1966, Soehartono 1997).

A member of the family Thymelaeaceae, *Aquilaria* is a relatively slow-growing, medium-sized tree, on average 15–25 m tall. Having a moderately straight stem, it can achieve a diameter (dbh) of up to 250 cm. Most *Aquilaria* species have smooth, thin, pale gray bark with dense, dark foliage of shiny elliptical to oblong leaves (7.5–12 cm long by 2.5–5.5 cm wide) (Ding Hou 1960). The small, pale blooms flowering in clusters on the short stalks of the leaf stems produce 3–5 cm long, bi-valved fruit capsules in August.

La Frankie (1994) found *A. malaccensis* widely distributed but relatively uncommon (2.5 stems per ha, >1 cm dbh) in the Pasoh Forest Reserve of peninsular Malaysia. Despite the fact that *Aquilaria* regenerates freely under natural conditions as seedlings around the mother tree or sprouts from the stumps of harvested trees, mother trees are becoming scarce in many areas because of over-exploitation (Beniwal 1989, Paoli et al. 1994, Hasnida et al. 2001, Soehartono and Newton 2002, Quan et al. 2003). Although this condition may not lead to local extinction of the species, it may severely affect the availability of the product and, thus, the local *gaharu* economy.

The occurrence of the tree itself does not guarantee the presence of the resin. Scientists estimate that only 10% of the *Aquilaria* trees in the forest may contain *gaharu* (Gibson 1977). The resin forms in response to wounding and subsequent fungal infection, and is found in many parts of the tree, according to some sources in the bark and the roots as well as the heartwood (Jalaluddin 1977). Under natural conditions, the resin is more commonly found in trees of about 20 years or older, with trees more than 50 years old reportedly having the highest concentration (Sadgopol 1959).

2.2 Properties of Essential Oil

An essential oil is a concentrated hydrophobic liquid containing volatile aroma compounds from plants. They are also known as volatile or ethereal oils, or simply as the “oil of” the plant material from which they were extracted, such as *oil of clove.* An oil is essential in the sense that it carries a distinctive scent or essence of the plant. Essential oils do not as a group need to have any specific chemical properties in common, beyond conveying characteristic fragrances. They are not to be confused with essential fatty acids. Essential oils are multi-component chemicals. The mixture of oil compounds that constitute the essential oil comprises polar and non-polar compounds (Fliesher and Fliesher; 1991, Bohra *et al.*, 1994; Masango, 2004).

2.2.1 Physical Properties

A vast majority of essential oils are colourless, particularly when fresh. *Gaharu* oil however can be distinguished by colours, specifically ‘reddish brown’ and ‘greenish brown’ (Fatmawati Adam *et al* 2005). Essential oils also known as volatile oils because are easily to evaporate. Unlike vegetable oils expressed from nuts and seeds, essential oils are not actually oily. Some essential oils are viscous; others are fairly solid and most are somewhat watery.

2.2.2 Chemical Properties

Essential oils, like all organic compounds, are made up of hydrocarbon molecules and can further be classified as terpenes, alcohols, esters, aldehydes, ketones and phenols etc (Nor Azah Mohd Ali, 2002). The terpenes in *Gaharu* oil can be further divided into monoterpenes and sesquiterpenes. Most monoterpenes in *Gaharu* oil have a structure consisting 10 carbon atoms and at least one double bond. Terpenes react readily with air in the presence of even the smallest heat source. This is the reason citrus oils degrade quickly unless properly stored. Sesquiterpenes on the other hand consist of 15 carbon atoms and have complex pharmacological actions which include anti-inflammatory and anti-allergy properties. Professor Otto Wallach attributes the fragrance of *Gaharu* oil mostly to the presence of terpenes and cites the terpenes as having greatly influenced the oil industry.

In addition, for oxygenated compounds, they are contains phenols and alcohols such as monoterpene and sesquiterpene alcohol. The phenols found in essential oils normally have a carbon side chain and here we can look at compounds such as thymol, eugenol and carvacrol. These components have great antiseptic, anti-bacterial and disinfectant qualities and also have greatly stimulating therapeutic properties.

Specifically the chemical compounds of interest discovered in *Aquilaria Malaccensis* Benth are α-agarofuran, (-)-10-epi-γ-eudesmol 6.2%, agarospirol 7.2%, jinkohol 5.2%, jinko-eremol 3.7%, kusunol 3.4%, jinkohol II 5.6%, and oxo-agarospirol 3.1% (Yoneda *et al*, 1984, Nakanishi *et al*, 1984). A more comprehensive and more recent list of compounds found in the Aquilaria species is shown in Table 2.1:

Table 2.1: List of compounds in different species of Aquilaria referred to from different sources

Compound	Species	Source
β-agarofuran	*Aquilaria agallocha*	Manfred Meier, Birgit Kohlenberg and Norbert A. Braun - Isolation of Anisyl Acetone from Agarwood Oil (February 2003)
Epi-γ-eudesmol		
Agarospirol		
Jinkoh-eremol		
Valerianol		
6,10,10-trimethyl-11-oxatricyclo-[7.2.10]dedecane-2-carbaldehyde		
2-isopropylidene-10-methyl-spiro[4.5]-dec-6-ene-6-carbaldehyde		
2-(1,2,6,7,8,8a-hexahydro-8,8a-dimethyl-2-naphthyl)-propan-2-ol		
Dihydrokaranone		
α-guaiene	*Aquilaria agallocha*	Masakazu Ishihara and Tomoyuki Tsuneya – Components of the Volatile Concentrate of Agarwood (June 1993)
α-bulnesene		
Nor-ketoargarofuran		
1,10-epoxybulnesene		
1,5-epoxy-nor ketoguaiene		
Kusunol		
Dehydrojinkoh-eremol		
Selina-3,11-dien-9-one		
Routundone		
Selina-3,11-dien-9-ol		

Selina-3,11-dien-14-al		
Neopetasane		
Selina-3,11-dien-14-ol		
Guaia-1(10),11-dien-9-one		
Selina-4,11-dien-14-1l		
Guaia-1,(10),11-dien-15-ol		
Sinenofuranol		
Guaia-1,(10),11-dien-15-al		
Karanone		
Oxo-agarospirol		
Guaia-1,(10),11-dien-15,2-olide		
Guaia-1,(10),11-dien-15-oic acid		
2-hydroxyguaia-1,(10),11-dien-15-oic acid		
Selina-4,11-dien-14-oic acid		
Selina-3,11-dien-14-oic acid		
9-hydroxyselina-4,11-dien-14-oic acid		
(s)-4a-methyl-2-(1-methylethyl)-3,4,4a,5,6,7-hexahydronaphthalene	*Aquilaria agallocha*	R. Naf, A. Velluz, R. Brauchli and w. Thommen – Agarwood Oil (Aquilaria agallocha Roxb.). Its Composition and Eight New Valencane-, Eremophilane- and Vetispirane-Derivatives (1995)
β-vetispirene		
4-phenyl-butan-2-one		
α-vetispirene		
Rel-(1R,2R)-9-(isopropyl-2-methyl-8-oxatricyclo[7.2.1.0]dodec-5-ene		
Rel-(1R,2R)-9-(isopropyl-2-methyl-8-oxatricyclo[7.2.1.0]dodeca-4,6-diene		
(2R,4aS)-2-(4a-methyl-1,2,3,4,4a,5,6,7-octahydro-2-naphthyl)-propan-2-ol		
2-(1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthyl)-propanal		
Valerianol		
(1S,2S,6S,9R)-6,10,10-trimethyl-11-oxatricyclo[7.2.1.0]dodecane-2-carbaldehyde		
4-(4-methoxyphenyl)-butan-2-one		

rel-(5R,10R)-2-isopropylidene-10-methyl-spiro[4.5]dec-6-ene-6-carbaldehyde		
rel-(2R,8S,8aS)-2-(1,2,6,7,8,8a-hexahydro-dimethyl-2-naphthyl)-propan-2-ol		
rel-(5R,7S,10R)-2-isopropylidene-10-methyl-6-methylene-spiro[4.5]decan-7-ol		
rel-(2R,8R,8aS)-2-(1,2,3,5,6,7,8,8a-octahydro-8,8a-dimethyl-2-naphthyl-prop-2-en-1-ol		

The list of compounds above omits recurring compounds and thus any one list may be an incomplete reproduction of the original. However, the compounds that consistently appear in almost every list besides the ones listed by Yoneda *et al* are: β-agarofuran, valerianol, dihydrokaranone, α-bulnesene, α-guaiene, β-vetispirene, α-vetispirene and 4-phenyl-butan-2-one.

2.3 Extraction of essential oils

The demand for *gaharu* oil has created the necessity to extract this oil from the resin using one of a vast number of methods available. Extraction of *gaharu* oil falls under the category of fragrance extraction which means the extraction of aromatic compounds from raw material. Among the methods commonly employed for fragrance extraction are water/steam distillation, solvent extraction, enfleurage, expression, carbon dioxide extraction, hydrodiffusion, percolation and maceration. The results of the extraction are either essential oils, absolutes, concretes or butters depending on the amount of waxes in the extracted product. Despite the vast variety of methods available the most frequently used methods of *gaharu* extraction are hydro-distillation and solvent extraction. The extraction method employed is of central interest because it determines the quality of the oil produced. An incorrect or wrongly carried out extraction procedure would produce inferior quality oil as it would change the chemical signature of the original *gaharu* oil.

2.3.1 Hydro-Distillation

Hydro distillation is used in the manufacture and extraction of essential oil. This is the simplest and usually the cheapest process of distillation. Hydro distillation seems to work best for powders and very tough materials like roots, wood, or nuts. The main advantages of this method are that less steam is used, shorter processing time and a higher oil yield.

In distillation, the plant material is heated, either by placing it in water which is brought to the boil or by passing steam through it. The heat and steam cause the cell structure of the plant material to burst and break down, thus freeing the essential oils. The essential oil molecules and steam are carried along a pipe and channelled through a cooling tank, where they return to the liquid form and are collected in a vat. The emerging liquid is a mixture of oil and water, and since essential oils are not water soluble they can be easily separated from the water and siphoned off. Essential oils which are lighter than water will float on the surface.

2.3.2 Solvent Extraction

Some plant material cannot tolerate the heated forms of extraction such as steam distillation. High pressure damages these plants and once damaged, their essential oils too are damaged and are no longer able to be extracted. For these plants solvents such as ether, ethanol, methanol, hexane, alcohol and petroleum are used instead. The problem with using solvents to extract essential oils is that most of the time, residual solvents or impurities remain in the product.

Plant material is first washed in a bath of hydrocarbon solvents. This process dissolves the necessary plant materials including the aromatic molecules, waxy matter and pigment and the dissolved matter mixes in with the solvent. The solvent mixture is then filtered and distilled using low pressure. After distillation and further

processing, either a resin or a concentrated concrete remain. Additional processing using alcohol does in fact help in the process of extracting the essential oils.

2.4 Analysis using GC/MS

GC/MS is the most frequently used technique for analyzing essential oil composition. This method of testing requires an analytical component, a gas chromatograph, coupled with a detection component, a mass spectrometer.

A small sample of an essential oil is introduced into the GC, where it is heated to vapor and then carried along a column by an inert gas, such as helium. As the vaporized oil passes through the column, it separates into individual molecular constituents as it interacts with the stationary phase of the column. The separated constituents then pass into the MS. In the MS module, the constituents become charged, or ionized. The ionized constituents are then amplified and detected as current by the MS.

Each constituent is represented by a peak in a chromatograph, and the peaks can be compared to a library of molecules to identify the substance. Even though a GC/MS can produce a “fingerprint” of an oil, it cannot detect some synthetic and natural diluents. It can, however, detect a mixture of two or more similar oils, an oil that has had the terpenes removed, an oil that has been rectified, and traces of solvents or mineral oils.

CHAPTER 3

METHODOLOGY

3.1 General Procedure

In conducting research into the compounds in the Gaharu essential oil extracted through several different extraction methods, the procedures involved can be divided into two distinct stages: the extraction of the essential oil and the analysis of the extracts. The extraction procedure can further be separated into the hydrodistillation procedure and the solvent extraction procedure which were both run in tandem.

3.2 Hydrodistillation

Prior to the hydrodistillation process, the already pre-grinded Gaharu wood (ground to an average particle diameter of 1mm) was first dried in an oven for one day at 60°C. Drying was necessary to remove any moisture that was accumulated during the storage of the ground Gaharu wood which may contain dissolved contaminants which would foil the objectives of the experiment. The necessary apparatus required for the extraction process were rinsed in a cleaning solvent solution for one day as well. The apparatus were then thoroughly rinsed with water and then with distilled water to remove any residues from previous experiments that would taint or change the signature of the essential oil.

Once the necessary pre-experimental preparations are complete, the apparatus are set up as in Figure 3.1. The flask containing the Gaharu wood and distilled water was wrapped with aluminum foil to minimize heat loss. Before switching on the heating mantle the cooling water is allowed to flow to ensure that the temperature at the initial stages of the experiment does not proceed beyond the optimum temperature range. This is especially important because a large number of compounds in the essential oil are sensitive to temperature and may decompose, denature or be otherwise altered.

The apparatus is left for 3 days before the measuring cylinder containing the mixture of essential oil and water is collected. The mixture is then separated using a rotary evaporator. The temperature of the rotary evaporator is arbitrarily set at a temperature above that of water to ensure that complete separation occurs. This form of separation is favoured since a higher percentage of separation is achievable without excessively high temperatures due to the higher surface area produced by the rotary motion.

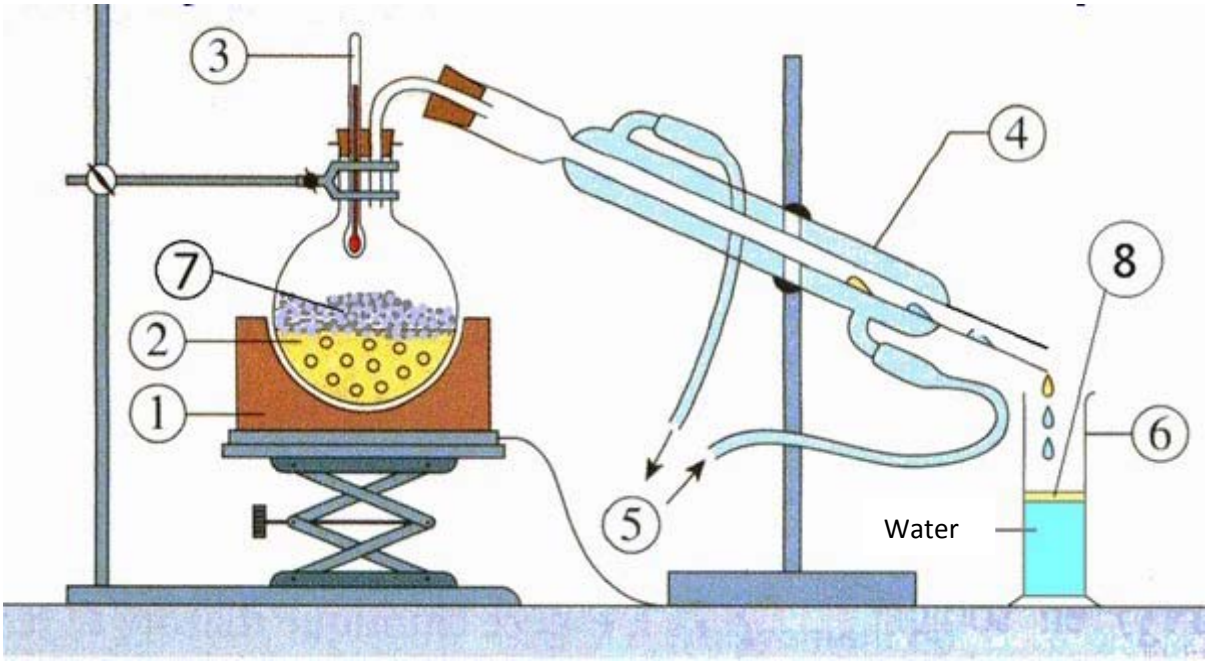


Figure 3.1: Hydrodistillation apparatus set-up

1. Heating mantle
2. Distilled water
3. Thermometer
4. Liebig condenser
5. Cooling water
6. Measuring cylinder
7. Gaharu wood grains
8. Essential oil

3.3 Solvent Extraction

Prior to the hydrodistillation process, the already pre-grinded Gaharu wood (ground to an average particle diameter of 1mm) was first dried in an oven for one day at 60°C. Drying was necessary to remove any moisture that was accumulated during the storage of the ground Gaharu wood which may contain dissolved contaminants which would foil the objectives of the experiment. The necessary apparatus required for the extraction process were rinsed in a cleaning solvent solution for one day as well. The apparatus were then thoroughly rinsed with water and then with the solvent to be used (acetone, dichloromethane or hexane) to remove any residues from previous experiments that would taint or change the signature of the essential oil.

Once the necessary pre-experimental preparations are complete, the apparatus are set up as in Figure 3.1. The ground gaharu grains are placed in a thimble and set in the soxhlet extraction column. The entire glass aperture of the apparatus was wrapped in aluminum foil to minimize heat losses. Before switching on the heating mantle the cooling water is allowed to flow to ensure that the temperature at the initial stages of the experiment does not proceed beyond the optimum temperature range. This is especially important because a large number of compounds in the essential oil are sensitive to temperature and may decompose, denature or be otherwise altered.

The apparatus is left for 5-6 hours before the measuring cylinder containing the mixture of essential oil and solvent is collected. The mixture is then separated using a rotary evaporator. The temperature of the rotary evaporator is arbitrarily set at a temperature above that of the solvent to ensure that complete separation occurs. This form of separation is favoured since a higher percentage of separation is achievable without excessively high temperatures due to the higher surface area produced by the rotary motion.

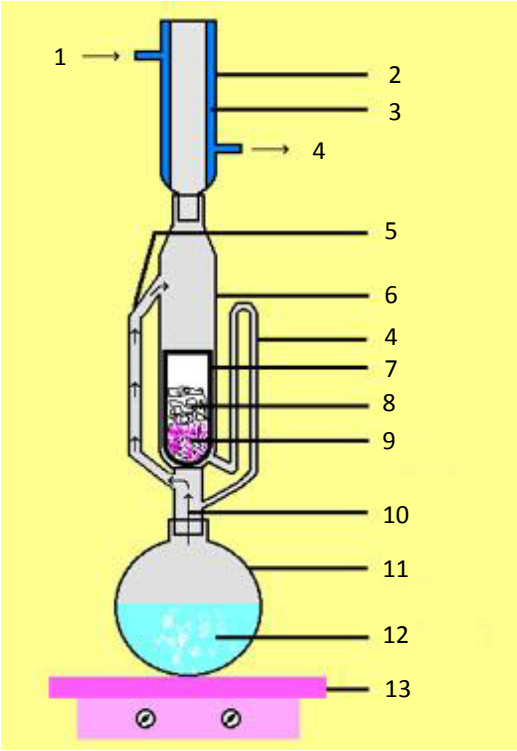


Figure 3.2: Solvent extraction apparatus set-up

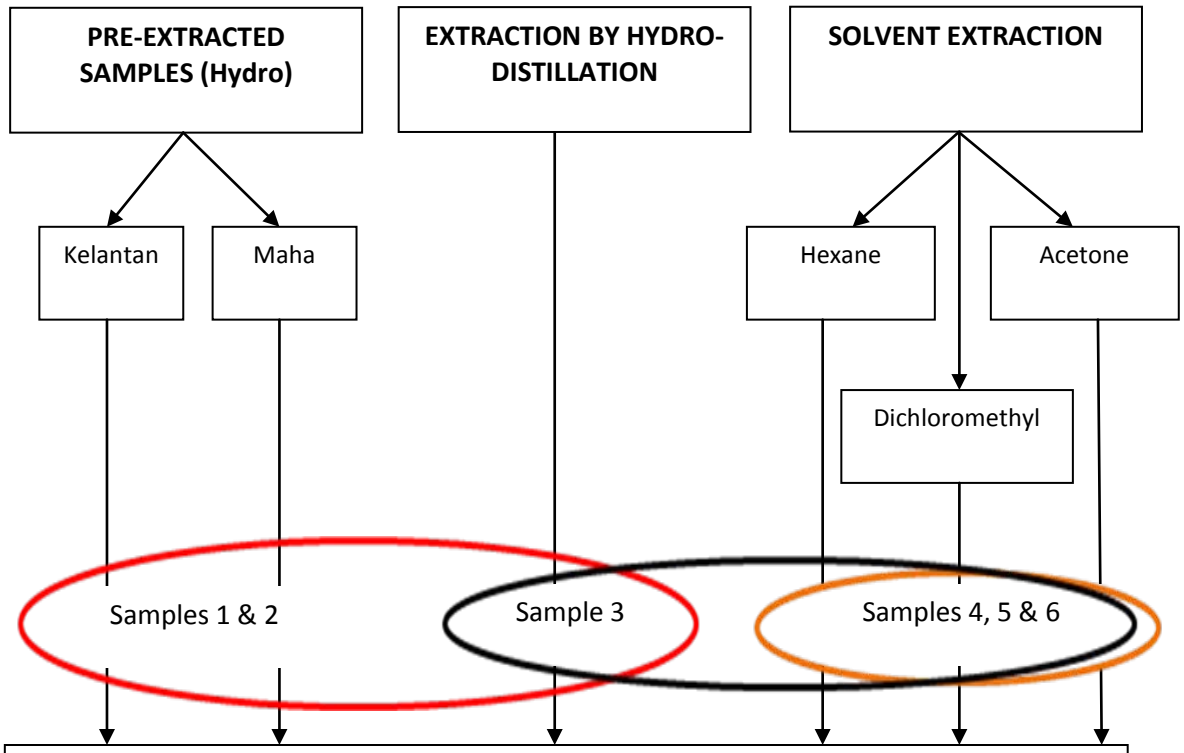
1. Cooling water in
2. Condenser tube
3. Water
4. Cooling water out
5. Bypass sidearm
6. Soxhlet extraction tube
7. Reflux sidearm
8. Cellulose thimble

9. Glass wool
10. Sample
11. Solvent vapour
12. Flask
13. Organic solvent
14. Heating mantle

3.4 Analysis of Extracts

Prior to analysis, the extracted samples from both the solvent extraction and the hydro-distillation procedures first had to be prepared for injection into the GCMS (Gas Chromatograph – Mass Spectrometer). For the sample obtained through hydrodistillation, enough essential oil was extracted to perform GCMS analysis.

However for the samples obtained through solvent extraction, the amount of essential oil obtained was too little to use the GCMS instrument with a significant level of confidence. Hence the first step in sample preparation was dilution to ensure that there was enough essential oil to proceed with analysis. Dilution was done by adding the respective solvents to the essential oil until enough solution was acquired to proceed with analysis. The vials used to store the samples were again washed with cleaning solvent, deionized water and then rinsed with the respective solvent used for extraction (acetone, dichloromethane, hexane or distilled water). Each sample then was filtered using a microfilter (0.4µm). This was done by drawing the liquid into a syringe and then removing the needle and fitting a microfilter at the head of the syringe. The liquid was then ejected from the syringe into a vial through the microfilter, thus effectively removing particles with sizes above 0.4µm. The prepared samples were then placed in the injection ports and GCMS analysis commenced. The results were collected and the analysis is presented in the following section. Figure 3.3 is a simplified explanation of how the analysis is to be conducted.



Legend:

Refers to the comparison between samples 1, 2 and 3. The variable being compared is the nature of the oil extracted where 1 and 2 refer to industrial grades whereas 3 refers to a lab grade sample.

Refers to the comparison between samples 3, 4, 5 and 6. The variable being compared is the extraction method with emphasis on compounds detected in the oil samples (including residues) and yield from extraction method.

Refers to the comparison between samples 4, 5 and 6. The variable being compared is the solvents used with emphasis on the polarity of solvent versus the polarity of the compounds extracted as well as number of compounds extracted.

Figure 3.3: Strategy for Analysis of Results

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Comparison of Solvent Extraction Samples

Of the three solvents used - acetone, dichloromethyl and hexane - the solvent that eluted the largest number of compounds at a quality of 70% and above was hexane (21 compounds). This finding comes as no surprise since an essential oil is essentially an oil and hence the compounds in it would be more likely to dissolve in a similar substance. In this case comparing between the solvents, hexane is a more oil-like substance compared to acetone and dichloromethyl which have varying degrees of polarity. An oil by definition is non-polar and tends to be viscous, hydrophobic and lipophilic. Hexane possesses all these properties and so does the gaharu essential oil to some extent.

However due to the organic nature of the essential oil, certain compounds in it are soluble in polar solvents but are not soluble in non-polar solvents like hexane. Despite the greater number of compounds detected in the hexane sample, an evaluation of which solvent is best used to identify marker compounds would require a closer examination of which compounds were detected in each sample. The compounds contributing to the unique nature of gaharu essential oil and hence determining its value should be prioritized.

Hence, a solvent capable of eluting such compounds would contribute to a superior solvent extraction procedure. The proceeding section highlights the compounds detected in each sample and discusses the implications of the findings.

4.1.1 Acetone

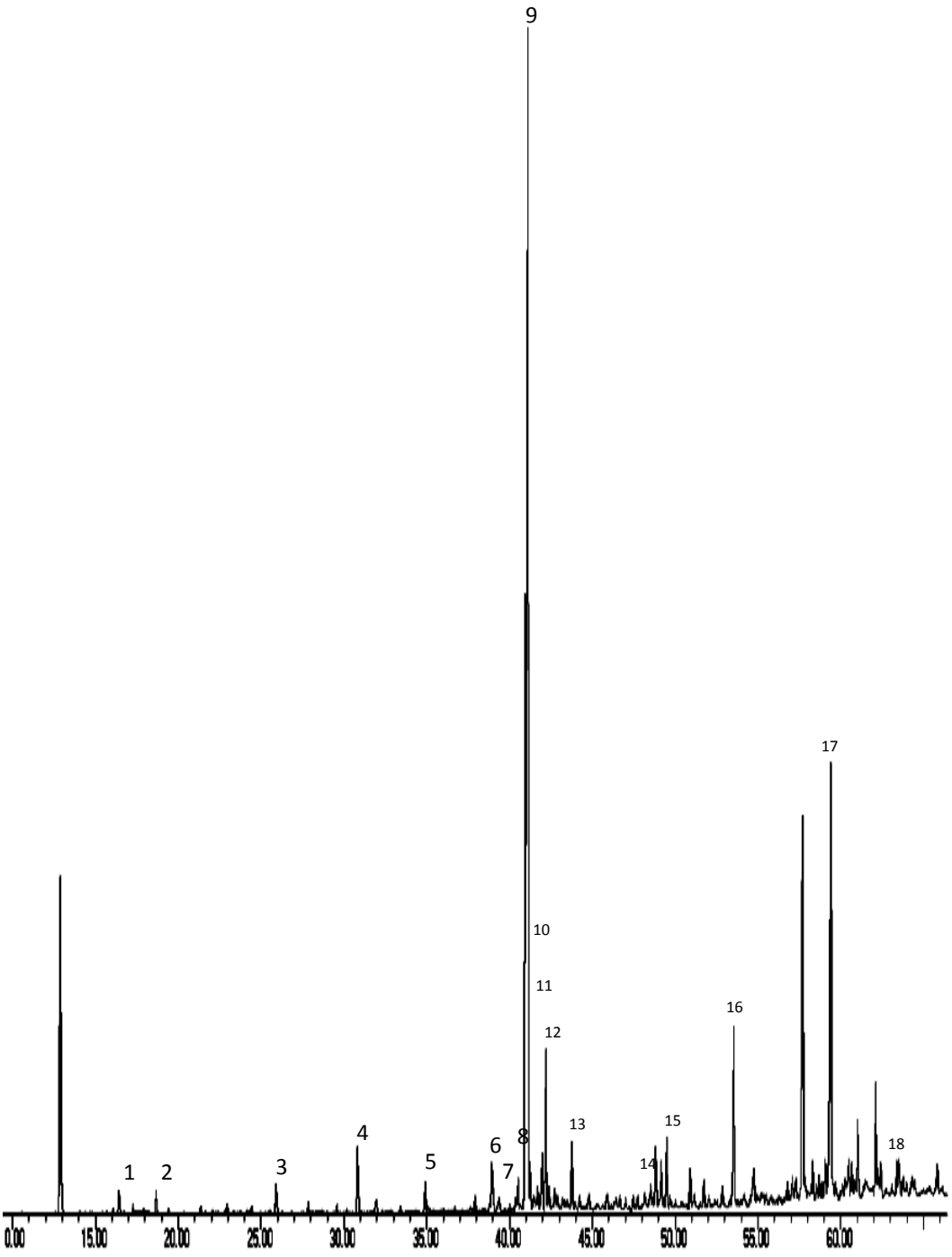


Figure 4.1: Spectrum of sample extracted using acetone

Table 4.1: Compound details for sample extracted using acetone

Peak no.	Area %	ID	Mol.formula	Cas#	Qual (%)
1	0.57	Diacetone Alcohol	$C_6H_{12}O_2$	4161-60-8	78
2	0.65	Benzaldehyde	C_6H_5CHO	100-52-7	96
3	0.79	δ-Guaiene	$C_{15}H_{24}$	3691-11-0	99
4	1.45	3-phenylbutan-2-one	$C_{10}H_{12}O$	769-59-5	97
5	0.72	Caryophyllene oxide	$C_{15}H_{24}O$	1139-30-6	93
6	1.37	Cadinene	$C_{15}H_{24}$	5951-61-1	95
7	0.56	α - Aromadendrene	$C_{15}H_{24}$	25246-27-9	95
8	-0.36	3-Allyl-6-methoxyphenol	$C_{10}H_{12}O_2$	501-19-9	98
9	28.2	Patchouli alcohol	$C_{15}H_{26}O$	5986-55-0	99
10	0.69	Agarospirol	$C_{15}H_{26}O$	23811-08-7	90
11	1.70	δ – Selinene	$C_{15}H_{24}$	28624-23-9	96
12	3.47	α – Selinene	$C_{15}H_{24}$	473-13-2	89
13	1.65	Aristolone	$C_{15}H_{22}O$	6831-17-0	70
14	0.57	1-Methyl-6-methylenebicyclo[3.2.0]heptanes	C_9H_{14}	210-90-0	83
15	1.72	Benzophenone	$C_{13}H_{10}O$	119-61-9	95
16	4.71	Benzyl Benzoate	$C_{14}H_{12}O_2$	120-51-4	96
17	12.8	2-Hydroxyethyl disulfide	$C_4H_{10}O_2S_2$	1892-29-1	96
18	0.71	2-Ethyl-6-isopropylphenyl isothiocyanate	$C_{12}H_{15}NS$	67330-54-5	70

18 compounds were identified at a quality of 70% and above from the acetone sample. The presence of diacetone alcohol which does not correspond with lists of compounds identified in gaharu essential oil suggests that this compound is a byproduct of using acetone as the solvent. Diacetone alcohol is formed from the condensation of two acetone molecules and most likely was not removed during the

rotary evaporation stage due to the much higher boiling point compared to acetone (diacetone alcohol has a boiling point of 166°C compared to 56.5°C for acetone).

Besides this, other important compounds detected include: δ-guaiene, caryophyllene oxide, cadinene, α-aromadendrene, agarospirol, δ-selinene, α-selinene, benzaldehyde, benzophenone, benzyl benzoate, 3-phenyl-butan-2-one, 3-allyl-6-methoxyphenol and aristolone. Other compounds such as patchouli alcohol and 2-hydroxyethyl disulfide are possible contaminants that are present due to the fact that the GCMS facility is a shared one and despite rigorous methodological care, sometimes traces still remain after a researcher has conducted and completed experimentation. As a whole, acetone succeeded in isolating 13 marker compounds of agarwood oil.

4.1.2 Dichloromethane

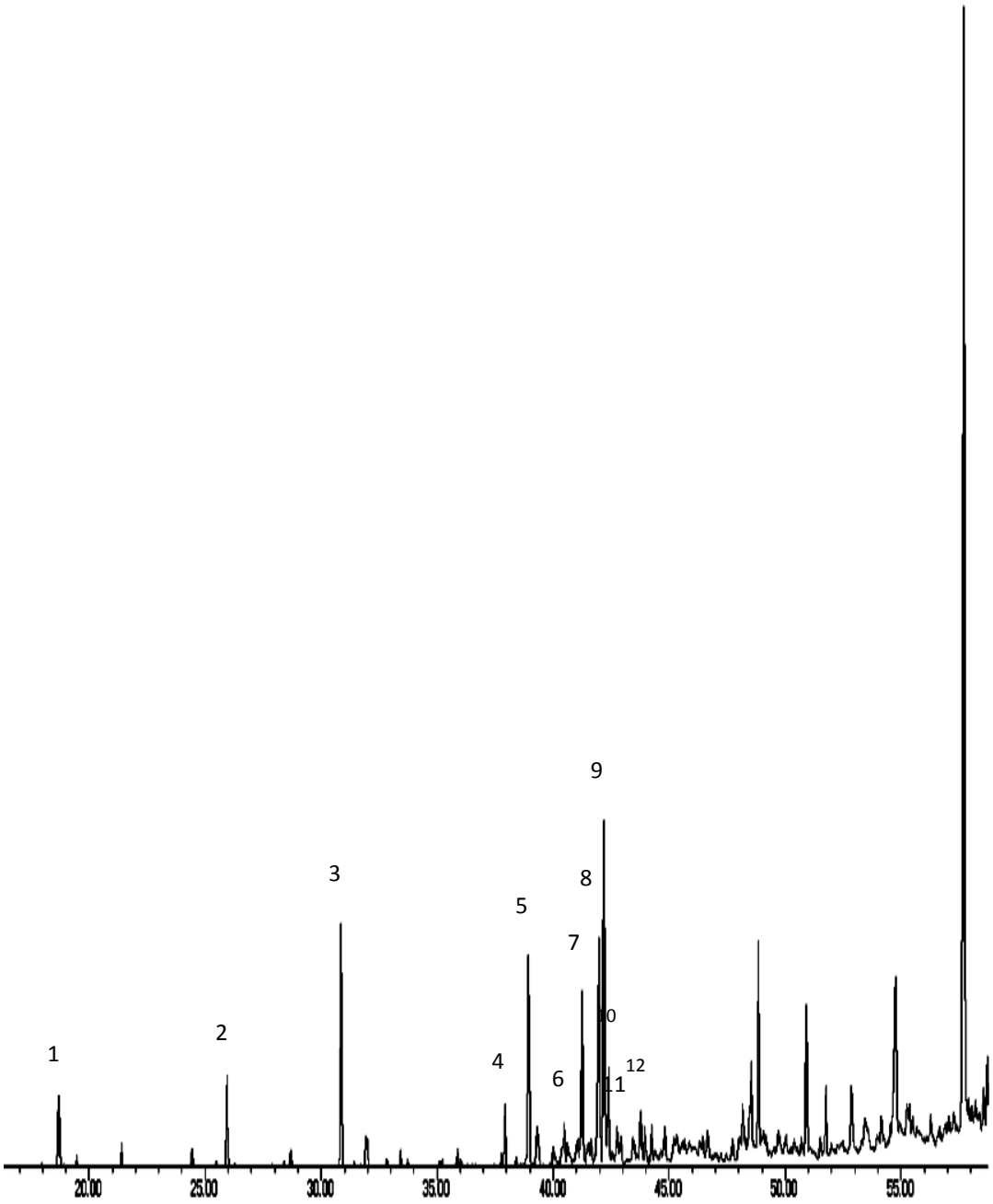


Figure 4.2: Spectrum for Sample Extracted using Dichloromethane

Table 4.2: Compound details for sample extracted using dichloromethane

Peak no.	Area %	ID	Mol.formula	Cas#	Qual (%)
1	0.61	Benzaldehyde	C_6H_5CHO	100-52-7	96
2	0.72	δ-Guaiene	$C_{15}H_{24}$	3691-11-0	99
3	1.55	Benzyl Acetone	$C_{10}H_{12}O$	2550-26-7	95
4	0.41	4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo [5.1.0.0(2,4)] octane	$C_{15}H_{22}O$	190-22-2	90
5	1.50	α – Gurjunene	$C_{15}H_{24}$	489-40-7	89
6	0.38	γ - Gurjunene	$C_{15}H_{24}$	22567-17-5	95
7	1.12	Hinesol	$C_{15}H_{26}O$	23811-08-7	86
8	1.90	Cadinene	$C_{15}H_{24}$	5951-61-1	95
9	2.16	Longifolene	$C_{15}H_{24}$	475-20-7	81
10	0.51	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene	$C_{15}H_{24}$	150320-52-8	70
11	0.19	β – Eudesmol	$C_{15}H_{26}O$	473-15-4	97
12	0.38	1R,3Z,9S2,6,10,10-Tetramethylbicyclo [7.2.0]undeca-2,6-diene	$C_{15}H_{24}$	140-07-4	92

12 compounds were identified at a quality of 70% and above from the acetone sample. Important compounds detected include: δ-guaiene, α-gurjunene, γ-gurjunene, hinesol, cadinene, longifolene, benzaldehyde, benzyl acetone and β-eudesmol. These compounds are those that contribute to the pleasant aroma associated with agarwood oil. As a whole, dichloromethyl succeeded in isolating nine important compounds that define agarwood oil.

4.1.3 Hexane

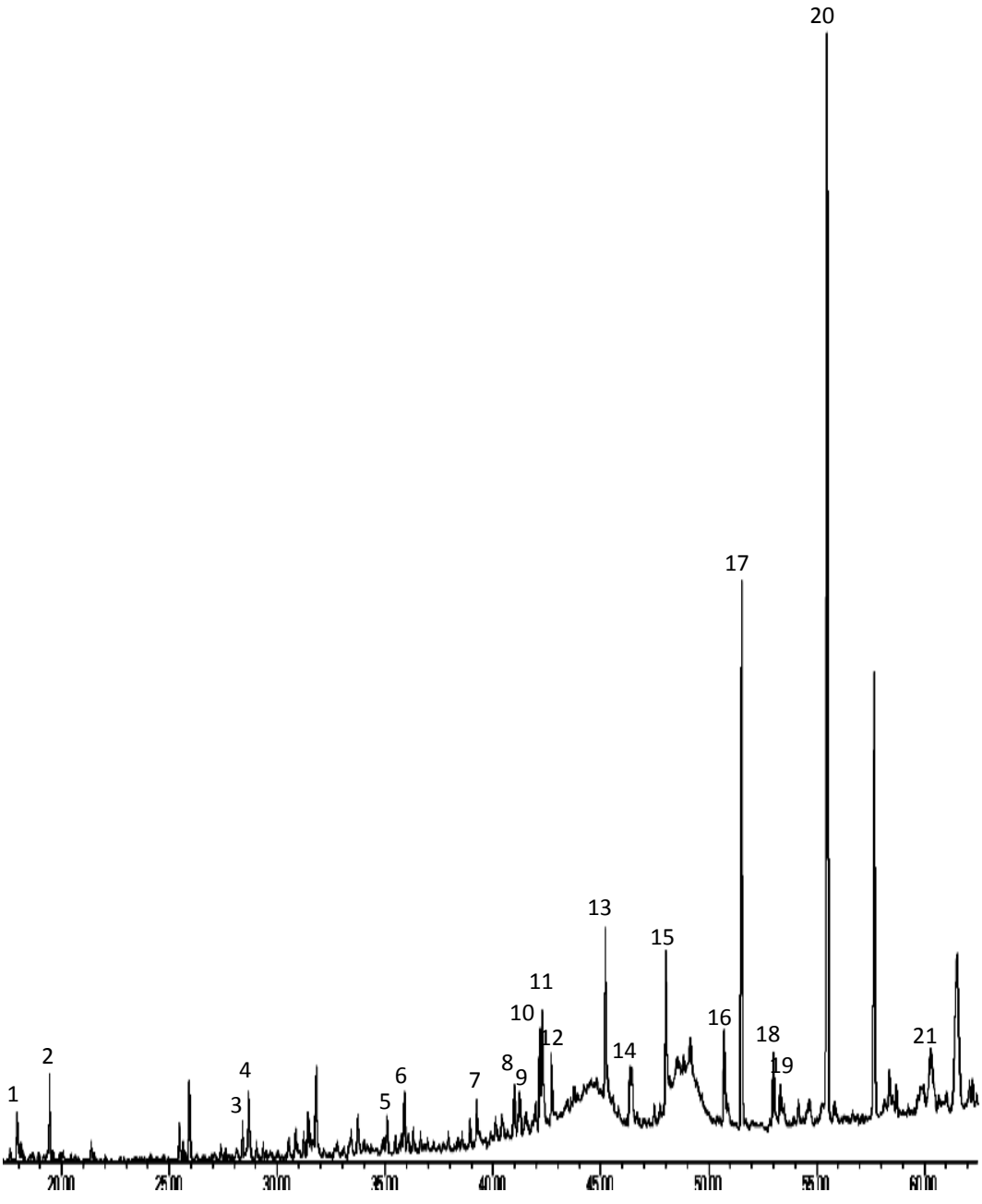


Figure 4.3: Spectrum for sample extracted using hexane

Table 4.3: Compound details for sample extracted using hexane

Peak no.	Area %	ID	Mol.formula	Cas#	Qual (%)
1	1.00	2-ethyl-1-Hexanol	$C_8H_{18}O$	104-76-7	83
2	1.62	Tetradecamethyl - Cycloheptasiloxane	$C_{14}H_{42}O_7Si_7$	107-50-6	90
3	0.63	α – Patchoulene	$C_{15}H_{24}$	560-32-7	76
4	2.00	Trimethyl - Cyclododecatriene	$C_{15}H_{24}$	21064-19-7	72
5	0.83	1-Tetradecanol Trifluoroacetate	$C_{16}H_{29}F_3O_2$	6222-02-2	91
6	1.15	Diphenyl ether	$C_{12}H_{10}O$	101-84-8	70
7	0.78	n-Heneicosane	$C_{21}H_{44}$	629-94-7	96
8	1.38	Patchouli alcohol	$C_{15}H_{26}O$	5986-55-0	97
9	1.27	Agarospirol	$C_{15}H_{26}O$	1460-73-7	95
10	1.28	Aromadendrene	$C_{15}H_{24}$	489-39-4	70
11	2.02	Docosane	$C_{22}H_{46}$	629-97-0	94
12	1.48	Methyl Palmitate	$C_{17}H_{34}O_2$	112-39-0	98
13	3.42	Octadecane	$C_{18}H_{38}$	593-45-3	96
14	0.50	Octadecanal	$C_{18}H_{36}O$	638-66-4	90
15	3.10	Tetracosane	$C_{24}H_{50}$	646-31-1	98
16	1.87	(E)-3-Eicosene	$C_{20}H_{40}$	74685-33-9	92
17	11.8	Diisobutyl Phthalate	$C_{16}H_{22}O_4$	84-69-5	86
18	1.60	Z-8-Hexadecene	$C_{16}H_{32}$	130-87-5	95
19	0.61	Pentadecane	$C_{15}H_{32}$	629-62-9	90
20	24.2	Butyl Isobutyl Phthalate	$C_{16}H_{22}O_4$	17851-53-5	94
21	2.02	2,2'-Methylenebis (4-ethyl-6-tert-butylphenol)	$C_{25}H_{36}O_2$	88-24-4	99

21 compounds were identified at a quality of 70% and above from the hexane sample. Important compounds detected include: heneicosane, agarospirol,

aromadendrene, docosane, methyl palmitate, tetracosane, 2-ethyl-1-hexanol, butyl isobutyl phthalate, diphenyl ether and diisobutyl phthalate. These compounds are those that contribute to the pleasant aroma associated with agarwood oil. The remaining compounds detected do not match lists of compounds composed from previous literature and have no appreciable scent. The lack of scent simply means that these compounds are of negligible interest in the identification of gaharu oil and do not serve as marker compounds. Hence a total of 11 marker compounds were detected in the gaharu essential oil with hexane as a solvent. Table 4.4 summarizes the results from the solvent extraction.

Table 4.4: Summary of compounds detected in solvent extraction samples.

Compound Name	Molecular Formula	Solvent Used		
		Acetone	Dichloromethyl	Hexane
α - Aromadendrene	$C_{15}H_{24}$	✓		✓
α – Gurjunene	$C_{15}H_{24}$		✓	
α – Selinene	$C_{15}H_{24}$	✓		
β – Eudesmol	$C_{15}H_{26}O$		✓	
δ-Guaiene	$C_{15}H_{24}$	✓	✓	
δ - Selinene	$C_{15}H_{24}$	✓		
γ - Gurjunene	$C_{15}H_{24}$		✓	
2-ethyl-1-Hexanol	$C_8H_{18}O$			✓
3-Allyl-6-methoxyphenol	$C_{10}H_{12}O_2$	✓		
3-phenylbutan-2-one	$C_{10}H_{12}O$	✓		
Agarospirol	$C_{15}H_{26}O$	✓		✓
Aristolone	$C_{15}H_{22}O$	✓		

Benzaldehyde	C_6H_5CHO	✓	✓	
Benzophenone	$C_{13}H_{10}O$	✓		
Benzyl Acetone	$C_{10}H_{12}O$		✓	
Benzyl Benzoate	$C_{14}H_{12}O_2$	✓		
Butyl Isobutyl Phthalate	$C_{16}H_{22}O_4$			✓
Cadinene	$C_{15}H_{24}$	✓	✓	
Caryophyllene oxide	$C_{15}H_{24}O$	✓		
Diisobutyl Phthalate	$C_{16}H_{22}O_4$			✓
Diphenyl ether	$C_{12}H_{10}O$			✓
Docosane	$C_{22}H_{46}$			✓
Heneicosane	$C_{21}H_{44}$			✓
Hinesol	$C_{15}H_{26}O$		✓	
Longifolene	$C_{15}H_{24}$		✓	
Methyl Palmitate	$C_{17}H_{34}O_2$			✓
Octadecanal	$C_{18}H_{36}O$			✓
Tetracosane	$C_{24}H_{50}$			✓
Total Marker Compounds Detected		13	9	11

4.2 Comparison of Hydrodistillation Samples

Of the three samples obtained through hydrodistillation, two were obtained via industrial scale hydrodistillation whereas the remaining sample was obtained from a lab scale hydrodistillation procedure. The three samples – lab, MAHA

(Malaysian Agriculture and Horticulture Agrotourism) and Kelantan were subjected to GCMS analysis and the results revealed that the MAHA sample eluted the greatest number of compounds at a quality of 70% and above (31 compounds).

This finding is unexpected since a lab scale procedure should be more efficient than an industrial scale one which leads us to the assumption that the industrial scale samples generally contain many contaminants or compounds that are of negligible interest when facing the task of identifying the essential oil of Aquilaria Malaccensis. To test this hypothesis, a closer examination of the compounds for each sample is necessary. This section aims to identify which sample is the best representative of gaharu essential oil so that the methods used to obtain that sample can be scrutinized and reproduced in the future for better results.

4.2.1 Lab Hydrodistillation

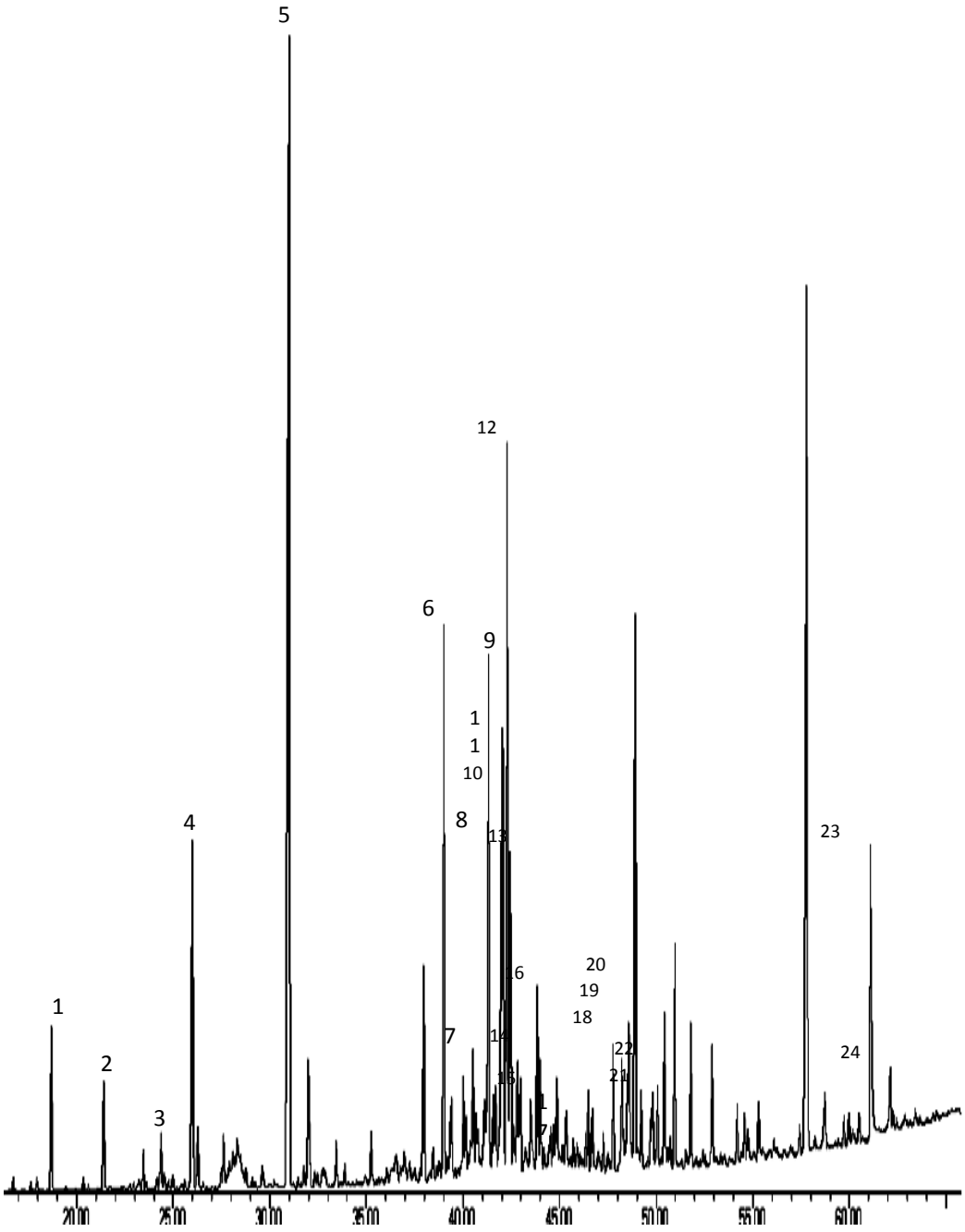


Figure 4.4: Spectrum for sample extracted using hydrodistillation in the lab

Table 4.5: Compound details for sample extracted using hydrodistillation in the lab

Peak no.	Area %	ID	Mol.formula	Cas#	Qual (%)
1	1.44	Benzaldehyde	C_6H_5CHO	100-52-7	96
2	1.00	α – Guaiene	$C_{15}H_{24}$	3691-12-1	99
3	0.58	Salicyl Aldehyde	$C_7H_6O_2$	90-02-8	97
4	3.84	δ-Guaiene	$C_{15}H_{24}$	3691-11-0	99
5	16.1	3-phenyl-2-Butanone	$C_{10}H_{12}O$	769-59-5	95
6	5.68	γ - Eudesmol	$C_{15}H_{26}O$	1209-71-8	93
7	0.85	γ - Gurjunene	$C_{15}H_{24}$	22567-17-5	95
8	4.29	Agarospirol	$C_{15}H_{26}O$	1460-73-7	91
9	0.47	Aromadendrene	$C_{15}H_{24}$	489-39-4	90
10	0.55	Hinesol	$C_{15}H_{26}O$	23811-08-7	93
11	6.50	Neoisolongifolene	$C_{15}H_{24}$	156-12-4	96
12	7.27	Eudesma-3,7(11)-diene	$C_{15}H_{24}$	6813-21-4	81
13	0.81	β – Eudesmol	$C_{15}H_{26}O$	473-15-4	98
14	0.52	1,2,4-Triethyl-Benzene	$C_{12}H_{18}$	877-44-1	70
15	0.65	Longifolene	$C_{15}H_{24}$	475-20-7	91
16	1.47	1R,3Z,9S2,6,10,10-Tetramethylbicyclo [7.2.0]undeca-2,6-diene	$C_{15}H_{24}$	140-07-4	94
17	0.61	Tricyclo[3.2.1.02,7]oct-3-ene, 2,3,4,5-Tetramethyl	$C_{12}H_{18}$	062338-44-7	89
18	0.60	Cycloheptane, 4-methylene-1-methyl-2-(2-methyl-1-propen-1-yl)-1-vinyl-	$C_{15}H_{24}$	159-38-5	90
19	-0.03	α – Caryophyllene	$C_{15}H_{24}$	596753-98-6	90
20	0.67	Cycloheptane, 4-methylene-1-methyl-2-(2-methyl-1-propen-1-yl)-1-vinyl-	$C_{15}H_{24}$	159-38-5	78
21	0.63	γ – Gurjunene	$C_{15}H_{24}$	22567-17-5	87
22	0.09	α - Aromadendrene	$C_{15}H_{24}$	25246-27-9	84

23	3.59	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	57-10-3	96
24	0.66	1,5-diphenyl-3-Pentanone	$C_{17}H_{18}O$	5396-91-8	80

24 compounds were identified from the sample hydroditillated in the lab at a 70% quality cut off point. Of the compounds detected, the important compounds identified include: benzaldehyde, α-guaiene, δ-guaiene, 3-phenyl-2-butanone, γ-eudesmol, γ-gurjunene, agarospirol, aromadendrene, hinesol, eudesma-3,7(11)-diene, β-eudesmol, longifolene, α-aromadendrene and palmitic acid.

Some other compounds detected include several branched unsaturated hydrocarbons. These compounds, while they may indeed come from gaharu oil, are not marker compounds and are not of interest in this study due to the fact that they do not possess the same aromatic qualities that make gaharu oil special like the other compounds listed. The lab hydrodistillated sample succeeded in eluting 14 marker compounds.

4.2.2 Kelantan Hydrodistillation

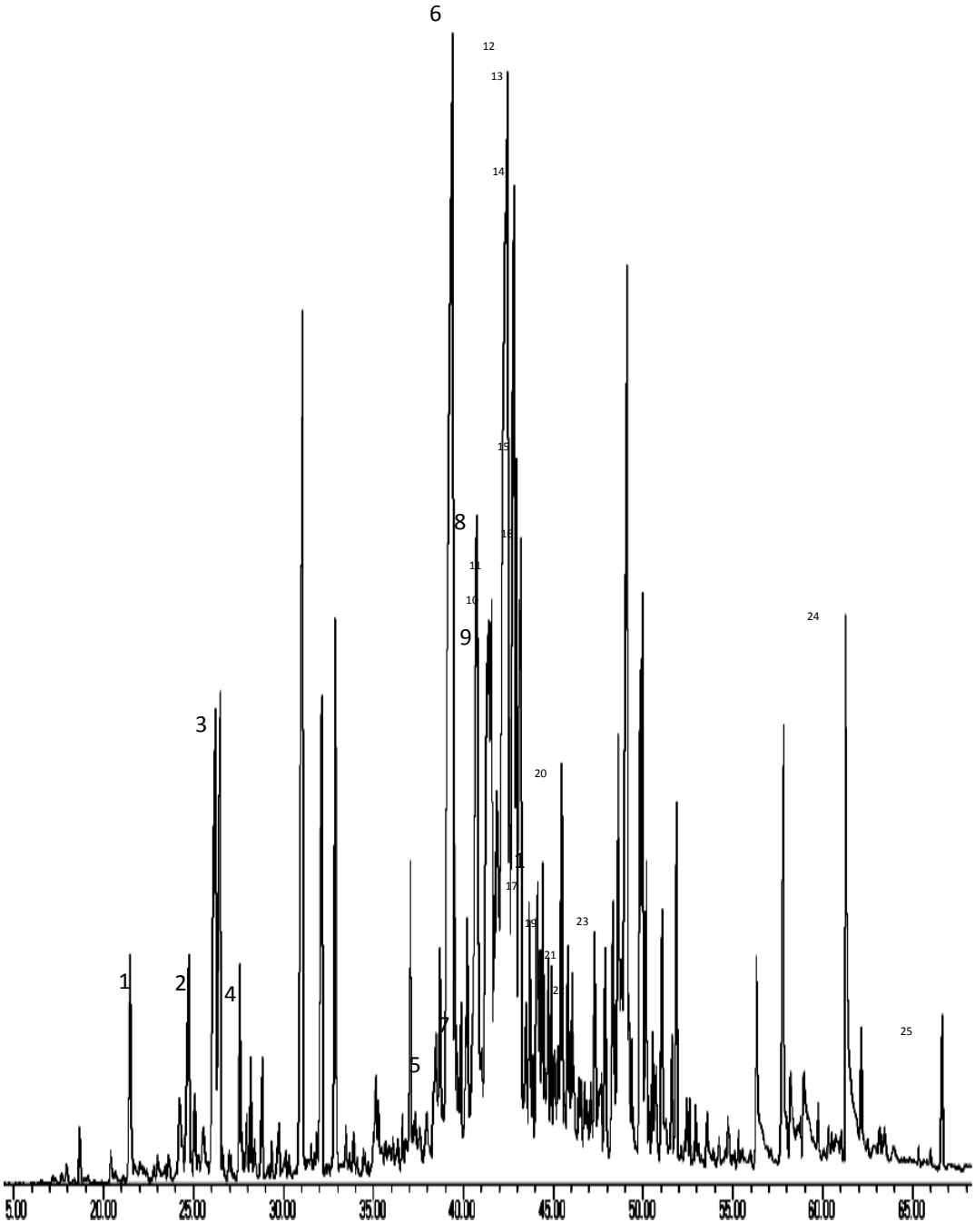


Figure 4.5: Spectrum for sample extracted using hydrodistillation (Kelantan)

Table 4.6: Compound details for sample extracted using hydrodistillation (Kelantan)

Peak no.	Area %	ID	Mol.formula	Cas#	Qual (%)
1	1.07	α - Guaiene	$C_{15}H_{24}$	3691-12-1	99
2	1.10	Aristolene	$C_{15}H_{24}$	150-14-9	87
3	3.27	α - Bulnesene	$C_{15}H_{24}$	3691-11-0	99
4	0.57	δ - Cadinene	$C_{15}H_{24}$	483-76-1	98
5	0.69	α - Elemol	$C_{15}H_{26}O$	639-99-6	90
6	12.6	γ - Eudesmol	$C_{15}H_{26}O$	1209-71-8	94
7	0.65	Dihydrokaranone	$C_{15}H_{22}O$	19598-45-9	78
8	5.11	γ - Cadinene	$C_{15}H_{24}$	39029-41-9	91
9	4.64	Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-	$C_{15}H_{24}$	5951-61-1	93
10	2.92	Hinesol	$C_{15}H_{26}O$	23811-08-7	90
11	2.42	Eremophilene	$C_{15}H_{24}$	10219-75-7	90
12	13.9	α - Gurjunene	$C_{15}H_{24}$	489-40-7	90
13	1.10	γ - Gurjunene	$C_{15}H_{24}$	22567-17-5	93
14	6.09	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene-	$C_{15}H_{24}$	150320-52-8	90
15	2.03	α - Eudesmol	$C_{15}H_{26}O$	473-16-5	98
16	2.72	β - Eudesmol	$C_{15}H_{26}O$	473-15-4	99
17	1.01	Viridiflorene	$C_{15}H_{24}$	21747-46-6	96
18	0.68	4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo [5.1.0.0(2,4)] octane	$C_{15}H_{22}O$	190-22-2	90
19	0.44	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	$C_{15}H_{24}$	192-43-5	83

20	1.43	Hexamethyl-Benzene	$C_{12}H_{18}$	87-85-4	83
21	0.56	Cycloisolongifolene	$C_{15}H_{24}$	151-28-0	90
22	0.33	Cycloheptane,4-methylene-1-methyl-2-(2-methyl-1-propen-1-yl)-1-vinyl-l	$C_{15}H_{24}$	159-38-5	95
23	0.30	1R,3Z,9S2,6,10,10-Tetramethylbicyclo [7.2.0]undeca-2,6-diene	$C_{15}H_{24}$	140-07-4	92
24	2.43	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	57-10-3	98
25	0.50	Mono(2-ethylhexyl) Phthalate	$C_{16}H_{22}O_4$	4376-20-9	91

25 compounds were detected from the Kelantan hydrodistillation sample. Of these compounds, the important ones include: α-guaiene, α-bulnesene, δ-cadinene, γ-eudesmol, dihydrokaranone, γ-cadinene, hinesol, α-gurjunene, γ-gurjunene, α-eudesmol, β-eudesmol, cycloisolongifolene and hexadecanoic acid.

Several compounds detected while producing a sweet scent were not of agarwood oil origin. These compounds include α-elemol, eremophilene and viridiflorene. α-elemol is primarily found in guava juice and commonly used as an additive to bring out flavor and scent. Eremophilene is obtainable from rose leaf oils and viridiflorene can be obtained from a host of sources including rosemary oil, eucalyptus leaf oil and tea tree oil. Other compounds detected included long chained unsaturated hydrocarbons which do not contribute to the pleasing scent of gaharu oil. The Kelantan sample succeeded in isolating 13 compounds of interest to this study.

4.2.3 MAHA Hydrodistillation

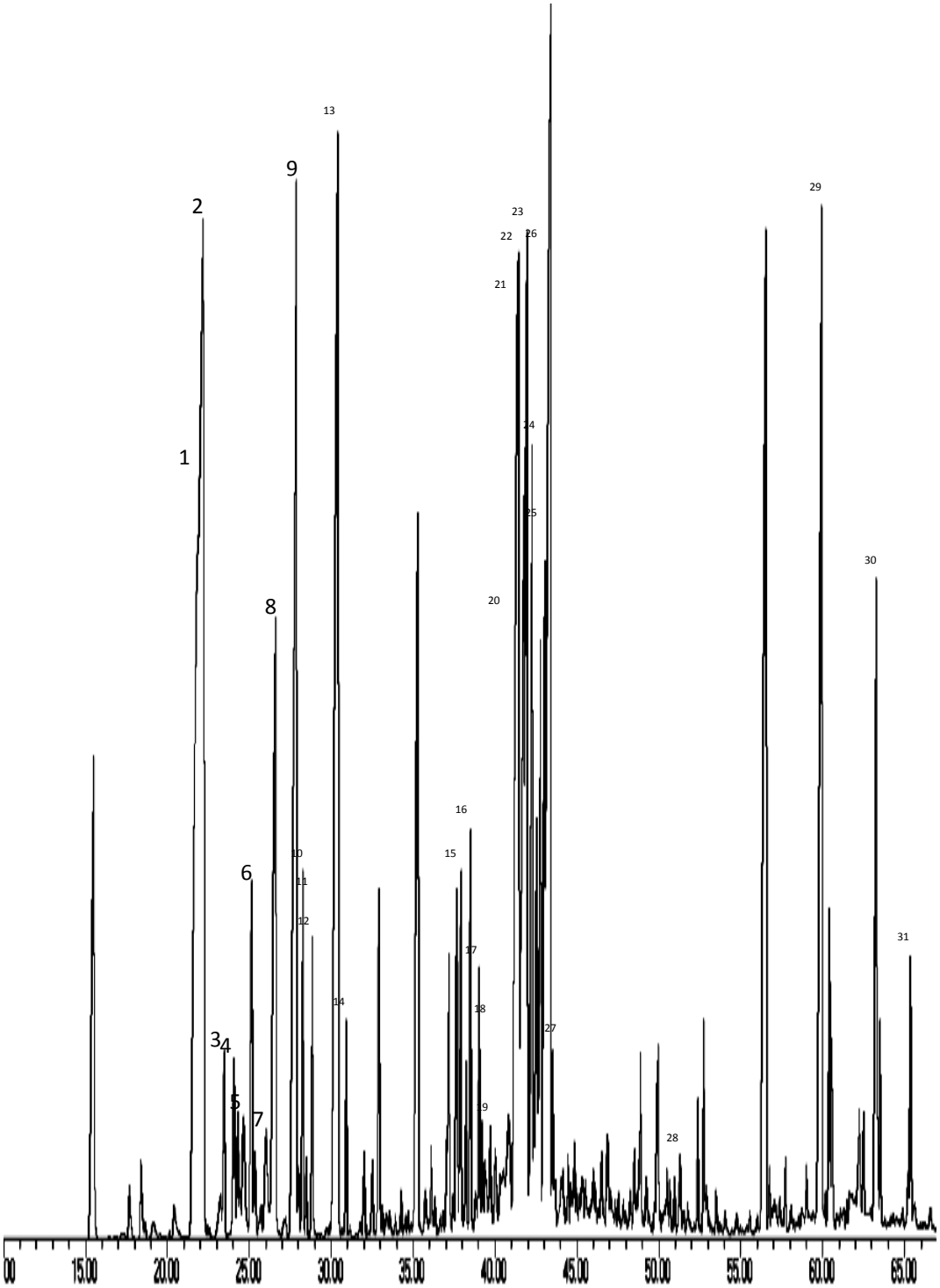


Figure 4.6: Spectrum for sample extracted using hydrodistillation (MAHA)

Table 4.7: Compound details for sample extracted using hydrodistillation (MAHA)

Peak no.	Area %	ID	Mol.formula	Cas#	Qual (%)
1	0.95	Selinane	$C_{15}H_{28}$	30824-81-8	99
2	0.76	p-t-Butylphenyl Glycidylether	$C_{13}H_{18}O_2$	3101-60-8	91
3	0.68	Alloaromadendrene	$C_{15}H_{24}$	25246-27-9	99
4	0.78	δ - Cadinene	$C_{15}H_{24}$	483-76-1	91
5	0.35	α - Caryophyllene	$C_{15}H_{24}$	6753-98-6	97
6	1.78	γ - Muurolene	$C_{15}H_{24}$	30021-74-0	98
7	0.69	6-ethenyl-6-methyl-1-propan-2-yl-3-propan-2-ylidene- cyclohexene	$C_{15}H_{24}$	5951-67-7	95
8	4.35	α - Muurolene	$C_{15}H_{24}$	31983-22-9	98
9	8.38	δ - Cadinene	$C_{15}H_{24}$	483-76-1	98
10	1.29	α - Curcumene	$C_{15}H_{22}$	644-30-4	99
11	0.23	1,2,3,4,6,8alpha-hexahydro-1-isopropyl-4,7-dimethylnaphthalene	$C_{15}H_{24}$	16728-99-7	98
12	1.14	α – Cadinene	$C_{15}H_{24}$	24406-05-1	96
13	8.91	Calamenene	$C_{15}H_{22}$	483-77-2	96
14	0.59	3-phenyl-butan-2-one	$C_{10}H_{12}O$	769-59-5	96
15	0.50	Ledol	$C_{15}H_{26}O$	577-27-5	95
16	1.31	α - Elemol	$C_{15}H_{26}O$	639-99-6	90
17	0.76	γ - Eudesmol	$C_{15}H_{26}O$	1209-71-8	94
18	0.29	Spathulenol	$C_{15}H_{24}O$	6750-60-3	90
19	0.08	α - Cedrene	$C_{15}H_{24}$	469-61-4	89
20	7.78	γ - Cadinene	$C_{15}H_{24}$	39029-41-9	87
21	1.24	Dihydroeudesmol	$C_{15}H_{28}O$	6770-16-7	78
22	3.44	α - Cadinol	$C_{15}H_{26}O$	481-34-5	78
23	3.62	α - Copaene	$C_{15}H_{24}$	3856-25-5	96

24	1.04	Cadalene	$C_{15}H_{18}$	483-78-3	98
25	2.07	α - Eudesmol	$C_{15}H_{26}O$	473-16-5	94
26	1.52	β - Eudesmol	$C_{15}H_{26}O$	473-15-4	99
27	0.32	1,4-Diisopropylbenzene	$C_{12}H_{18}$	100-18-5	76
28	0.32	Cycloisolongifolene	$C_{15}H_{24}$	151-28-0	90
29	6.65	6-(2-Formylhydrazino)-N,N'-Bis (isopropyl)-1,3,5-triazine-2,4-diamine	$C_{10}H_{19}N_7O$	084305-82-8	91
30	2.03	6-Iodo-2-methylquinazolin-4(3H)-on	$C_9H_7IN_2O$	090347-75-4	90
31	0.72	2,2-diphenylchromane	$C_{21}H_{18}O$	010419-28-0	91

31 compounds were detected from the MAHA hydrodistillation sample. Of these compounds, the important ones are: selinane, alloaromadendrene, δ-cadinene, δ-caryophyllene, γ-muurolene, α-muurolene, α-cadinene, 3-phenyl-butan-2-one, γ-eudesmol, γ-cadinene, α-eudesmol, β-eudesmol and cycloisolongifolene.

Other compounds detected include: p-t-butylphenyl glycidylether, α-curcumene, calamenene, ledol, spathulenol, α-cedrene, dihydroeudesmol, α-elemol, α-copaene and 1,4-diisopropylbenzene which although are compounds which induce a pleasant scent are not compounds found naturally in the essential oil of Aquilaria Malaccensis. Calamenene for example is obtained mostly from calamus rhizome oil, α-elemol is primarily found in guava juice, ledol is obtainable from a variety of sources but mostly from marsh tea oils, spathulenol can be obtained from eucalyptus leaves and the list goes on.

The compounds detected which do not constitute essential oil components are basically additives to increase the quantity of oil, to bring out a more complex blend of scents and flavors as well as to lengthen the ability of the oil or absolute to withstand oxidation and free radical attack. The MAHA sample while succeeding in eluting an astounding 31 compound was only able to isolate 14 compounds which belong to agarwood oil.

Table 4.8: Summary of compounds detected in each hydrodistillation sample

Compound Name	Molecular Formula	Sample Used		
		Lab	Kelantan	MAHA
α – Aromadendrene	$C_{15}H_{24}$	✓		
α – Bulnesene	$C_{15}H_{24}$		✓	
α – Cadinene	$C_{15}H_{24}$			✓
α - Caryophyllene	$C_{15}H_{24}$			✓
α - Eudesmol	$C_{15}H_{26}O$		✓	✓
α – Guaiene	$C_{15}H_{24}$	✓	✓	
α – Gurjunene	$C_{15}H_{24}$		✓	
α - Muurolene	$C_{15}H_{24}$			✓
β – Eudesmol	$C_{15}H_{26}O$	✓	✓	✓
δ - Cadinene	$C_{15}H_{24}$		✓	✓
δ-Guaiene	$C_{15}H_{24}$	✓		
γ - Cadinene	$C_{15}H_{24}$		✓	✓
γ – Eudesmol	$C_{15}H_{26}O$	✓	✓	✓
γ – Gurjunene	$C_{15}H_{24}$	✓	✓	
γ - Muurolene	$C_{15}H_{24}$			✓
3-phenylbutan-2-one	$C_{10}H_{12}O$	✓		✓
Agarospirol	$C_{15}H_{26}O$	✓		
Alloaromadendrene	$C_{15}H_{24}$			✓
Aromadendrene	$C_{15}H_{24}$	✓		
Benzaldehyde	C_6H_5CHO	✓		

Cycloisolongifolene	$C_{15}H_{24}$		✓	✓
Dihydrokaranone	$C_{15}H_{22}O$		✓	
Eudesma-3,7(11)-diene	$C_{15}H_{24}$	✓		
Hexadecanoic Acid	$C_{16}H_{32}O_2$	✓	✓	
Hinesol	$C_{15}H_{26}O$	✓	✓	
Longifolene	$C_{15}H_{24}$	✓		
Selinane				✓
Total Marker Compounds Detected in each Sample		14	13	13

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Solvent Extraction

Generally the three solvents used in solvent extraction elicited poorer results compared to the hydrodistillation technique. Solvent extraction managed to elute 9-13 marker compounds whereas hydrodistillation averages 13-14 compounds. Solvents with varying degrees of polarity were selected with the aim of testing the polarity range in which a majority of marker compounds in the agarwood essential oil fell. The proceeding section discusses the conclusions reached from analysis of the results.

5.1.1 Acetone

Acetone is a polar solvent with a dipole moment of 2.91D. This solvent is considered to be the most suitable of the three tested to be used for solvent extraction having successfully eluted 13 marker compounds of agarwood oil. The success of this solvent is mostly associated with the nature of the marker compounds which are mostly polar as well. The compounds eluted by acetone are more similar to those eluted by dichloromethane than those eluted by hexane. The strong forces of attraction due acetone's polarity ensure that many significant compounds dissolve in it making acetone an attractive solvent to be used for extraction of gaharu essential oil.

5.1.2 Dichloromethane

Dichloromethane is a semi-polar solvent having a dipole moment of 1.14D. This solvent eluted only 12 compounds in total and only 9 were marker compounds. This solvent is suitable to be used if one wishes to identify agarwood oil without much noise (additional compounds that are not relevant). However, if the objective is to obtain a more comprehensive and accurate analysis this solvent would perform poorly. The reason for this is that the polarity of dichloromethane is insufficient to dissolve certain marker compounds such as agarospirol, most phenols and ketones and essentially most compounds with a functional group containing oxygen atoms. This eliminates many of the fragrance inducing compounds in agarwood oil and hence reduces the attractiveness of selecting dichloromethane as a solvent.

5.1.3 Hexane

Hexane is a non-polar solvent with a dipole moment of 0.08D. This solvent successful eluted 21 compounds which is greater than acetone and dichloromethane. However, of the 21 compounds isolated only agarospirol and aromadendrene are common compounds eluted with acetone. Hexane has no common compounds eluted with dichloromethane. This is due to the fact that hexane is non-polar and a vast majority of the marker compounds in agarwood oil are polar. The polarities of some of the compounds exist due to the cyclic nature of the compounds causing temporary polarities to be induced in the electron clouds in the rings. This weak form of polarity is compensated by hexane's VDW (Van der Waal's) forces which binds some of the weaker polar compounds.

However when it comes to more polar compounds, the polarity repels hexane's relatively weak van der waal's forces of attraction. Since a majority of the marker compounds are of such nature, hexane is not as desirable as a solvent for extraction compared to acetone.

5.2 Hydrodistillation

Hydrodistillation in this study produced superior results to solvent extraction. Water once again proves its worth as universal solvent with the hydrodistillation procedures eluting 24-31 compounds compared to only 12-21 compounds for solvent extraction. Although this process is tedious and takes a comparatively longer period (3 days for hydrodistillation compared to only 6 hours for solvent extraction) it produces the desired results in the sense that a more comprehensive compound analysis can be obtained. The aim of the proceeding section is to present the conclusions drawn from the analysis of the different hydrodistillation samples.

5.2.1 Lab Hydrodistillation

The lab sample which underwent hydrodistillation succeeded in eluting 24 compounds which was less than that detected in the Kelantan and MAHA samples. However the number of marker compounds detected in the lab sample exceeded those in the Kelantan and MAHA samples which indicates that lab scale experimentation is indeed more efficient.

However the difference in marker compounds detected was small. The lab sample eluted 14 marker compounds whereas the industrial scale samples eluted 13 compounds each. This leads us to the conclusion that the hydrodistillation process itself is the most efficient method for essential oil extraction. Even with the personal touch and careful methodological procedures implemented in the lab, almost negligible difference can be observed in the compounds detected.

5.2.2 Kelantan Hydrodistillation

25 compounds were detected in the Kelantan sample of which only 13 were marker compounds. The remaining compounds were additives meant to bring out

flavor and scent. Since the sample was one obtained from an industrial facility it is safe to conclude that some compounds in the essential oil are not of gaharu origin. The Kelantan facility hydrodistillation process managed to extract many of the cyclic aromatic compounds, some of which were not extracted in the lab scale process. This is probably due to the higher process temperatures in industrial scale facilities which aid in dissolving relatively non-polar and difficult to dissolve compounds such as cyclic aromatic compounds.

5.2.3 MAHA Hydrodistillation

31 compounds were detected in the MAHA sample of which only 13 were marker compounds. The remaining compounds were not of agarwood oil origin and were additives meant to enhance the fragrance and preserve the longevity of the absolute. The MAHA sample had a more complex mixture of marker compounds involving many isomers such as α-, δ-, and γ-cadinene, α-, β- and γ-eudesmol and several other isomers. There were also a greater number of additives coming from a variety of sources such as eucalyptus leaf oils, tea tree oils and guava juice extracts which made up the bulk of the components detected in the MAHA sample.

5.3 Recommendation

The results of this study point towards several guidelines for future experimentation. Firstly that hydrodistillation is a superior technique for extraction of agarwood essential oil unless a better solvent can be discovered. In the event that solvent extraction is used, acetone dissolves the most marker compounds compared to dichloromethane and hexane due to its polar nature. Hence if analysis is necessary within a short period of time (say 5-6 hours) solvent extraction using acetone should be employed.

Dichloromethane on the other hand only elutes 12 compounds but 9 of those 12 are marker compounds for agarwood oil. Hence dichloromethane would be a suitable solvent for easily and quickly identifying gaharu oil without excessive noise. If the objective is extraction where time and noise elimination are not important, hydrodistillation should be employed since water is a better solvent due to its polarity (water has a dipole moment of 1.85D) as well as hydrogen bonding.

The comparison between industrial scale and lab scale hydrodistillation differed by very little. Lab hydrodistillation procedures do not produce significantly better results than industrial scale hydrodistillation hence making hydrodistillation the overall best process for mass production of gaharu essential oil extracts since scaling up comes at very small cost to the quality of product

Future research should further explore the potential of solvent extraction. While this method may have performed poorly compared to hydroditillation in this particular research, there is a vast array of solvents available that could possibly perform better. While hydroditillation does extract gaharu essential oil better, it also has its drawbacks. Hydrodistillation takes a much longer time – ranging from three days to a week for one batch of quality essential oil to be produced. In contrast solvent extraction takes only a few hours before optimum results can be obtained.

In this study, solvents of different polarities were used to determine the polarity best suited for extraction of agarwood oil. The results indicate that the most polar solvent was best suited for the job. Future studies should examine a wider range of solvents and the choice of solvents should lean towards more polar compounds. Since water is currently the best apparent solvent for extraction, solvents with dipole moments approaching that of water should be taken as the median and solvents with polarities less and more than that of water should be incorporated into the experiment to improve control and provide results that can be used to better explain the phenomena of extraction. Future studies can even be made quantitative by correlating the dipole moment of many solvents with the number of marker compounds eluted, hence making for an empirical research into solvent extraction.

In this study, grade C agarwood chips were used for extraction. Future studies should employ better grades so that the difference in the grades can be quantitatively established and measured. Other variables such as the size of grains, solvent concentration, solvent viscosity, the temperature used for extraction and if possible the pressure should also be varied and manipulated in an attempt to find the combination of variables that gives optimum results.

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REFERENCES

Beniwal, B. S. 1989. Silvical characteristics of *Aquilaria agallocha. Indian Forester* 115:17–21.

Burkill, I. H. 1966. *A dictionary of the economic products of the Malay Peninsula.* Ministry of Agriculture and Cooperatives, Kuala Lumpur, Malaysia.

Chakrabarty, K., Kumar, A. and Menon, V. (1994). *Trade in Agarwood* . TRAFFIC India and WWF-India, Delhi 51pp.

Chang, Y. S., M. A. Nor Azah, A. Abu Said, E. H. Lok, S. Reader, and A. Spiers. 2002. *Gaharu*. FRIM Technical Information Bulletin No. 69. Forest Research Institute of Malaysia, Kuala Lumpur, Malaysia.

Chung, R. C. K., and Purawaningsih. 1999. *Aquilaria malaccensis* Lamk. Pages ? *in* L. Oyen, and X. D. Nguyen, editors. *Plant resources of South-East Asia No. 19: essential-oil plants.* Backhuys Publishers, Leiden, the Netherlands.

Fatmawati Adam (2005). *Preliminary Study on Chemical Profiles of Gaharu Essential Oils (Aquilaria Malaccensis) Produced by Conventinal Hydrodistillation Process.*

Hasnida, H. N., M.Y. Aziah, M. Salbiah, Z. Fadhilah, I. Haliza, and H. J. M. Azmy. 2001. Multiplication of shoots from *in vitro* germinated seedlings of *Eurycoma longifolia* and *Aquilaria malaccensis.* Pages 269–276 *in Tropical Forestry research in the new millennium: meeting the challenges.* Proceedings of the International Conference on Forestry and Forest Products Research, 1–3 October 2001, Kuala Lumpur, Malaysia.

Ishihara, M., Tsuneya, T., Shiga. M. and Uneyama, K. 1993. Components of the Volatile Concentrate of Agarwood. *Journal of Essential Oil Research* 5(3): 283-289

Jalaluddin, M. 1977. A Useful Pathological Condition of Wood. *Economic Botany* 31(2): 222-224.

La Frankie, J. (1994). Population Dynamics of Some Tropical Trees That Yield Non-timber Forest Products. *Economic Botany* 48(3): 301-309

Masango Phineas (2005), Cleaner Production of Essential Oils by Steam Distillation. *Journal of Cleaner Production* 13 (2005) 833-839.

Nakanishi, T., Yamagata, E., Yoneda, K. and Miura, I. and Mori, H. (1983) journal Chemical Society Perkin Trans. 1, 601

Newton, A. C., R. R. B. Leakey, W. Powell, K. Chalmers, R. Wangh, Z. Tchoundjeu, P. J. Mathias, P. G. Alderson, J. Meseu, P. Baker, and S. Ramnarine. 1994. Domestication of mahoganies. Pages 256–266 *in* R. Leakey and A. C. Newton, editors. *Tropical trees, the potential for domestication and rebuilding of forest resources.* HMSO Books, London, UK.

Ng, L.T., Chang, Y.S. and Kadir, A.A. (1997). A Review on Agar (*gaharu*) Producing *Aquilaria* Species. *Journal of Tropical Forest Products* 2(2): 272-285.

Paoli, G. D., D. R. Peart, M. Leighton, and I. Samsoedin. 2001. An ecological and economic assessment of the non-timber forest product *gaharu* wood in Gunung Palung National Park, West Kalimantan, Indonesia. *Conservation Biology* 15(6):1721–1732.

Quan Le Tran, Qui Kim Tran, K. Kouda, N. T. Nguyen, Y. Maruyama, I. Saiki, and S. Kadota. 2003. A survey on agarwood in Vietnam. *Journal of Traditional Medicine* 20(3):124–131.

Ruthven, D. M. (1997). Encyclopedia of Separation Technology. Volume 1. New York: John Willey & Sons.

Sadgopol, D. 1959. Experimental studies on the development of essential oils and their components in aromatic plants. *La France et Sa Parfums* 3: 62–71.

Soehartono, T. and Mardiastuti, A. (1997). The Current Trade in Gaharu in West Kalimantan. *Jurnal Ilmiah Biodiversitas Indonesia* 1(1).

Tsutomo Nakanishi, Etsuko Yamagata, Kaisuke Yoneda, Tsukasa Nagashima, Ichiro Kawasaki, Toshio Yoshida, Hideo Morill and Iwao Miurall (1983) “Three Fragrant sesquiterpene of Agarwood”. Faculty of Pharmaceutical Sciences, Osaka University, japan. Pages 2066-2067

Y. S. Chang, M. A. Nor Azah, A. Abu Said, E. H. Lok, S. Reader & A. Spiers (2002) “Gaharu” FRIM Technology Information. No 69.

APPENDIX A

A.1 GC-MS Compound Analysis Results

Data Path : D:\Data\PSM-GAHARU(2008)\

Data File : SOXHLET.ACETONE.D

Acq On : 17 Oct 2008 8:57

Operator : SNT

Sample : ACETONE.SOXHLET

Misc :

ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\Database\NIST05a.L Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint1.e

Table A.1: GC-MS analysis results for solvent extraction with acetone

Pk#	RT	Area%	Library/ID	CAS#	Qa
1	3.621	0.71	C:\Database\NIST05a.L		
Trichloromethane				8712 000067-66-3	97
Trichloromethane				8714 000067-66-3	93
Trichloromethane				8713 000067-66-3	91
2	12.893	8.59	C:\Database\NIST05a.L		
2-Pentanone, 4-hydroxy-4-methyl-				7951 000123-42-2	53
2-Pentanone, 4-hydroxy-4-methyl-				7952 000123-42-2	45
2-Pentanone, 4-hydroxy-4-methyl-				7945 000123-42-2	36
3	16.439	0.57	C:\Database\NIST05a.L		
2-Pentanone, 4-hydroxy-				4168 004161-60-8	78
Acetic acid, hexyl ester				20093 000142-92-7	12
3-Buten-2-one, 3-methyl-				1407 000814-78-8	9
4	18.672	0.65	C:\Database\NIST05a.L		

Benzaldehyde	4937	000100-52-7	96
Benzaldehyde	4934	000100-52-7	95
Benzaldehyde	4936	000100-52-7	95
5 25.925 0.79 C:\Database\NIST05a.L			
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-	60035	003691-11-0	99
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-	60033	003691-11-0	98
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-	60031	003691-11-0	97
6 30.849 1.45 C:\Database\NIST05a.L			
2-Butanone, 3-phenyl-	21739	000769-59-5	97
2-Butanone, 4-phenyl-	21740	002550-26-7	96
2-Butanone, 4-phenyl-	21741	002550-26-7	95
7 34.919 0.72 C:\Database\NIST05a.L			
Caryophyllene oxide	71352	001139-30-6	93
Caryophyllene oxide	71353	001139-30-6	93
Caryophyllene oxide	71350	001139-30-6	91
8 38.946 1.37 C:\Database\NIST05a.L			
Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-	60045	005951-61-1	95
1H-Cyclopropa[a]naphthalene, 1a,2,3,3a,4,5,6,7b-octahydro-1,1,3a,7-tetramethyl-, [1aR-(1a.alpha.,3a.alpha.,7b.alpha.)]-	60074	000489-29-2	95
.delta.-Selinene	59822	028624-23-9	95
9 40.516 0.56 C:\Database\NIST05a.L			
1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-	60073	025246-27-9	95
1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1.alpha.,3a.beta.,4.alpha.,8a.beta.)]	60018	000475-20-7	87
Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-	60067	022567-17-5	83
10 40.965 0.36 C:\Database\NIST05a.L			
3-Allyl-6-methoxyphenol	31757	000501-19-9	98
Eugenol	31716	000097-53-0	98
Eugenol	31715	000097-53-0	98
11 41.125 28.24 C:\Database\NIST05a.L			
Patchouli alcohol	72916	005986-55-0	99
1(2H)-Naphthalenone, octahydro-4a,8a-dimethyl-7-(1-methylethyl)-, [4	73001	001803-39-0	30

aR-(4a.alpha.,7.beta.,8a.alpha.)]-				
.+/-.-4-Acetyl-1-methylcyclohexene			16987 070286-20-3	22
12	41.264	0.69	C:\Database\NIST05a.L	
Hinesol			72894 023811-08-7	90
1H-Cycloprop[e]azulene, decahydro-			60080 000489-39-4	83
1,1,7-trimethyl-4-methylene-, [1aR				
-(1a.alpha.,4a.alpha.,7.alpha.,7a.				
beta.,7b.alpha.)]-				
Naphthalene, 1,2,3,5,6,7,8,8a-octa			60048 004630-07-3	64
hydro-1,8a-dimethyl-7-(1-methyleth				
enyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-				
13	41.980	1.70	C:\Database\NIST05a.L	
.delta.-Selinene			59822 028624-23-9	96
Tricyclo[4.1.0.0(2,4)]heptane, 3,3			59968 056348-21-1	93
,7,7-tetramethyl-5-(2-methyl-1-pro				
penyl)-				
1,4-Methanoazulene, decahydro-4,8,			60023 000475-20-7	90
8-trimethyl-9-methylene-, [1S-(1.a				
lpha.,3a.beta.,4.alpha.,8a.beta.)]				
14	42.194	3.47	C:\Database\NIST05a.L	
Naphthalene, 1,2,3,4,4a,5,6,8a-oct			60063 000473-13-2	89
ahydro-4a,8-dimethyl-2-(1-methylet				
henyl)-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				
Azulene, 1,2,3,5,6,7,8,8a-octahydr			60033 003691-11-0	87
o-1,4-dimethyl-7-(1-methylethenyl)				
-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-				
Azulene, 1,2,3,5,6,7,8,8a-octahydr			60034 003691-11-0	86
o-1,4-dimethyl-7-(1-methylethenyl)				
-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-				
15	43.785	1.65	C:\Database\NIST05a.L	
2H-Cyclopropa[a]naphthalen-2-one,			69993 006831-17-0	70
1,1a,4,5,6,7,7a,7b-octahydro-1,1,7				
,7a-tetramethyl-, (1a.alpha.,7.alp				
ha.,7a.alpha.,7b.alpha.)-				
2(3H)-Naphthalenone, 4,4a,5,6,7,8-			69988 019598-45-9	55
hexahydro-4a,5-dimethyl-3-(1-methy				
lethylidene)-, (4ar-cis)-				
2(1H)Naphthalenone, 3,5,6,7,8,8a-h			69976 1000188-66-5	49
exahydro-4,8a-dimethyl-6-(1-methylethenyl)-				
16	48.549	0.57	C:\Database\NIST05a.L	
1-Methyl-6-methylenebicyclo[3.2.0]			9743 1000210-90-0	83
heptane				
Naphthalene, 1,2,3,5,6,7,8,8a-octa			60047 004630-07-3	52
hydro-1,8a-dimethyl-7-(1-methyleth				
enyl)-, [1R-(1.alpha.,7.beta.,8a.a				
lpha.)]-				
4,6,6-Trimethyl-2-(3-methylbuta-1,			69975 1000190-22-2	49
3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane				
17	48.848	1.29	C:\Database\NIST05a.L	

1,4-Methanoazulen-7(1H)-one, octah ydro-4,8,8,9-tetramethyl-, (+)-	71426	018319-28-3	49
6-Isopropenyl-4,8a-dimethyl-1,2,3, 5,6,7,8,8a-octahydro-naphthalen-2-ol	71438	1000189-10-2	43
2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7- octahydro-naphthalen-2-yl)-prop-2-en-1-ol	71444	1000190-51-8	38
18 49.180 1.37 C:\Database\NIST05a.L			
N-(2-Oxo-2,3-dihydro-1H-benzoimida zol-5-yl)-butyramide	70303	1000274-22-8	35
Benzene, 1-isothiocyanato-2-methyl	22617	000614-69-7	27
Tricyclo[4.3.1.1(3,8)]undecane,1-bromo-	76877	021898-96-4	27
19 49.489 1.72 C:\Database\NIST05a.L			
Benzophenone	44594	000119-61-9	95
Benzophenone	44599	000119-61-9	95
Benzophenone	44597	000119-61-9	94
20 50.910 0.89 C:\Database\NIST05a.L			
9-Isopropyl-1-methyl-2-methylene-5 -oxatricyclo[5.4.0.0(3,8)]undecane	71434	1000185-86-6	38
Caryophyllene	59802	000087-44-5	25
1H-3a,7-Methanoazulen-5-ol, octahy dro-3,8,8-trimethyl-6-methylene-	71429	028231-03-0	22
21 51.754 0.67 C:\Database\NIST05a.L			
Ethanone, 1-[4-(trifluoromethoxy)p henyl]-	60400	085013-98-5	35
Azulene, 1,2,3,5,6,7,8,8a-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1S-(1.alpha.,7.alpha.,8a.beta.)]-	60033	003691-11-0	30
Glaucyl alcohol	71328	087745-32-2	25
22 53.548 4.71 C:\Database\NIST05a.L			
Benzyl Benzoate	65862	000120-51-4	96
Benzyl Benzoate	65860	000120-51-4	96
Benzyl Benzoate	65863	000120-51-4	94
23 54.756 1.14 C:\Database\NIST05a.L			
1,3-Benzenedicarboxylic acid, 4-me thyl-, dimethyl ester	62521	023038-61-1	30
7-Isobutoxy-5,9-dihydro-6,8-dioxa- 7-bora-benzocycloheptene	71016	1000317-66-9	27
Benzofuran-2-one, 4-amino-2,3-dihydro-3,3-dimethyl-	40909	1000129-51-7	25
24 57.074 0.55 C:\Database\NIST05a.L			
Anthracene, 9-butyl-	81253	001498-69-7	60
2-Allyl-1,4-dimethoxy-3-vinyloxyme thylbenzene	81012	1000188-16-6	49
dl-9-Cyano-2-oxo-cis-decalin semicarbazone	80886	002740-39-8	46
25 57.714 10.13 C:\Database\NIST05a.L			
1,3-Cyclopentadiene, 5,5-dimethyl- 1-ethyl-	9746	1000162-25-7	38
Phenol, 3,4-dimethyl-, methylcarba mate	42272	002425-10-7	38

Phenol, 3,5-dimethyl-	9631	000108-68-9	38
26 58.323 0.79 C:\Database\NIST05a.L			
Tricyclo[5.1.0.0(2,4)]oct-5-ene-5-propanoic acid, 3,3,8,8-tetramethyl-	81134	074793-63-8	14
3-Butyl-4,5-dimethyl-4-hydroxyhexahydropyrimidin-2-thione	68122	088070-31-9	11
2,4-Pentadienoic acid, 2-acetyl-4-methyl-5-(2-furyl)-, methyl ester	80933	349496-09-9	11
27 58.719 0.52 C:\Database\NIST05a.L			
Benzene, 1-methyl-3,5-bis(1-methylethyl)-	40378	003055-14-9	43
Acetamide, N-(4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl)-, (1.alpha.,2.beta.,5.alpha.)-	52033	133180-86-6	25
Benzene, (2,2-dimethyl-1-methylenepropyl)-	29583	005676-29-9	25
28 59.082 0.95 C:\Database\NIST05a.L			
Pyrene, 1,2,3,3a,4,5,5a,6,7,8,8a,9,10,10a-tetradecahydro-	68677	126188-35-0	38
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	29572	022531-20-0	35
1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetrahydro-	29509	055255-94-2	20
29 59.413 12.80 C:\Database\NIST05a.L			
Ethanol, 2,2'-dithiobis-	26018	001892-29-1	96
Ethanol, 2,2'-dithiobis-	26017	001892-29-1	94
2-(Diethyl-phosphinoyl)-acetamide	31515	013298-22-1	28
30 60.492 0.94 C:\Database\NIST05a.L			
Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,4.alpha.,7.alpha.)]-	60028	003691-12-1	51
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-	60033	003691-11-0	38
Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,4.alpha.,7.alpha.)]-	60027	003691-12-1	35
31 60.684 0.73 C:\Database\NIST05a.L			
.gamma.-Himachalene	59843	1000140-08-0	53
2(1H)Naphthalenone, 3,5,6,7,8,8a-hexahydro-4,8a-dimethyl-6-(1-methylethenyl)-	69976	1000188-66-5	49
2-Amino-4-cyanomethyl-6-piperidino-1,3,5-triazine	69370	1000241-05-9	45
32 61.047 1.76 C:\Database\NIST05a.L			
5,5'-Ethylenebis(4-phenyl-2-thiazolamine)	164464	102077-35-0	27
9-Methyltetracyclo[7.3.1.0(2.7).1(7.11)]tetradecane	59892	1000215-30-5	27
2,5-Pyrrolidinedione, 3-methyl-1-phenyl-	49264	075619-07-7	20
33 62.115 2.53 C:\Database\NIST05a.L			
Cyclopentane-3'-spirotricyclo[3.1.0.0(2,4)]hexane-6'-spirocyclopentane	48802	078578-93-5	25
Bicyclo[6.3.0]undeca-1(8),9-diene,11,11-dimethyl-	40394	1000163-44-3	22
Tridecane, 3-methyl-2,12-diphenyl-	189548	1000161-64-9	16

5,7,9-tris(1-phenylethyl)-					
34	62.436	0.65	C:\Database\NIST05a.L		
Bicyclo[4.1.0]heptan-2-one, 3,4,4-trimethyl-3-(3-methyl-1,3-butadienyl)-, [1.alpha.,3.alpha.(E),6.alpha.]-(.+-.)-				69989	102146-81-6 55
Benzenamine, 3,5-dimethyl-				9312	000108-69-0 46
Benzenamine, 3,5-dimethyl-				9311	000108-69-0 46
35	63.408	0.52	C:\Database\NIST05a.L		
Megastigmatrienone				49924	038818-55-2 50
Cyclopenta[1,3]cyclopropa[1,2]cycloheptene-3(3aH)-one, 1,2,3b,6,7,8-hexahydro-6,6-dimethyl-				49990	091531-58-7 47
Megastigmatrienone				49925	038818-55-2 30
36	63.536	0.71	C:\Database\NIST05a.L		
2-Ethyl-6-isopropylphenyl isothiocyanate				60638	067330-54-5 70
(-)-Spathulenol				71327	077171-55-2 55
1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9- methylene-, (4aS-cis)-				59998	003853-83-6 51
37	65.843	0.92	C:\Database\NIST05a.L		
5-Pyrimidinamine, 2-chloro-4-ethoxy-				38633	054484-70-7 18
1,3,5-Trisilacyclohexane, 1,1-dimethyl-				29653	054424-15-6 11
4-Methyl-2H-benzopyrane				20723	021776-94-3 11
38	69.465	1.19	C:\Database\NIST05a.L		
Cycloheptane, 4-methylene-1-methyl-2-(2-methyl-1-propen-1-yl)-1-vinyl-				59957	1000159-38-5 56
Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-				59912	013877-93-5 35
Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-				59917	242794-76-9 35
39	69.924	1.13	C:\Database\NIST05a.L		
Pentacyclo[7.5.0.0(2,8).0(5,14).0(7,11)]tetradecane				48786	079772-15-9 38
3-Bromo-2-methyl-2-hydroxyindan-1-one-3-carboxilic acid				114204	091063-07-9 30
Cyclopentane-3'-spirotricyclo[3.1.0.0(2,4)]hexane-6'-spirocyclopentane				48802	078578-93-5 25

Table A.2: GC-MS analysis results for solvent extraction with dichloromethane

Pk#	RT	Area%	Library/ID	CAS#	Qual
1	3.151	1.24	C:\Database\NIST05a.L		
Methylene Chloride				1499 000075-09-2	94
Methylene Chloride				1500 000075-09-2	64
Methylene Chloride				1497 000075-09-2	50

2	3.194	2.32	C:\Database\NIST05a.L		
Methylene Chloride				1499 000075-09-2	94
Methylene Chloride				1500 000075-09-2	64
Methylene Chloride				1498 000075-09-2	50
3	3.269	10.01	C:\Database\NIST05a.L		
Methylene Chloride				1499 000075-09-2	91
Methylene Chloride				1498 000075-09-2	72
Methylene Chloride				1500 000075-09-2	72
4	3.472	60.46	C:\Database\NIST05a.L		
Methylene Chloride				1499 000075-09-2	95
Methylene Chloride				1498 000075-09-2	94
Methylene Chloride				1497 000075-09-2	91
5	18.693	0.61	C:\Database\NIST05a.L		
Benzaldehyde				4937 000100-52-7	96
Benzaldehyde				4935 000100-52-7	95
Benzaldehyde				4936 000100-52-7	94
6	25.936	0.72	C:\Database\NIST05a.L		
Azulene, 1,2,3,5,6,7,8,8a-octahydr				60035 003691-11-0	99
o-1,4-dimethyl-7-(1-methylethenyl)					
-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-					
Azulene, 1,2,3,5,6,7,8,8a-octahydr				60033 003691-11-0	99
o-1,4-dimethyl-7-(1-methylethenyl)					
-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-					
Azulene, 1,2,3,5,6,7,8,8a-octahydr				60031 003691-11-0	98
o-1,4-dimethyl-7-(1-methylethenyl)					
-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-					
7	30.860	1.55	C:\Database\NIST05a.L		
2-Butanone, 4-phenyl-				21740 002550-26-7	95
2-Butanone, 4-phenyl-				21741 002550-26-7	95
2-Butanone, 4-phenyl-				21737 002550-26-7	94
8	31.939	0.07	C:\Database\NIST05a.L		
2H-2,4a-Methanonaphthalen-8(5H)-on				71452 023787-90-8	42
e, 1,3,4,6,7,8a-hexahydro-1,1,5,5-tetramethyl-					
Ethanol, 2-(2-cyclohexylphenoxy)-				71171 054852-66-3	35
2,6,10-Trimethyl-12-oxatricyclo[7.				71413 1000189-02-9	18
3.1.0(1,6)]tridec-2-ene					
9	37.932	0.41	C:\Database\NIST05a.L		
4,6,6-Trimethyl-2-(3-methylbuta-1,				69975 1000190-22-2	90
3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane					
Cyclohexane, 1-ethenyl-1-methyl-2,				60003 000515-13-9	55
4-bis(1-methylethenyl)-, [1S-(1.al					
pha.,2.beta.,4.beta.)]-					
9-Oxabicyclo[4.3.0]non-6-en-8-one,				69762 1000160-28-8	38
7-(1-cyclopenten-3-one-1-yl)-					
10	38.946	1.50	C:\Database\NIST05a.L		
1H-Cycloprop[e]azulene, 1a,2,3,4,4				60090 000489-40-7	89
a,5,6,7b-octahydro-1,1,4,7-tetrame					
thyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-					
2-Naphthalenemethanol, 1,2,3,4,4a,				72998 001209-71-8	89

5,6,7-octahydro-.alpha.,.alpha.,4a ,8-tetramethyl-, (2R-cis)-				
Naphthalene, 1,2,4a,5,8,8a-hexahyd ro-4,7-dimethyl-1-(1-methylethyl)- , (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-			60045	005951-61-1 87
11	39.320	0.41	C:\Database\NIST05a.L	
2H-1-Benzopyran-2-one, 4-methyl-7- (2-propenyloxy)-			68495	003993-57-5 53
Phenol, 4-bromo-2-methoxy-5-methyl			68826	040992-09-4 30
Tiaprofenic Acid			98510	033005-95-7 27
12	40.485	0.38	C:\Database\NIST05a.L	
Azulene, 1,2,3,3a,4,5,6,7-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-			60069	022567-17-5 95
Azulene, 1,2,3,3a,4,5,6,7-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-			60067	022567-17-5 95
1H-Cycloprop[e]azulene, decahydro- 1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-			60080	000489-39-4 90
13	41.254	1.12	C:\Database\NIST05a.L	
Hinesol			72894	023811-08-7 86
Naphthalene, 1,2,3,5,6,7,8,8a-octa hydro-1,8a-dimethyl-7-(1-methyleth enyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-			60046	004630-07-3 70
Naphthalene, 1,2,3,5,6,7,8,8a-octa hydro-1,8a-dimethyl-7-(1-methyleth enyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-			60048	004630-07-3 64
14	41.980	1.90	C:\Database\NIST05a.L	
Naphthalene, 1,2,4a,5,8,8a-hexahyd ro-4,7-dimethyl-1-(1-methylethyl)- , (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-			60043	005951-61-1 95
Tricyclo[4.1.0.0(2,4)]heptane, 3,3 ,7,7-tetramethyl-5-(2-methyl-1-propenyl)-			59968	056348-21-1 93
Neoisolongifolene			59831	1000156-12-4 92
15	42.194	2.16	C:\Database\NIST05a.L	
1,4-Methanoazulene, decahydro-4,8, 8-trimethyl-9-methylene-, [1S-(1.a lpha.,3a.beta.,4.alpha.,8a.beta.)]			60018	000475-20-7 81
Naphthalene, 1,2,3,4,4a,5,6,8a-oct ahydro-4a,8-dimethyl-2-(1-methylet henyl)-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-			60063	000473-13-2 78
Azulene, 1,2,3,5,6,7,8,8a-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1S-(1.alpha.,7.alpha.,8a.beta.)]-			60033	003691-11-0 64
16	42.397	0.51	C:\Database\NIST05a.L	
Bicyclo[4.4.0]dec-1-ene, 2-isoprop yl-5-methyl-9-methylene-			59918	150320-52-8 70
1,4-Methanoazulene, decahydro-4,8,			60024	000475-20-7 64

8-trimethyl-9-methylene-, [1S-(1.a lpha.,3a.beta.,4.alpha.,8a.beta.)]					
Isoledene				59783 1000156-10-8	60
17	42.771	0.19	C:\Database\NIST05a.L		
2-Naphthalenemethanol, decahydro-. alpha.,.alpha.,4a-trimethyl-8-meth ylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				73009 000473-15-4	97
2-Naphthalenemethanol, decahydro-. alpha.,.alpha.,4a-trimethyl-8-meth ylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				73010 000473-15-4	93
1H-Indene, 1-ethylideneoctahydro-7 a-methyl-, cis-				32229 056362-87-9	64
18	43.785	0.38	C:\Database\NIST05a.L		
1R,3Z,9S-2,6,10,10-Tetramethylbicy clo[7.2.0]undeca-2,6-diene				59923 1000140-07-4	92
Longifolene-(V4)				59820 061262-67-7	89
1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.beta.,7.alpha.,7a.b eta.,7b.alpha.)]-				60077 025246-27-9	83
19	44.255	0.21	C:\Database\NIST05a.L		
6,7-Dimethyl-3,4-dihydro-1H-[1,4]d iazepino[3,2,1-hi]indol-2-one				67128 063594-54-7	46
1(2H)Phenanthrenone, 3,4,4a,9,10,1 0a-hexahydro-4a-methyl-				67362 062318-99-4	38
4-(2-Hydroxyphenyl)pyrimidine				37720 068535-55-7	35
20	48.186	0.25	C:\Database\NIST05a.L		
9H-Cycloisolongifolene, 8-oxo-				69939 1000155-43-0	50
Isolongifolen-5-one				69932 1000159-37-1	46
Benzene, 1,4-dimethyl-2,5-bis(1-methylethyl)-				50034 010375-96-9	41
21	48.475	0.21	C:\Database\NIST05a.L		
.alpha.-Caryophyllene				59848 006753-98-6	62
1,3,6-Octatriene, 3,7-dimethyl-, (Z)-				15283 003338-55-4	60
Santolina triene				15184 002153-66-4	58
22	48.550	0.31	C:\Database\NIST05a.L		
4,6,6-Trimethyl-2-(3-methylbuta-1, 3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane				69975 1000190-22-2	43
Cycloheptane, 4-methylene-1-methyl -2-(2-methyl-1-propen-1-yl)-1-vinyl-				59957 1000159-38-5	38
Cyclolongifolene oxide, dehydro-				69941 1000156-11-4	38
23	48.849	1.23	C:\Database\NIST05a.L		
6-Isopropenyl-4,8a-dimethyl-1,2,3, 5,6,7,8,8a-octahydro-naphthalen-2-ol				71438 1000189-10-2	43
1,4-Methanoazulen-7(1H)-one, octah ydro-4,8,8,9-tetramethyl-, (+)-				71426 018319-28-3	38
Cycloisolongifolene, 8-hydroxy-, endo-				71391 1000151-49-2	25
24	50.910	0.95	C:\Database\NIST05a.L		
Caryophyleine-(I3)				59836 136296-37-2	35
4-Hexadecen-6-yne, (Z)-				71496 074744-54-0	18

1,5,9,11-Tridecatetraene, 12-methyl-, (E,E)-				50030	062338-27-6 14
25	51.765	0.44	C:\Database\NIST05a.L		
Acetic acid, [(2,4,6-triethylbenzoyl)thio]-				111694	067902-78-7 47
Azulene, 1,2,3,5,6,7,8,8a-octahydr				60033	003691-11-0 38
o-1,4-dimethyl-7-(1-methylethenyl)					
-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-					
6S-2,3,8,8-Tetramethyltricyclo[5.2				59906	137235-48-4 38
.2.0(1,6)]undec-2-ene					
26	52.865	0.48	C:\Database\NIST05a.L		
1H-Benzimidazole, 2-ethyl-				21357	001848-84-6 43
3-Pyridinecarbonitrile, 6-ethyl-5-methyl-				21387	110253-41-3 43
Benzene, 1-(1-methyl-2-propenyl)-4				48792	057438-46-7 27
-(2-methylpropyl)-					
27	54.756	1.52	C:\Database\NIST05a.L		
4-Pyrimidinamine, 5-(2-thienyl)-				41162	058758-95-5 35
2-(2-Hydroxypropionyl)phenylglyoxylic acid				72313	091345-20-9 25
Pyrazolo[3,4-b]pyridin-6-one, 1,7-				41181	057411-62-8 25
dihydro-1,3,4-trimethyl-					
28	57.704	8.40	C:\Database\NIST05a.L		
Phenol, 3,5-dimethyl-				9619	000108-68-9 38
Phenol, 2-ethyl-				9607	000090-00-6 38
Phenol, 3,4-dimethyl-,methylcarbamate				42272	002425-10-7 38
29	58.569	0.24	C:\Database\NIST05a.L		
Caryophyllene-(I1)				59838	1000158-18-5 56
4,4-Dimethyl-3-(3-methylbut-3-enyl				58548	079718-83-5 38
idene)-2-methylenebicyclo[4.1.0]heptane					
1,2,3,6-Tetrahydropyridine, 4-[4-hydroxyphenyl]-				39749	090684-15-4 38
30	58.719	0.35	C:\Database\NIST05a.L		
5-Isopropylidene-4,6-dimethylnona-				61468	1000195-14-9 27
3,6,8-trien-2-ol					
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-				29565	002613-76-5 25
Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-				29611	005557-93-7 25
GAHARU PHD.M Sat Oct 18 16:26:17 2008 CHEMSTATION					

Table A.3: GC-MS analysis results for solvent extraction with hexane

Pk#	RT	Area%	Library/ID	CAS#	Qual
1	6.249	1.94	C:\Database\NIST05a.L		
Cyclopentasiloxane, decamethyl-				161015	000541-02-6 95
Cyclopentasiloxane, decamethyl-				161017	000541-02-6 94
Cyclopentasiloxane, decamethyl-				161016	000541-02-6 91
2	12.573	1.64	C:\Database\NIST05a.L		
Cyclohexasiloxane, dodecamethyl-				179152	000540-97-6 91
Cyclohexasiloxane, dodecamethyl-				179153	000540-97-6 90

2-Chloro-4-(4-methoxyphenyl)-6-(4-nitrophenyl)pyrimidine			148181	063673-76-7 43
3	14.015	0.80	C:\Database\NIST05a.L	
Nonanal			19202	000124-19-6 86
Nonanal			19204	000124-19-6 83
Nonanal			19203	000124-19-6 74
4	17.946	1.00	C:\Database\NIST05a.L	
1-Hexanol, 2-ethyl-			13237	000104-76-7 83
1-Hexanol, 2-ethyl-			13235	000104-76-7 83
1-Hexanol, 2-ethyl-			13229	000104-76-7 72
5	19.452	1.62	C:\Database\NIST05a.L	
Cycloheptasiloxane, tetradecamethyl-			185541	000107-50-6 90
3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane			187800	071579-69-6 32
Tetrasiloxane, 3,5-diethoxy-1,1,1,7,7,7-hexamethyl-3,5-bis(trimethylsiloxy)-			185549	072439-78-2 27
6	25.476	0.80	C:\Database\NIST05a.L	
.beta.-Vatirenene			58513	1000293-04-2 49
Benzene, 1-(1-formylethyl)-4-(1-buten-3-yl)-			48728	1000161-46-6 46
2(1H)-Quinolinone, 1-methyl-			29124	000606-43-9 38
7	25.925	1.45	C:\Database\NIST05a.L	
Cyclooctasiloxane, hexadecamethyl-			188231	000556-68-3 62
Silane, [[4-[1,2-bis[(trimethylsilyl)oxy]ethyl]-1,2-phenylene]bis(oxy)]bis[trimethyl-			180820	056114-62-6 53
Benzoic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester			161136	010586-16-0 47
8	28.382	0.63	C:\Database\NIST05a.L	
1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hexahydro-1,4,9,9-tetramethyl-, (1.alpha.,3a.alpha.,7.alpha.,8a.beta.)-			60042	000560-32-7 76
1,5,6,7-Tetrahydro-4-indolone			15024	013754-86-4 47
1-Cycloheptene, 1,4-dimethyl-3-(2-methyl-1-propene-1-yl)-4-vinyl-			59937	1000159-38-6 46
9	28.681	2.00	C:\Database\NIST05a.L	
1,5,9-Cyclododecatriene, 1,5,9-trimethyl-			59880	021064-19-7 72
1,7-Octadiene, 2-methyl-6-methylene-			15276	001686-30-2 64
1,5,9-Cyclododecatriene, 1,5,9-trimethyl-			59878	021064-19-7 64
10	31.426	0.55	C:\Database\NIST05a.L	
2,6,11,15-Tetramethyl-hexadeca-2,6,8,10,14-pentaene			107082	038259-79-9 40
Phenylacetic acid, 3-methylbut-2-enyl ester			59665	151091-17-7 38
4-Aza-5-thiatricyclo[5.2.1.0(3,7)]decane, 4-(2-butenoyl)-10,10-dimethyl-5,5-dioxo-			113782	1000156-44-2 25
11	31.800	1.77	C:\Database\NIST05a.L	
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester			115959	074381-40-1 50
Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester			115958	1000140-77-5 50

Oxalic acid, neopentyl-nonyl ester			115941 1000309-73-3	45
12	33.734 1.09	C:\Database\NIST05a.L		
1-Adamantyl methyl ketone			41627 001660-04-4	47
1-Adamantyl methyl ketone			41628 001660-04-4	47
4-Hydroxy-2-methylacetophenone			23479 000875-59-2	47
13	35.090 0.83	C:\Database\NIST05a.L		
Acetic acid, trifluoro-, tetradecyl ester			130785 006222-02-2	91
4-Trifluoroacetoxytridecane			121959 1000245-47-3	87
Pentafluoropropionic acid, tetradecyl ester			156947 006222-06-6	80
14	35.891 1.15	C:\Database\NIST05a.L		
Diphenyl ether			36402 000101-84-8	70
Diphenyl ether			36401 000101-84-8	60
Diphenyl ether			36400 000101-84-8	45
15	39.246 0.78	C:\Database\NIST05a.L		
Heneicosane			122436 000629-94-7	96
Heptacosane, 1-chloro-			174384 062016-79-9	87
Heptacosane			165300 000593-49-7	83
16	40.987 1.38	C:\Database\NIST05a.L		
Patchouli alcohol			72910 005986-55-0	97
Patchouli alcohol			72914 005986-55-0	96
Patchouli alcohol			72916 005986-55-0	94
17	41.243 1.27	C:\Database\NIST05a.L		
Agarospirol			72903 001460-73-7	95
Hinesol			72894 023811-08-7	90
10s,11s-Himachala-3(12),4-diene			59868 060909-28-6	68
18	42.183 1.28	C:\Database\NIST05a.L		
1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-			60080 000489-39-4	70
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-			60034 003691-11-0	66
(-)-Isoaromadendrene-(V)			59859 1000156-14-3	62
19	42.290 2.02	C:\Database\NIST05a.L		
Docosane			131156 000629-97-0	94
Heneicosane, 11-(1-ethylpropyl)-			159851 055282-11-6	91
Docosane			131155 000629-97-0	90
20	42.717 1.48	C:\Database\NIST05a.L		
Hexadecanoic acid, methyl ester			105639 000112-39-0	98
Hexadecanoic acid, methyl ester			105646 000112-39-0	95
Pentadecanoic acid, 14-methyl-, methyl ester			105661 005129-60-2	95
21	45.217 3.42	C:\Database\NIST05a.L		
Octadecane			94930 000593-45-3	96
Tetratetracontane			188836 007098-22-8	91
Nonadecane, 9-methyl-			113498 013287-24-6	91
22	46.360 0.50	C:\Database\NIST05a.L		
Octadecanal			104240 000638-66-4	90
1,15-Hexadecadiene			73063 021964-51-2	76

1,13-Tetradecadiene			52921	021964-49-8 76
23	48.026	3.10	C:\Database\NIST05a.L	
Tetracosane			146923	000646-31-1 98
Tetracosane			146921	000646-31-1 98
Heptadecane			85523	000629-78-7 96
24	48.539	0.27	C:\Database\NIST05a.L	
8-Naphthol, 1-(benzyloxy)-			92179	326875-68-7 64
Acetamide, N-(4-cyanomethylphenyl)-2-phenyl-			92082	1000303-53-0 59
1-Benzyl-5-methylsulfanyl-3-nitro-1H-[1,2,4]triazole			91479	1000275-74-7 59
25	49.158	1.41	C:\Database\NIST05a.L	
8-Naphthol, 1-(benzyloxy)-			92179	326875-68-7 64
1-Benzyl-5-methylsulfanyl-3-nitro-1H-[1,2,4]triazole			91479	1000275-74-7 64
Naphthalene, 2-[(phenylmethyl)thio]-			92193	007570-97-0 59
26	50.718	1.87	C:\Database\NIST05a.L	
3-Eicosene, (E)-			112107	074685-33-9 92
Heptacosane, 1-chloro-			174384	062016-79-9 91
Pentacosane			153747	000629-99-2 90
27	51.530	11.76	C:\Database\NIST05a.L	
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester			110591	000084-69-5 86
Phthalic acid, butyl tetradecyl ester			175178	1000308-91-3 83
Phthalic acid, isobutyl octyl ester			144805	1000309-04-5 83
28	53.004	1.60	C:\Database\NIST05a.L	
Z-8-Hexadecene			74523	1000130-87-5 95
1-Nonadecene			102860	018435-45-5 93
1-Octadecanol			105753	000112-92-5 93
29	53.324	0.61	C:\Database\NIST05a.L	
Pentadecane			66065	000629-62-9 90
Nonahexacontanoic acid			190763	040710-32-5 74
1-Bromodocosane			167801	006938-66-5 74
30	55.493	24.18	C:\Database\NIST05a.L	
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester			110593	017851-53-5 94
Dibutyl phthalate			110572	000084-74-2 94
Phthalic acid, butyl hexyl ester			128446	1000308-99-5 86
31	57.672	10.76	C:\Database\NIST05a.L	
(-)-.alpha.-Panasinsen			59853	056633-28-4 47
Phenol, 3,5-dimethyl-, methylcarbamate			42274	002655-14-3 45
Phenol, 3,5-dimethyl-			9619	000108-68-9 43
32	58.388	0.74	C:\Database\NIST05a.L	
5-Allyl-5-acetamido-6-imino-hexahydro-2-thioxopyrimidin-4-one			85666	114477-58-6 46
2-t-Butyl-4-quinolinealdehyde			66578	1000255-75-1 25
2-Chlorobenzoic acid, hexadecyl ester			165225	070152-86-2 25
33	60.310	2.02	C:\Database\NIST05a.L	
Phenol, 2,2'-methylenebis[6-(1,1-d			160660	000088-24-4 99

imethylethyl)-4-ethyl-					
Phenol, 2,2'-methylenebis[6-(1,1-d				160659 000088-24-4	99
imethylethyl)-4-ethyl-					
Phenol, 2,2'-methylenebis[6-(1,1-d				160661 000088-24-4	76
imethylethyl)-4-ethyl-					
34	61.507	9.92	C:\Database\NIST05a.L		
3-Buten-2-one, 4-(2,6,6-trimethyl-				51302 014901-07-6	46
1-cyclohexen-1-yl)-					
4-Pyrimidinamine, 5-(2-thienyl)-				41162 058758-95-5	27
Diethyl 1,4-benzenediacetate				91859 036076-26-3	25
35	63.397	1.48	C:\Database\NIST05a.L		
Cyclopenta[1,3]cyclopropa[1,2]cycl				49990 091531-58-7	30
ohepten-3(3aH)-one, 1,2,3b,6,7,8-h					
exahydro-6,6-dimethyl-					
Phenol, 2-methoxy-4-(2-propenyl)-,acetate				61150 000093-28-7	25
1-(3-Methylbutyl)-2,3,6-trimethylbenzene				50021 084651-14-9	25
36	66.591	0.89	C:\Database\NIST05a.L		
1,2-Benzenedicarboxylic acid, mono				110586 004376-20-9	45
(2-ethylhexyl) ester					
2-Methyl-6-tert-octylphenol				71382 019546-31-7	42
Phthalic acid, monocyclohexyl este				90508 007517-36-4	35
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Table A.4: GC-MS analysis results for lab hydrodistillation sample

Pk#	RT	Area%	Library/ID	CAS#	Qual
1	18.693	1.44	C:\Database\NIST05a.L		
Benzaldehyde				4937 000100-52-7	96
Benzaldehyde				4936 000100-52-7	95
Benzaldehyde				4935 000100-52-7	95
2	21.396	1.00	C:\Database\NIST05a.L		
Azulene, 1,2,3,4,5,6,7,8-octahydro				60026 003691-12-1	99
-1,4-dimethyl-7-(1-methylethenyl)-					
, [1S-(1.alpha.,4.alpha.,7.alpha.)]-					
Azulene, 1,2,3,4,5,6,7,8-octahydro				60027 003691-12-1	97
-1,4-dimethyl-7-(1-methylethenyl)-					
, [1S-(1.alpha.,4.alpha.,7.alpha.)]-					
.beta.-Humulene				59811 000116-04-1	74
3	24.376	0.58	C:\Database\NIST05a.L		
Benzaldehyde, 2-hydroxy-				9587 000090-02-8	97
Benzaldehyde, 2-hydroxy-				9583 000090-02-8	95
Benzaldehyde, 3-hydroxy-				9584 000100-83-4	90
4	25.989	3.84	C:\Database\NIST05a.L		

Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-			60035 003691-11-0	99
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-			60033 003691-11-0	99
Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,7.alpha.,8a.beta.)]-			60034 003691-11-0	96
5	26.277	0.68	C:\Database\NIST05a.L	
2-(3-Isopropyl-4-methyl-pent-3-en-1-ynyl)-2-methyl-cyclobutanone			59759 1000193-37-3	60
Ethanone, 1-(5,6,7,8-tetrahydro-2,8,8-trimethyl-4H-cyclohepta[b]furan-5-yl)-			71257 071596-88-8	43
1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-			60076 025246-27-9	42
6	27.613	0.35	C:\Database\NIST05a.L	
.beta.-Vatirenene			58513 1000293-04-2	64
Isolongifolene, 9,10-dehydro-			58523 1000151-67-1	50
Aromadendrene, dehydro-			58517 1000156-12-5	50
7	30.999	16.17	C:\Database\NIST05a.L	
2-Butanone, 3-phenyl-			21739 000769-59-5	95
Benzene, (1-methylbutyl)-			21888 002719-52-0	64
6-Methyl-1,2,3,5,8,8a-hexahydronaphthalene			21943 107914-86-3	59
8	31.992	1.65	C:\Database\NIST05a.L	
2H-2,4a-Ethanonaphthalen-8(5H)-one, hexahydro-2,5,5-trimethyl-			71422 032391-46-1	22
Benzo[b]dihydropyran, 6-hydroxy-4,4,5,7,8-pentamethyl-			71232 050442-70-1	18
5-Acetyl-2-ethylsulfanyl-6-methyl-nicotinonitrile			70862 303146-26-1	18
9	33.445	0.46	C:\Database\NIST05a.L	
Cyclohexane, 1,2-dimethyl-3,5-bis(1-methylethenyl)-			51375 062337-99-9	38
Phenol, 3-ethyl-			9604 000620-17-7	25
Phenol, 3-ethyl-			9603 000620-17-7	25
10	35.240	0.55	C:\Database\NIST05a.L	
1,3,5-Cycloheptatriene, 2,5-diethyl-7,7-dimethyl-			40393 1000156-99-5	38
1,3,5-Cycloheptatriene, 3,4-diethyl-7,7-dimethyl-			40392 1000156-99-7	35
1,3-Butanedione, 2-sec-butyl-1-phenyl-			69840 010225-40-8	25
11	37.964	2.04	C:\Database\NIST05a.L	
Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1.alpha.,2.beta.,4.beta.)]-			60003 000515-13-9	42
Benzene, 1,2,4-triethyl-			30810 000877-44-1	40
1,5-Cycloundecadiene, 8,8-dimethyl-9-methylene-			50038 062338-54-9	38
12	39.021	5.68	C:\Database\NIST05a.L	
2-Naphthalenemethanol, 1,2,3,4,4a,5,6,7-octahydro-.alpha.,.alpha.,4a			72998 001209-71-8	93

,8-tetramethyl-, (2R-cis)-				
1H-Cycloprop[e]azulene, 1a,2,3,4,4	60090	000489-40-7	89	
a,5,6,7b-octahydro-1,1,4,7-tetrame				
thyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-				
.delta.-Selinene	59826	028624-23-9	89	
13 39.395 1.08 C:\Database\NIST05a.L				
Bicyclo[5.3.0]decane, 2-methylene-	59925	1000159-39-3	38	
5-(1-methylvinyl)-8-methyl-				
cis-Z-.alpha.-Bisabolene epoxide	71387	1000131-71-2	35	
1H-Cycloprop[e]azulen-7-ol, decahy	71464	006750-60-3	27	
dro-1,1,7-trimethyl-4-methylene-,				
[1ar-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]-				
14 40.025 0.71 C:\Database\NIST05a.L				
2H-Pyran-3-ol, tetrahydro-2,2,6-tr	83896	022567-36-8	53	
imethyl-6-(4-methyl-3-cyclohexen-1				
-yl)-, [3S-[3.alpha.,6.alpha.(R*)]]-				
1-Propene, 3-cyano-1-phenyl-	19384	1000164-96-2	18	
Quinoline, 4-methyl-	19367	000491-35-0	18	
15 40.527 0.85 C:\Database\NIST05a.L				
Azulene, 1,2,3,3a,4,5,6,7-octahydr	60069	022567-17-5	95	
o-1,4-dimethyl-7-(1-methylethenyl)				
-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-				
Azulene, 1,2,3,3a,4,5,6,7-octahydr	60067	022567-17-5	92	
o-1,4-dimethyl-7-(1-methylethenyl)				
-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-				
.beta.-Panasinsene	59841	1000159-39-0	90	
16 40.655 0.26 C:\Database\NIST05a.L				
Humulen-(v1)	59795	1000159-39-4	47	
Bicyclo[2.2.1]heptane, 2-cycloprop	40400	1000159-45-7	38	
ylidene-1,7,7-trimethyl-				
Bicyclo[5.2.0]nonane, 2-methylene-	59917	242794-76-9	35	
4,8,8-trimethyl-4-vinyl-				
17 41.104 0.25 C:\Database\NIST05a.L				
2-Naphthalenemethanol, 1,2,3,4,4a,	72997	001209-71-8	99	
5,6,7-octahydro-.alpha.,.alpha.,4a				
,8-tetramethyl-, (2R-cis)-				
Naphthalene, 1,2,4a,5,8,8a-hexahyd	60045	005951-61-1	99	
ro-4,7-dimethyl-1-(1-methylethyl)-				
, (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-				
2-Naphthalenemethanol, 1,2,3,4,4a,	72998	001209-71-8	91	
5,6,7-octahydro-.alpha.,.alpha.,4a				
,8-tetramethyl-, (2R-cis)-				
18 41.328 4.29 C:\Database\NIST05a.L				
Agarospirol	72903	001460-73-7	91	
Hinesol	72894	023811-08-7	90	
Naphthalene, 1,2,3,5,6,7,8,8a-octa	60046	004630-07-3	76	
hydro-1,8a-dimethyl-7-(1-methyleth				
enyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-				
19 41.585 0.47 C:\Database\NIST05a.L				

1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-	60080	000489-39-4	90
Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-	60046	004630-07-3	64
Azulene, 1,2,3,4,5,6,7,8-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1S-(1.alpha.,4.alpha.,7.alpha.)]-	60026	003691-12-1	62
20 41.681 0.55 C:\Database\NIST05a.L			
Hinesol	72894	023811-08-7	93
1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1.alpha.,3a.beta.,4.alpha.,8a.beta.)]	60024	000475-20-7	51
Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-	60046	004630-07-3	49
21 42.044 6.50 C:\Database\NIST05a.L			
Neoisolongifolene	59831	1000156-12-4	96
1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1.alpha.,3a.beta.,4.alpha.,8a.beta.)]	60023	000475-20-7	89
Aristolene	59784	1000150-14-9	83
22 42.300 7.27 C:\Database\NIST05a.L			
Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a,8-dimethyl-2-(1-methylethylidene)-, (4aR-trans)-	60004	006813-21-4	81
1,4-Methanoazulene, decahydro-4,8,8-trimethyl-9-methylene-, [1S-(1.alpha.,3a.beta.,4.alpha.,8a.beta.)]	60018	000475-20-7	70
1,4-Methano-1H-indene, octahydro-4-methyl-8-methylene-7-(1-methylethyl)-, [1S-(1.alpha.,3a.beta.,4.alpha.,7.alpha.,7a.beta.)]-	60092	003650-28-0	43
23 42.461 2.67 C:\Database\NIST05a.L			
Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene-	59918	150320-52-8	52
Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-	59980	000483-76-1	50
1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-	60040	000546-28-1	45
24 42.824 0.81 C:\Database\NIST05a.L			
2-Naphthalenemethanol, decahydro-.alpha.,.alpha.,4a-trimethyl-8-methylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-	73009	000473-15-4	98
2-Naphthalenemethanol, decahydro-.alpha.,.alpha.,4a-trimethyl-8-methylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-	73010	000473-15-4	94

1H-Indene, 1-ethylideneoctahydro-7 a-methyl-, (1Z,3a.alpha.,7a.beta.)			32243	056324-69-7 35
25	42.963	0.52	C:\Database\NIST05a.L	
Benzene, 1,2,4-triethyl-			30816	000877-44-1 70
Ethanone, 1-(2,4,5-trimethylphenyl)-			30730	002040-07-5 55
Benzene, 1,2,4-triethyl-			30810	000877-44-1 55
26	43.508	0.65	C:\Database\NIST05a.L	
1,4-Methanoazulene, decahydro-4,8, 8-trimethyl-9-methylene-, [1S-(1.a lpha.,3a.beta.,4.alpha.,8a.beta.)]			60018	000475-20-7 91
1,4-Methanoazulene, decahydro-4,8, 8-trimethyl-9-methylene-, [1S-(1.a lpha.,3a.beta.,4.alpha.,8a.beta.)]			60024	000475-20-7 90
Neoisolongifolene			59831	1000156-12-4 90
27	43.849	1.47	C:\Database\NIST05a.L	
1R,3Z,9S-2,6,10,10-Tetramethylbicy clo[7.2.0]undeca-2,6-diene			59923	1000140-07-4 94
1H-Cycloprop[e]azulene, decahydro- 1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-			60076	025246-27-9 91
Aromadendrene			59796	109119-91-7 91
28	43.999	0.97	C:\Database\NIST05a.L	
Disiloxane, 1-ethenyl-1,1,3,3-tetramethyl-			29688	055967-52-7 41
2-Butyl(dimethyl)silyloxypentane			58250	1000282-49-8 32
2-(5-Aminopentyl)benzimidazole			59001	039650-63-0 25
29	44.853	0.77	C:\Database\NIST05a.L	
1H-Cycloprop[e]azulene, decahydro- 1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-			60075	025246-27-9 53
1s,4R,7R,11R-1,3,4,7-Tetramethyltr icyclo[5.3.1.0(4,11)]undec-2-en-8-one			69972	137235-42-8 46
Cyclolongifolene oxide, dehydro-			69941	1000156-11-4 46
30	45.334	0.61	C:\Database\NIST05a.L	
Tricyclo[3.2.1.02,7]oct-3-ene, 2,3,4,5-tetramethyl-			30912	062338-44-7 89
Benzene, 1,2,4-triethyl-			30816	000877-44-1 62
Benzo[b]thiophene, 2-ethyl-			30619	001196-81-2 55
31	46.498	0.67	C:\Database\NIST05a.L	
Disiloxane, 1-ethenyl-1,1,3,3-tetramethyl-			29688	055967-52-7 30
(3,7-Dimethyl-octa-2,4,6-trienylid eneamino)-acetonitrile			48671	1000187-75-7 30
1H-Isoindole-4-carboxylic acid, 2- (3-methoxypropyl)-3-oxo-2,3-dihydro-			91156	1000316-43-1 25
32	46.691	0.50	C:\Database\NIST05a.L	
Silane, triethoxypropyl-			61843	002550-02-9 50
Propanal, 2-(4-ethoxyphenyl)-2-methyl-			51130	093622-71-0 50
1,3,6-Trimethyladamantane			41740	024139-37-5 49
33	47.791	1.30	C:\Database\NIST05a.L	
Humulen-(v1)			59795	1000159-39-4 49

Cyclolongifolene oxide, dehydro-		69941	1000156-11-4	35
1-Propyl-3-(propen-1-yl)adamantane		70021	057040-46-7	30
34	48.229 0.60 C:\Database\NIST05a.L			
Cycloheptane, 4-methylene-1-methyl -2-(2-methyl-1-propen-1-yl)-1-vinyl-		59957	1000159-38-5	90
2-Naphthalenecarboxylic acid, 8-et henyl-3,4,4a,5,6,7,8,8a-octahydro-5-methylene-		69905	001451-36-1	56
Isolongifolen-5-one		69932	1000159-37-1	51
35	48.517 0.03 C:\Database\NIST05a.L			
.alpha.-Caryophyllene		59847	006753-98-6	90
.alpha.-Caryophyllene		59849	006753-98-6	62
1,2-Dihydropyridine, 1-(1-oxobutyl)-		23982	1000132-46-2	60
36	48.592 0.67 C:\Database\NIST05a.L			
Cycloheptane, 4-methylene-1-methyl -2-(2-methyl-1-propen-1-yl)-1-vinyl-		59957	1000159-38-5	78
4,6,6-Trimethyl-2-(3-methylbuta-1, 3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane		69975	1000190-22-2	50
Naphthalene, 1,2,3,5,6,7,8,8a-octa hydro-1,8a-dimethyl-7-(1-methyleth enyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-		60047	004630-07-3	43
37	48.913 5.01 C:\Database\NIST05a.L			
1,4-Methanoazulen-7(1H)-one, octah ydro-4,8,8,9-tetramethyl-, (+)-		71426	018319-28-3	49
2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7- ctahydro-naphthalen-2-yl)-prop-2-en-1-ol		71444	1000190-51-8	43
6.beta.Bicyclo[4.3.0]nonane, 5.bet a.-iodomethyl-1.beta.-isopropenyl- 4.alpha.,5.alpha.-dimethyl-,		143324	1000195-85-9	27
38	49.222 0.63 C:\Database\NIST05a.L			
Azulene, 1,2,3,3a,4,5,6,7-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-		60069	022567-17-5	87
Azulene, 1,2,3,3a,4,5,6,7-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-		60066	022567-17-5	60
1H-Cycloprop[e]azulene, decahydro- 1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-		60080	000489-39-4	50
39	49.746 0.09 C:\Database\NIST05a.L			
1H-Cycloprop[e]azulene, decahydro- 1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-		60077	025246-27-9	84
2(3H)-Naphthalenone, 4,4a,5,6,7,8- hexahydro-4a,5-dimethyl-3-(1-methy lethylidene)-, (4ar-cis)-		69988	019598-45-9	81
2(1H)Naphthalenone, 3,5,6,7,8,8a-h exahydro-4,8a-dimethyl-6-(1-methylethenyl)-		69976	1000188-66-5	58
40	50.077 0.87 C:\Database\NIST05a.L			
1,3-Diethyladamantane		51347	025074-51-5	52

4(1H)-Pteridinone, 2-amino-				31521 002236-60-4	49
Cycloheptane, 4-methylene-1-methyl -2-(2-methyl-1-propen-1-yl)-1-vinyl-				59957 1000159-38-5	45
41	50.429	1.40	C:\Database\NIST05a.L		
1,2,3,4-Tetrahydro-3-isopropyl-5-m ethylnaphthalene				48785 1000241-59-1	64
Biphenylene, 1,2,3,6,7,8,8a,8b-oct ahydro-4,5-dimethyl-				48796 106988-87-8	50
Bicyclo[4.2.0]oct-1-ene, exo-7-(1- cyclohexen-1-yl)-				48787 1000142-22-1	49
42	50.953	2.20	C:\Database\NIST05a.L		
Caryophyleine-(I3)				59836 136296-37-2	35
gamma.-Neoclovene				59837 1000156-11-7	35
Bicyclo[5.2.0]nonane, 4-methylene- 2,8,8-trimethyl-2-vinyl-				59916 1000159-38-2	18
43	51.797	1.29	C:\Database\NIST05a.L		
Acetic acid, [(2,4,6-triethylbenzoyl)thio]-				111694 067902-78-7	50
2,5-Pyrrolidinedione, 3-methyl-1-phenyl-				49264 075619-07-7	25
cis-Acrylic acid, 3[(3-(2,2-dimeth ylcyclopropyl)-2,2-dimethylcyclopropyl)] -, methyl ester				72803 1000061-89-5	22
44	52.897	1.06	C:\Database\NIST05a.L		
1H-Benzimidazole, 2-ethyl-				21357 001848-84-6	43
Benzene, 1-(1-methyl-2-propenyl)-4 -(2-methylpropyl)-				48792 057438-46-7	38
2H-Isoindole, 5,6-dimethyl-				20463 070187-63-2	35
45	54.189	0.54	C:\Database\NIST05a.L		
Benzenemethanol, 4-methyl-				9653 000589-18-4	38
Phenol, 3,5-dimethyl-				9619 000108-68-9	30
1,6-Dimethylhepta-1,3,5-triene				9726 1000196-61-0	30
46	54.574	0.39	C:\Database\NIST05a.L		
Octaethylene glycol				161142 1000289-34-2	38
2,5,8,11,14-Pentaoxahexadecan-16-o				92938 023778-52-1	27
Pentaethylene glycol				83342 004792-15-8	27
47	55.300	0.53	C:\Database\NIST05a.L		
Octaethylene glycol				161142 1000289-34-2	38
1,4,7,10,13,16-Hexaoxanonadecane, 18-(2-propenyl)-				135590 1000163-64-0	35
Hexagol				112857 002615-15-8	35
48	57.789	11.49	C:\Database\NIST05a.L		
Benzenemethanol, 4-methyl-				9648 000589-18-4	41
Phenol, 2-ethyl-				9607 000090-00-6	38
Phenol, 3,4-dimethyl-, methylcarbamate				42272 002425-10-7	38
49	58.740	0.83	C:\Database\NIST05a.L		
1,4,7,10,13,16-Hexaoxacyclooctadecane				100941 017455-13-9	42
Octaethylene glycol				161142 1000289-34-2	38
3,6,9,12,15-Pentaoxanonadecan-1-ol				120685 001786-94-3	38
50	61.090	3.59	C:\Database\NIST05a.L		

n-Hexadecanoic acid				96235 000057-10-3	96
n-Hexadecanoic acid				96234 000057-10-3	96
n-Hexadecanoic acid				96233 000057-10-3	94
51	62.126	0.66	C:\Database\NIST05a.L		
3-Pentanone, 1,5-diphenyl-				84022 005396-91-8	80
3-Pentanone, 1,5-diphenyl-				84020 005396-91-8	42
2-Cyanophenyl .beta.-phenylpropionate				92690 040123-48-6	35
52	66.655	0.60	C:\Database\NIST05a.L		
Octaethylene glycol monododecyl ether				186450 003055-98-9	83
1,4,7,10,13,16-Hexaoxacyclooctadecane				100940 017455-13-9	72
1,4,7,10,13,16-Hexaoxacyclooctadecane				100938 017455-13-9	64
GAHARU PHD.M Sat Oct 18 16:29:27 2008 CHEMSTATION					

Table A.5: GC-MS analysis results for Kelantan hydrodistillation sample

Pk#	RT	Area%	Library/ID	CAS#	Qual
1	21.481	1.07	C:\Database\NIST05a.L		
Azulene, 1,2,3,4,5,6,7,8-octahydro -1,4-dimethyl-7-(1-methylethenyl)- , [1S-(1.alpha.,4.alpha.,7.alpha.)]-				60026 003691-12-1	99
Azulene, 1,2,3,4,5,6,7,8-octahydro -1,4-dimethyl-7-(1-methylethenyl)- , [1S-(1.alpha.,4.alpha.,7.alpha.)]-				60027 003691-12-1	97
Azulene, 1,2,3,5,6,7,8,8a-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1S-(1.alpha.,7.alpha.,8a.beta.)]-				60033 003691-11-0	78
2	24.718	1.10	C:\Database\NIST05a.L		
Aristolene				59784 1000150-14-9	87
Longifolene-(V4)				59820 061262-67-7	59
Naphthalene, 1,2,4a,5,6,8a-hexahyd ro-4,7-dimethyl-1-(1-methylethyl)- ,[1R-(1.alpha.,4a.alpha.,8a.alpha.)]-				60029 017627-24-6	58
3	26.213	3.27	C:\Database\NIST05a.L		
Azulene, 1,2,3,5,6,7,8,8a-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1S-(1.alpha.,7.alpha.,8a.beta.)]-				60033 003691-11-0	99
Azulene, 1,2,3,5,6,7,8,8a-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1S-(1.alpha.,7.alpha.,8a.beta.)]-				60031 003691-11-0	98
Azulene, 1,2,3,5,6,7,8,8a-octahydr o-1,4-dimethyl-7-(1-methylethenyl) -, [1S-(1.alpha.,7.alpha.,8a.beta.)]-				60035 003691-11-0	98
4	26.480	2.83	C:\Database\NIST05a.L		
Ethanone, 1-(5,6,7,8-tetrahydro-2,				71257 071596-88-8	50

8,8-trimethyl-4H-cyclohepta[b]furan-5-yl)-					
2H-1-Benzopyran, 6,7-dimethoxy-2,2-dimethyl-			71064	000644-06-4	38
Benzenamine, N,N-diethyl-4-(2-nitroethenyl)-			70985	064462-51-7	30
5	27.581	0.57	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,5,6,8a-hexahydr			59980	000483-76-1	98
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-					
Naphthalene, 1,2,3,5,6,8a-hexahydr			59978	000483-76-1	95
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-					
Naphthalene, 1,2,4a,5,8,8a-hexahyd			60036	000523-47-7	91
ro-4,7-dimethyl-1-(1-methylethyl)-					
, [1S-(1.alpha.,4a.beta.,8a.alpha.)]-					
6	32.142	2.50	C:\Database\NIST05a.L		
5-Acetyl-2-ethylsulfanyl-6-methyl-nicotinonitrile			70862	303146-26-1	30
5-(2,5-Dimethoxy-phenyl)-2H-pyrazol-3-ol			70834	1000278-26-9	22
Pyrrolo[1,2-a]thieno[2,3-d]pyrimid			70870	056929-61-4	22
in-4(6H)-one, 7,8-dihydro-2,3-dimethyl-					
7	32.879	2.27	C:\Database\NIST05a.L		
.beta.-Neoclovene			59830	056684-96-9	40
1,3,5-Cycloheptatriene, 2,5-diethyl-7,7-dimethyl-			40393	1000156-99-5	38
Benzenethanol, O,.beta.,.beta.,2,3			71407	1000128-94-8	30
,5,6-heptamethyl-					
8	37.077	1.04	C:\Database\NIST05a.L		
7-Tetradecyne			52910	035216-11-6	44
3,7-Cyclodecadien-1-one, 3,7-dimet			69970	006902-91-6	41
hyl-10-(1-methylethylidene)-, (E,E)-					
Trichloroacetic acid, tridec-2-ynyl ester			147474	1000299-26-2	30
9	38.722	0.69	C:\Database\NIST05a.L		
Cyclohexanemethanol, 4-ethenyl-.al			73011	000639-99-6	90
pha.,.alpha.,4-trimethyl-3-(1-meth					
ylethenyl)-, [1R-(1.alpha.,3.alpha.,4.beta.)]-					
Cyclohexanemethanol, 4-ethenyl-.al			73014	000639-99-6	90
pha.,.alpha.,4-trimethyl-3-(1-meth					
ylethenyl)-, [1R-(1.alpha.,3.alpha.,4.beta.)]-					
Cyclohexanemethanol, 4-ethenyl-.al			73016	000639-99-6	68
pha.,.alpha.,4-trimethyl-3-(1-meth					
ylethenyl)-, [1R-(1.alpha.,3.alpha,4.beta.)]-					
10	39.427	12.64	C:\Database\NIST05a.L		
2-Naphthalenemethanol, 1,2,3,4,4a,			72998	001209-71-8	94
5,6,7-octahydro-.alpha.,.alpha.,4a					
,8-tetramethyl-, (2R-cis)-					
.delta.-Selinene			59826	028624-23-9	86
Naphthalene, 2,3,4,4a,5,6-hexahydr			59949	000473-14-3	86
o-1,4a-dimethyl-7-(1-methylethyl)-					
11	39.534	0.73	C:\Database\NIST05a.L		
2-Cyclopenten-1-one, 3-methoxy-5-methyl-			10850	007180-60-1	30
Ethanone, 1-(2-thienyl)-			10785	000088-15-3	30
Ethanone, 1-(3-thienyl)-			10786	001468-83-3	30
12	40.250	0.65	C:\Database\NIST05a.L		
2(3H)-Naphthalenone, 4,4a,5,6,7,8-			69988	019598-45-9	78

hexahydro-4a,5-dimethyl-3-(1-methy lethylidene)-, (4ar-cis)-				
5(1H)-Azulenone, 2,4,6,7,8,8a-hexa hydro-3,8-dimethyl-4-(1-methylethy lidene)-, (8S-cis)-		69984	006754-66-1	50
6-Fluoro-3,4-dihydro-2H-pyrano[2,3 -b]quinolin-5-amine		69631	122910-26-3	38
13	40.741 5.11	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,4,4a,5,6,8a-oct ahydro-7-methyl-4-methylene-1-(1-m ethylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-		60057	039029-41-9	91
.beta.-Panasinsene		59841	1000159-39-0	86
Cyclohexene, 6-ethenyl-6-methyl-1- (1-methylethyl)-3-(1-methylethylidene)-, (S)-		59984	005951-67-7	83
14	41.414 4.64	C:\Database\NIST05a.L		
Naphthalene, 1,2,4a,5,8,8a-hexahyd ro-4,7-dimethyl-1-(1-methylethyl)- , (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-		60043	005951-61-1	93
1H-Cycloprop[e]azulene, 1a,2,3,4,4 a,5,6,7b-octahydro-1,1,4,7-tetrame thyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-		60090	000489-40-7	92
Naphthalene, 1,2,4a,5,8,8a-hexahyd ro-4,7-dimethyl-1-(1-methylethyl)- , (1.alpha.,4a.beta.,8a.alpha.)-(.+/-.)-		60045	005951-61-1	91
15	41.574 2.92	C:\Database\NIST05a.L		
Hinesol		72894	023811-08-7	90
10s,11s-Himachala-3(12),4-diene		59868	060909-28-6	86
1H-Cyclopropa[a]naphthalene, decah ydro-1,1,3a-trimethyl-7-methylene- , [1aS-(1a.alpha.,3a.alpha.,7a.beta.,7b.alpha.)]-		60072	020071-49-2	64
16	41.862 2.42	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,5,6,7,8,8a-octa hydro-1,8a-dimethyl-7-(1-methyleth enyl)-, [1S-(1.alpha.,7.alpha.,8a.alpha.)]-		60053	010219-75-7	90
Naphthalene, 1,2,3,5,6,7,8,8a-octa hydro-1,8a-dimethyl-7-(1-methyleth enyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-		60046	004630-07-3	90
Naphthalene, 1,2,3,4,4a,5,6,8a-oct ahydro-7-methyl-4-methylene-1-(1-m ethylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-		60057	039029-41-9	86
17	42.471 13.96	C:\Database\NIST05a.L		
1H-Cycloprop[e]azulene, 1a,2,3,4,4 a,5,6,7b-octahydro-1,1,4,7-tetrame thyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-		60083	000489-40-7	90
1,4-Methanoazulene, decahydro-4,8, 8-trimethyl-9-methylene-, [1S-(1.a lpha.,3a.beta.,4.alpha.,8a.beta.)]		60023	000475-20-7	90
Naphthalene, 1,2,4a,5,6,8a-hexahyd ro-4,7-dimethyl-1-(1-methylethyl)-		60008	031983-22-9	78

, (1.alpha.,4a.alpha.,8a.alpha.)-				
18	42.568	1.10	C:\Database\NIST05a.L	
Azulene, 1,2,3,3a,4,5,6,7-octahydr			60067	022567-17-5 93
o-1,4-dimethyl-7-(1-methylethenyl)				
-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-				
1H-Cycloprop[e]azulene, decahydro-			60080	000489-39-4 83
1,1,7-trimethyl-4-methylene-, [1aR				
-(1a.alpha.,4a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-				
Naphthalene, decahydro-4a-methyl-1			59991	000515-17-3 64
-methylene-7-(1-methylethylidene)-, (4aR-trans)-				
19	42.835	6.09	C:\Database\NIST05a.L	
Bicyclo[4.4.0]dec-1-ene, 2-isoprop			59918	150320-52-8 90
yl-5-methyl-9-methylene-				
1,6-Cyclodecadiene, 1-methyl-5-met			59960	023986-74-5 60
hylene-8-(1-methylethyl)-, [s-(E,E)]-				
Naphthalene, 1,2,3,4,4a,5,6,8a-oct			60005	006813-21-4 58
ahydro-4a,8-dimethyl-2-(1-methylet				
hylidene)-, (4aR-trans)-				
20	42.941	2.03	C:\Database\NIST05a.L	
2-Naphthalenemethanol, 1,2,3,4,4a,			73025	000473-16-5 98
5,6,8a-octahydro-.alpha.,.alpha.,4				
a,8-tetramethyl-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				
2-Naphthalenemethanol, 1,2,3,4,4a,			72998	001209-71-8 95
5,6,7-octahydro-.alpha.,.alpha.,4a				
,8-tetramethyl-, (2R-cis)-				
.beta.-Panasinsene			59841	1000159-39-0 72
21	43.134	2.72	C:\Database\NIST05a.L	
2-Naphthalenemethanol, decahydro-.			73010	000473-15-4 99
alpha.,.alpha.,4a-trimethyl-8-meth				
ylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				
2-Naphthalenemethanol, decahydro-.			73009	000473-15-4 86
alpha.,.alpha.,4a-trimethyl-8-meth				
ylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				
Benzene, 1-butyl-4-methoxy-			32049	018272-84-9 30
22	43.230	2.02	C:\Database\NIST05a.L	
Bicyclo[2.2.2]octa-2,5-diene, 1,2,			30909	062338-43-6 46
3,6-tetramethyl-				
Spiro(1,3-benzodioxole-2,1'-cycloheptane)			59661	024362-85-4 43
Benzene, hexamethyl-			30800	000087-85-4 42
23	43.689	1.01	C:\Database\NIST05a.L	
1H-Cycloprop[e]azulene, 1a,2,3,5,6			60086	021747-46-6 96
,7,7a,7b-octahydro-1,1,4,7-tetrame				
thyl-, [1aR-(1a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]-				
1H-Cycloprop[e]azulene, 1a,2,3,4,4			60089	000489-40-7 95
a,5,6,7b-octahydro-1,1,4,7-tetrame				
thyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7b.alpha.)]-				
Azulene, 1,2,3,3a,4,5,6,7-octahydr			60067	022567-17-5 93
o-1,4-dimethyl-7-(1-methylethenyl)				
-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-				

24	44.074	0.68	C:\Database\NIST05a.L		
4,6,6-Trimethyl-2-(3-methylbuta-1, 3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane				69975	1000190-22-2 90
.beta.-Neoclovene				59830	056684-96-9 84
1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR -(1a.alpha.,4a.beta.,7.alpha.,7a.beta.,7b.alpha.)]-				60077	025246-27-9 78
25	44.127	0.74	C:\Database\NIST05a.L		
1,4-Methanoazulen-7(1H)-one, octahydro-4,8,8,9-tetramethyl-, (+)-				71426	018319-28-3 41
Naphtho[2,3-d]-1,3-dioxol-5-ol, 3a ,4,9,9a-tetrahydro-2,2-dimethyl-, cis-				71101	052187-19-6 25
Cycloheptane, 4-methylene-1-methyl -2-(2-methyl-1-propen-1-yl)-1-vinyl-				59957	1000159-38-5 25
26	44.426	0.88	C:\Database\NIST05a.L		
(+)-3-Carene, 4-isopropenyl-				40362	161395-29-5 45
2-Furancarboxaldehyde, 5-(2-furanylmethyl)-				40069	033488-56-1 42
Ethanal, 2-methyl-2-[4-(1-methylethyl)phenyl]-				40325	1000131-87-5 42
27	44.896	0.44	C:\Database\NIST05a.L		
2-Isopropenyl-4a,8-dimethyl-1,2,3, 4,4a,5,6,7-octahydronaphthalene				59939	1000192-43-5 83
2-(3-Isopropyl-4-methyl-pent-3-en-1-ynyl)-2-methyl-cyclobutanone				59759	1000193-37-3 78
Naphthalene, 1,2,3,4,4a,5,6,8a-oct ahydro-4a,8-dimethyl-2-(1-methylet henyl)-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				60063	000473-13-2 60
28	45.473	1.43	C:\Database\NIST05a.L		
Benzene, hexamethyl-				30803	000087-85-4 83
Tricyclo[3.2.1.02,7]oct-3-ene, 2,3,4,5-tetramethyl-				30912	062338-44-7 60
Benzene, 1,4-bis(1-methylethyl)-				30849	000100-18-5 55
29	45.826	0.56	C:\Database\NIST05a.L		
Cycloisolongifolene, 8,9-dehydro-				58528	1000151-28-0 90
Aromadendrene, dehydro-				58517	1000156-12-5 86
7-Tetracyclo[6.2.1.0(3.8)0(3.9)]un decanol, 4,4,11,11-tetramethyl-				71428	074842-43-6 83
30	46.050	0.33	C:\Database\NIST05a.L		
Cycloheptane, 4-methylene-1-methyl -2-(2-methyl-1-propen-1-yl)-1-vinyl-				59957	1000159-38-5 95
2,3,3-Trimethyl-2-(3-methylbuta-1, 3-dienyl)-6-methylenecyclohexanone				69967	077822-57-2 81
4,6,6-Trimethyl-2-(3-methylbuta-1, 3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane				69975	1000190-22-2 50
31	47.321	0.89	C:\Database\NIST05a.L		
11-Isopropylidenetricyclo[4.3.1.1(2,5)]undec-3-en-10-one				58508	1000191-49-3 38
Tricyclo[4.4.0.0(2,7)]dec-3-ene-3-methanol, 1-methyl-8-(1-methylethyl)-				71440	115728-41-1 15
Shizukanolide				78685	070578-36-8 14
32	47.908	0.81	C:\Database\NIST05a.L		

9H-Cycloisolongifolene, 8-oxo-			69939 1000155-43-0	50
1-Propyl-3-(propen-1-yl)adamantane			70021 057040-46-7	46
Cyclolongifolene oxide, dehydro-			69941 1000156-11-4	42
33	48.336	0.91	C:\Database\NIST05a.L	
1-Propyl-3-(propen-1-yl)adamantane			70021 057040-46-7	53
Acetic acid, 3-(2,2-dimethyl-6-met			92150 1000192-69-2	49
hylene-cyclohexylidene)-1-methyl-butyl ester				
4-Amino-1-methyl-1,5-naphthyridin-2-one			39973 1000213-36-1	43
34	48.624	1.46	C:\Database\NIST05a.L	
.alpha.-Caryophyllene			59846 006753-98-6	62
.alpha.-Caryophyllene			59847 006753-98-6	53
1,4,7,-Cycloundecatriene, 1,5,9,9-			59900 1000062-61-9	53
tetramethyl-, Z,Z,Z-				
35	48.688	0.30	C:\Database\NIST05a.L	
1R,3Z,9S-2,6,10,10-Tetramethylbicy			59923 1000140-07-4	92
clo[7.2.0]undeca-2,6-diene				
Cycloheptane, 4-methylene-1-methyl			59957 1000159-38-5	90
-2-(2-methyl-1-propen-1-yl)-1-vinyl-				
Aromadendrene oxide-(2)			71361 1000151-98-6	87
36	49.116	4.62	C:\Database\NIST05a.L	
Cycloisolongifolene, 8-hydroxy-, endo-			71391 1000151-49-2	46
2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-			71444 1000190-51-8	38
octahydro-naphthalen-2-yl)-prop-2-en-1-ol				
3-(2-Isopropyl-5-methylphenyl)-2-m			71230 005451-67-2	35
ethylpropionic acid				
37	49.842	1.75	C:\Database\NIST05a.L	
11-Isopropylidenetricyclo[4.3.1.1(			58508 1000191-49-3	64
2,5)]undec-3-en-10-one				
1-Acetyl-2,6-naphthalenediol			58281 108804-50-8	43
5H-Naphtho[1,8-bc]thiophen-5-one,			58322 010243-18-2	43
3,4-dihydro-2-methyl-				
38	49.959	2.01	C:\Database\NIST05a.L	
Cycloheptane, 4-methylene-1-methyl			59957 1000159-38-5	53
-2-(2-methyl-1-propen-1-yl)-1-vinyl-				
.beta.-[2-Methoxy-4,6-dimethylphenyl]butyric acid			72607 1000129-26-2	50
3-(6-Methoxy-2,4-dimethylphenyl)pr			72623 1000126-61-1	43
opionic acid, methyl ester				
39	50.173	1.10	C:\Database\NIST05a.L	
1,4-Methanophthalazine, 1,4,4a,5,6			61406 109746-14-7	53
,7,8,8a-octahydro-1,4,9,9-tetramet				
hyl-, (1.alpha.,4.alpha.,4a.alpha.,8a.alpha.)-				
1,3,6-Trimethyladamantane			41740 024139-37-5	52
1,3,4-Trimethyladamantane			41741 1000214-98-3	50
40	51.049	0.79	C:\Database\NIST05a.L	
Tridecane, 3-methyl-2,12-diphenyl-			189548 1000161-64-9	16
5,7,9-tris(1-phenylethyl)-				
Bicylo[4.1.0]heptane, 7-bicyclo[4.			48793 1000152-39-9	15
1.0]hept-7-ylidene-				

1-Butanone, 2-hydroxy-1-phenyl-				31801	016183-46-3 10
41	51.872	1.11	C:\Database\NIST05a.L		
Cyclopropanecarboxylic acid, 3-(3-methoxy-2-methyl-3-oxo-1-propenyl) -2,2-dimethyl-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl est er, [1R-[1.alpha.[S*(Z)],3.beta.(E)]]-				163056	001172-63-0 27
2,5-Pyrrolidinedione, 3-methyl-1-phenyl-				49264	075619-07-7 18
Pyrido[3,4-d]pyrimidin-4(3H)-one, 3,6,8-trimethyl-				49174	022389-79-3 18
42	56.326	0.57	C:\Database\NIST05a.L		
Benzenemethanol, .alpha.-1-pentynyl-				39001	108946-34-5 44
1H-Benzoimidazole, 1-(2-cyclohexylethyl)-2-ethyl-				96320	1000303-65-8 42
5,19-Cyclo-5.beta.-androst-6-ene-3,17-dione				114899	033585-88-5 42
43	57.800	2.31	C:\Database\NIST05a.L		
Phenol, 3,4-dimethyl-, methylcarbamate				42272	002425-10-7 41
Phenol, 2-iodo-4-methyl-				81363	016188-57-1 38
Benzenemethanol, 4-methyl-				9648	000589-18-4 38
44	61.272	2.43	C:\Database\NIST05a.L		
n-Hexadecanoic acid				96235	000057-10-3 98
n-Hexadecanoic acid				96234	000057-10-3 97
n-Hexadecanoic acid				96233	000057-10-3 93
45	66.634	0.50	C:\Database\NIST05a.L		
1,2-Benzenedicarboxylic acid, mono (2-ethylhexyl) ester				110586	004376-20-9 91
Di-n-octyl phthalate				168497	000117-84-0 90
1,2-Benzenedicarboxylic acid, diisooctyl ester				168521	027554-26-3 68
FAME CJO.M Mon Feb 23 16:01:54 2009 CHEMSTATION					

Table A.6: GC-MS analysis results for MAHA hydrodistillation sample

Pk#	RT	Area%	Library/ID	CAS#	Qual
1	15.499	2.86	C:\Database\NIST05a.L		
Naphthalene, decahydro-1,4a-dimeth yl-7-(1-methylethyl)-, [1S-(1.alph a.,4a.alpha.,7.alpha.,8a.beta.)]-				63071	030824-81-8 83
1-Cyclohexanol, 2-(3-methyl-1,3-bu tadienyl)-1,3,3-trimethyl-				62973	1000196-01-6 49
Cyclohexane, 1,3-dimethyl-2-methylene-, trans-				10394	020348-74-7 43
2	21.855	6.35	C:\Database\NIST05a.L		
Naphthalene, decahydro-1,4a-dimeth yl-7-(1-methylethyl)-, [1S-(1.alph a.,4a.alpha.,7.alpha.,8a.beta.)]-				63071	030824-81-8 99
Naphthalene, decahydro-1,4a-dimeth yl-7-(1-methylethyl)-, [1S-(1.alph				63072	030824-81-8 95

a.,4a.alpha.,7.alpha.,8a.beta.)]-				
10.alpha.-Eremophilane		63044	003242-05-5	60
3	22.165 8.89	C:\Database\NIST05a.L		
Naphthalene, decahydro-1,4a-dimeth		63071	030824-81-8	99
yl-7-(1-methylethyl)-, [1S-(1.alph				
a.,4a.alpha.,7.alpha.,8a.beta.)]-				
Naphthalene, decahydro-1,4a-dimeth		63072	030824-81-8	91
yl-7-(1-methylethyl)-, [1S-(1.alph				
a.,4a.alpha.,7.alpha.,8a.beta.)]-				
10.alpha.-Eremophilane		63044	003242-05-5	70
4	22.240 1.85	C:\Database\NIST05a.L		
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-		61349	003101-60-8	91
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-		61347	003101-60-8	87
Phenol, 3,5-bis(1,1-dimethylethyl)		61448	001138-52-9	58
5	24.088 0.68	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,5,6,8a-hexahydr		59980	000483-76-1	91
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-				
Naphthalene, 1,2,3,5,6,8a-hexahydr		59979	000483-76-1	87
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-				
(+)-Epi-bicyclosesquiphellandrene		59869	054324-03-7	86
6	25.167 1.48	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,4,4a,5,6,8a-oct		60068	030021-74-0	98
ahydro-7-methyl-4-methylene-1-(1-m				
ethylethyl)-, (1.alpha.,4a.alpha.,8a.alpha.)-				
Naphthalene, 1,2,4a,5,6,8a-hexahyd		59954	000483-75-0	98
ro-4,7-dimethyl-1-(1-methylethyl)-				
Naphthalene, 1,2,3,4,4a,5,6,8a-oct		60070	030021-74-0	97
ahydro-7-methyl-4-methylene-1-(1-m				
ethylethyl)-, (1.alpha.,4a.alpha.,8a.alpha.)-				
7	26.598 3.63	C:\Database\NIST05a.L		
Naphthalene, 1,2,4a,5,6,8a-hexahyd		60010	031983-22-9	98
ro-4,7-dimethyl-1-(1-methylethyl)-				
, (1.alpha.,4a.alpha.,8a.alpha.)-				
Naphthalene, 1,2,4a,5,6,8a-hexahyd		60009	031983-22-9	98
ro-4,7-dimethyl-1-(1-methylethyl)-				
, (1.alpha.,4a.alpha.,8a.alpha.)-				
.alpha.-Muurolene		59829	010208-80-7	97
8	27.880 7.19	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,5,6,8a-hexahydr		59980	000483-76-1	98
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-				
Naphthalene, 1,2,3,5,6,8a-hexahydr		59979	000483-76-1	95
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-				
Naphthalene, 1,2,4a,5,8,8a-hexahyd		60036	000523-47-7	93
ro-4,7-dimethyl-1-(1-methylethyl)-				
, [1S-(1.alpha.,4a.beta.,8a.alpha.)]-				
9	28.275 1.09	C:\Database\NIST05a.L		
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-		58537	000644-30-4	99
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-		58538	000644-30-4	96
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-		58536	000644-30-4	94

10	28.863	0.93	C:\Database\NIST05a.L	
Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1.alpha.,4a.beta.,8a.alpha.)]-			60030	024406-05-1 96
.alpha.-Muurolene			59829	010208-80-7 90
Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1.alpha.,4a.alpha.,8a.alpha.)-			60008	031983-22-9 90
11	30.401	7.62	C:\Database\NIST05a.L	
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-			58550	000483-77-2 96
Naphthalene, 1,2,3,4-tetrahydro-1,5,8-trimethyl-			39070	021693-51-6 86
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-			39075	000475-03-6 86
12	30.914	0.47	C:\Database\NIST05a.L	
2-Butanone, 3-phenyl-			21739	000769-59-5 96
2-Butanone, 4-phenyl-			21741	002550-26-7 95
2-Butanone, 4-phenyl-			21740	002550-26-7 95
13	32.922	1.07	C:\Database\NIST05a.L	
Naphthalene, 1,2-dihydro-1,1,6-trimethyl-			37894	030364-38-6 53
Quinoline, 5,8-dimethyl-			27977	002623-50-9 53
Cadala-1(10),3,8-triene			58518	1000140-05-6 50
14	37.173	0.79	C:\Database\NIST05a.L	
N-Acrylonitryl-2,2,6,6-tetramethyl piperidine-4-one			61225	077376-90-0 25
1,3-Dimethyladamantan-5-carboxylic acid, n-hexyl ester			119878	107995-66-4 25
cis-3-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane			23010	1000215-29-0 25
15	37.665	1.29	C:\Database\NIST05a.L	
1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-			60040	000546-28-1 43
Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-			59947	016728-99-7 42
.alpha.-Cubebene			59821	017699-14-8 41
16	37.921	1.14	C:\Database\NIST05a.L	
Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-			59947	016728-99-7 58
Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, [1S-(1.alpha.,4a.beta.,8a.alpha.)]-			60032	000523-47-7 49
Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]-			60046	004630-07-3 43
17	38.508	1.09	C:\Database\NIST05a.L	
Cyclohexanemethanol, 4-ethenyl-.alpha.,.alpha.,4-trimethyl-3-(1-methylethenyl)-, [1R-(1.alpha.,3.alpha.,4.beta.)]-			73014	000639-99-6 90
Cyclohexanemethanol, 4-ethenyl-.alpha.,.alpha.,4-trimethyl-3-(1-meth			73015	000639-99-6 87

ylethenyl)-, [1R-(1.alpha.,3.alpha.,4.beta.)]-					
Cyclohexanemethanol, 4-ethenyl-.al			73011	000639-99-6	83
pha.,.alpha.,4-trimethyl-3-(1-meth					
ylethenyl)-, [1R-(1.alpha.,3.alpha.,4.beta.)]-					
18	39.053	0.64	C:\Database\NIST05a.L		
2-Naphthalenemethanol, 1,2,3,4,4a,			72998	001209-71-8	94
5,6,7-octahydro-.alpha.,.alpha.,4a					
,8-tetramethyl-, (2R-cis)-					
2-Naphthalenemethanol, 1,2,3,4,4a,			72997	001209-71-8	93
5,6,7-octahydro-.alpha.,.alpha.,4a					
,8-tetramethyl-, (2R-cis)-					
.delta.-Selinene			59826	028624-23-9	89
19	41.425	7.72	C:\Database\NIST05a.L		
Naphthalene, 1,2,3,4,4a,5,6,8a-oct			60062	039029-41-9	87
ahydro-7-methyl-4-methylene-1-(1-m					
ethylethyl)-, (1.alpha.,4a.beta.,8a.alpha.)-					
Epizonarene			59794	1000156-10-7	86
1H-Cyclopropa[a]naphthalene, 1a,2,			60096	017334-55-3	86
3,5,6,7,7a,7b-octahydro-1,1,7,7a-t					
etramethyl-, [1aR-(1a.alpha.,7.alp					
ha.,7a.alpha.,7b.alpha.)]-					
20	41.734	3.85	C:\Database\NIST05a.L		
4a,trans-8a-Perhydro-cis-2-(2-hydr			74487	006770-16-7	78
oxy-2-propyl)-4a,cis-8-dimethylnaphthalene					
2,4-Heptadiene, 2,6-dimethyl-			10358	004634-87-1	30
5-Thiophen-2-yl-2H-pyrazol-3-ol			33809	1000278-27-0	27
21	41.948	4.76	C:\Database\NIST05a.L		
.alpha.-Cadinol			72908	000481-34-5	78
.tau.-Muurolol			72907	019912-62-0	70
Cyclohexene, 6-ethenyl-6-methyl-1-			59984	005951-67-7	47
(1-methylethyl)-3-(1-methylethylidene)-, (S)-					
22	42.268	3.28	C:\Database\NIST05a.L		
Copaene			59780	003856-25-5	96
1-Naphthalenol, 1,2,3,4,4a,7,8,8a-			73023	036564-42-8	95
octahydro-1,6-dimethyl-4-(1-methyl					
ethyl)-, [1S-(1.alpha.,4.alpha.,4a.beta.,8a.beta.)]-					
.alpha.-Cubebene			59821	017699-14-8	93
23	42.546	1.34	C:\Database\NIST05a.L		
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-			56008	000483-78-3	98
Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-			56006	000483-78-3	91
Azulene, 1,4-dimethyl-7-(1-methylethyl)-			56002	000489-84-9	87
24	42.792	2.05	C:\Database\NIST05a.L		
2-Naphthalenemethanol, 1,2,3,4,4a,			73024	000473-16-5	94
5,6,8a-octahydro-.alpha.,.alpha.,4					
a,8-tetramethyl-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-					
2-Naphthalenemethanol, 1,2,3,4,4a,			73025	000473-16-5	83
5,6,8a-octahydro-.alpha.,.alpha.,4					
a,8-tetramethyl-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-					
.delta.-Selinene			59826	028624-23-9	66

25	43.048	2.47	C:\Database\NIST05a.L	
2-Naphthalenemethanol, decahydro-.			73010	000473-15-4 99
alpha.,.alpha.,4a-trimethyl-8-meth				
ylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				
2-Naphthalenemethanol, decahydro-.			73009	000473-15-4 96
alpha.,.alpha.,4a-trimethyl-8-meth				
ylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.)]-				
Benzene, 1-(1,1-dimethylethyl)-4-methoxy-			32092	005396-38-3 41
26	43.379	8.65	C:\Database\NIST05a.L	
Imidazole, 2-trifluoroacetyl-			32285	105480-29-3 25
Naphthalene, 1,2,3,5,6,8a-hexahydr			59977	000483-76-1 25
o-4,7-dimethyl-1-(1-methylethyl)-,(1S-cis)-				
3-Isopropenyl-trans-8a-methyl-6-ox			72775	013567-75-4 25
o-perhydro-trans-4a-naphthol				
27	52.747	0.51	C:\Database\NIST05a.L	
Galaxolide 2			97604	1000285-26-7 64
Furo[2,3-H]coumarine, 2-(1-hydroxy			97372	350682-01-8 53
ethyl)-1,6-dimethyl-				
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin			97609	000088-29-9 50
28	56.518	5.81	C:\Database\NIST05a.L	
5,19-Cyclo-5.beta.-androst-6-ene-3,17-dione			114899	033585-88-5 47
Benzene, 1,2,3,4-tetramethyl-4-(1-methylethenyl)-			39077	061142-76-5 35
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-			39073	030316-17-7 35
29	59.936	5.56	C:\Database\NIST05a.L	
6-(2-Formylhydrazino)-N,N'-bis(iso			93717	084305-82-8 91
propyl)-1,3,5-triazine-2,4-diamine				
2-Propenamide, 2-cyano-N,N-dimethy			87316	125535-35-5 56
l-3-[4-(dimethylamino)phenyl]-				
9(11)-Dehydrotestosterone			116164	002398-99-4 46
30	60.417	0.94	C:\Database\NIST05a.L	
2H-Isoindole, 4,5,6,7-tetramethyl-			38542	070187-61-0 41
Phenol, 5-methyl-2-(pyrrol-1-yl)-			38514	1000302-46-2 38
2-Pyrrolidinone, 5-hydroxy-5-methyl-1-phenyl-			50510	029879-80-9 35
31	60.567	0.68	C:\Database\NIST05a.L	
2-Pentanone, 3-(phenylmethylene)-			38997	003437-89-6 22
3-Isopropylidenephthalide			38891	004767-54-8 11
8.alpha.,9.beta.-Estra-1,3,5(10)-t			114922	019592-58-6 11
rien-17-one, 3-methoxy-				
32	63.248	2.15	C:\Database\NIST05a.L	
6-Iodo-2-methylquinazolin-4(3H)-on			116304	090347-75-4 90
Estra-1,3,5(10)-trien-17-one, 3,15			116122	002208-13-1 45
-dihydroxy-, (15.alpha.)-				
5-(Adamantyl-1)salicylic acid, methyl ester			116103	126145-52-6 40
33	63.515	0.51	C:\Database\NIST05a.L	
Estra-1,3,5(10)-trien-17-one, 3,15			116122	002208-13-1 47
-dihydroxy-, (15.alpha.)-				
Estra-1,3,5(10)-triene-3,17-diol,			116181	003597-38-4 46
1-methyl-, (17.beta.)-				
17.beta.-Hydroxy-3-methoxy-estra-1			116187	1000215-86-6 44

,3,5(10)-triene (8.beta.,9.beta.,14.alpha.)					
34	65.363	0.68	C:\Database\NIST05a.L		
2H-1-Benzopyran, 3,4-dihydro-2,2-diphenyl-				116256	010419-28-0 91
Estra-1,3,5(10)-trien-17-ol, 3-met				116176	001035-77-4 43
hoxy-, (17.beta.)-					
Estra-1,3,5(10)-trien-17-ol, 3-met				116185	006570-46-3 42
hoxy-, (8.alpha.,17.beta.)-					
FAME CJO.M Mon Feb 23 16:03:20 2009 CHEMSTATION					

APPENDIX B

B.1 Sample Total Ion Chromatograms

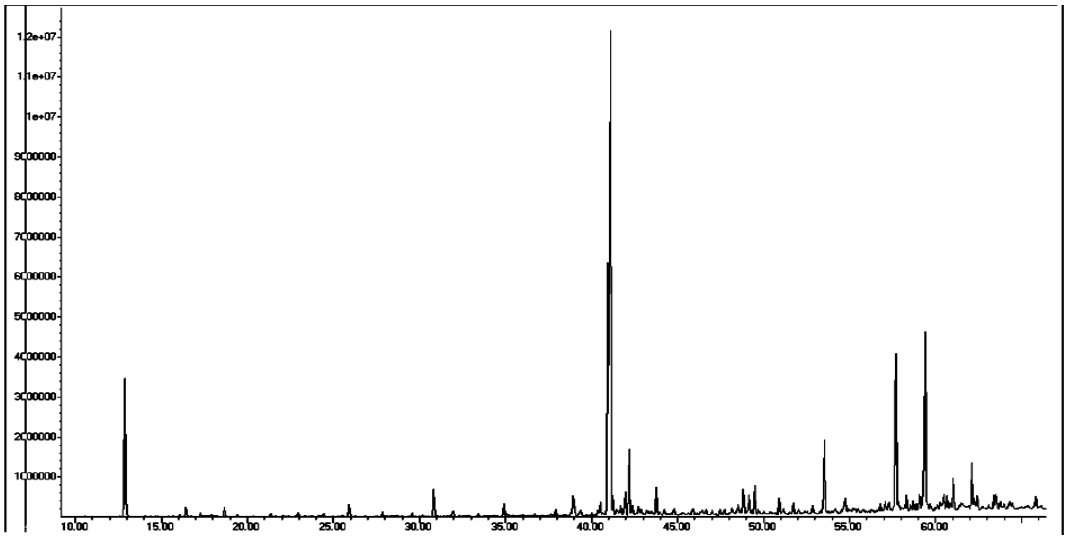

Figure B.1: One dimensional total ion current chromatogram for sample extracted with acetone

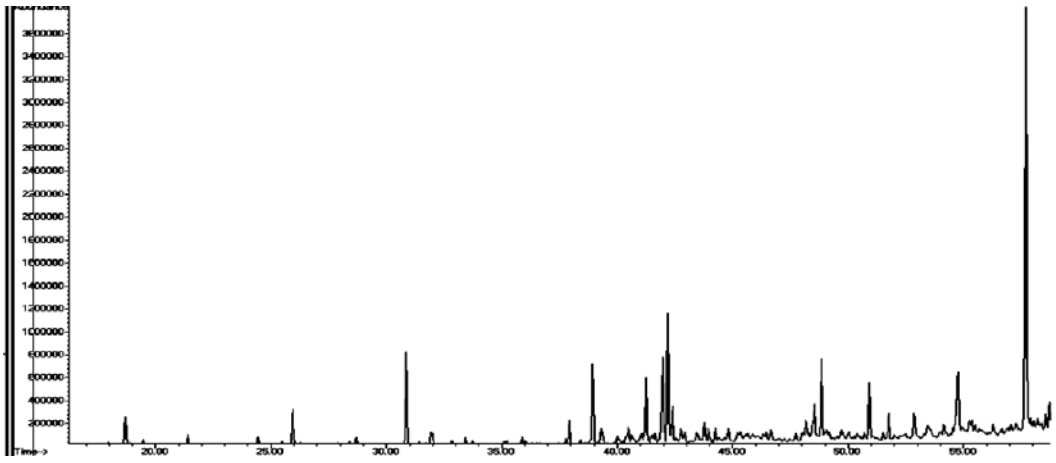

Figure B.2: One dimensional total ion current chromatogram for sample extracted with dichloromethane

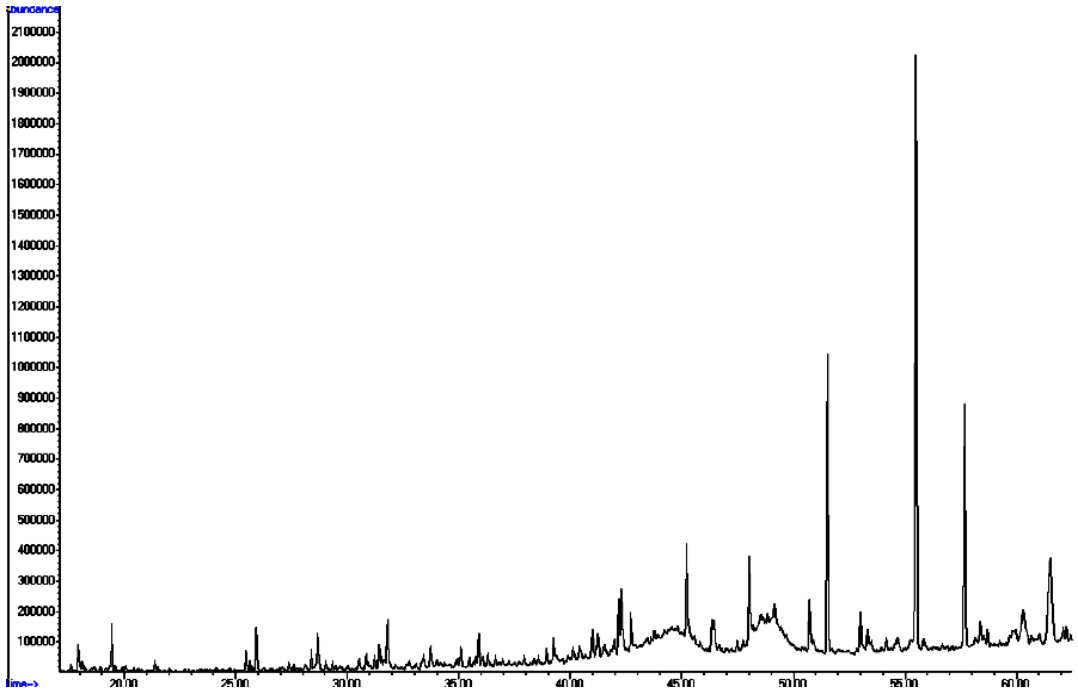

Figure B.3: One dimensional total ion current chromatogram for sample extracted with hexane

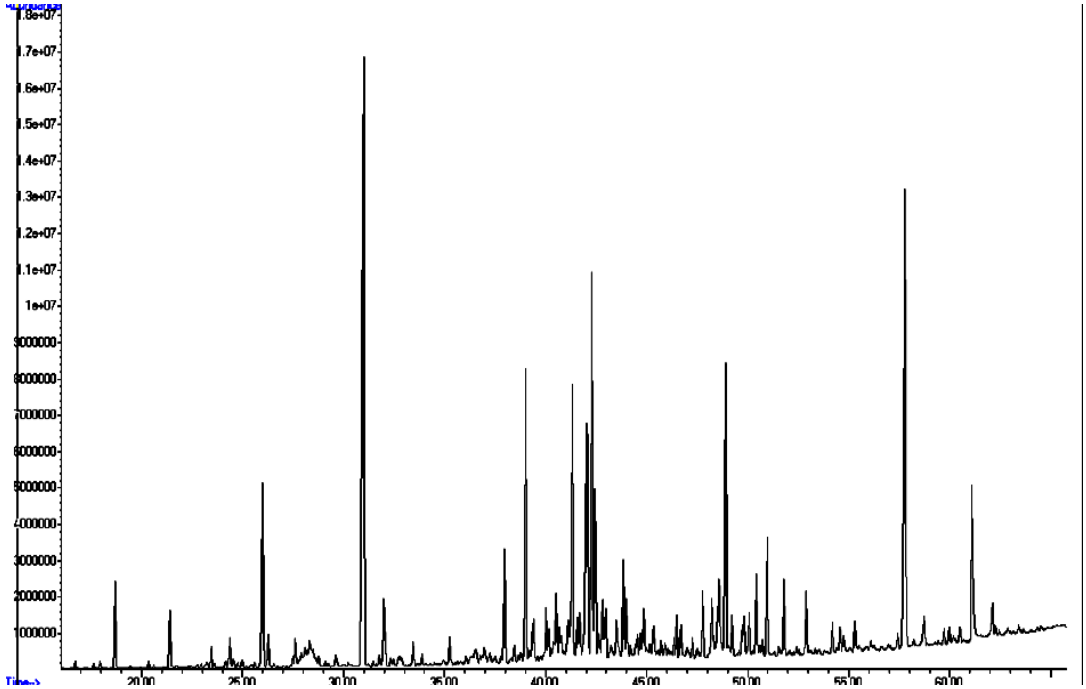

Figure B.4: One dimensional total ion current chromatogram for sample extracted via lab scale hydrodistillation

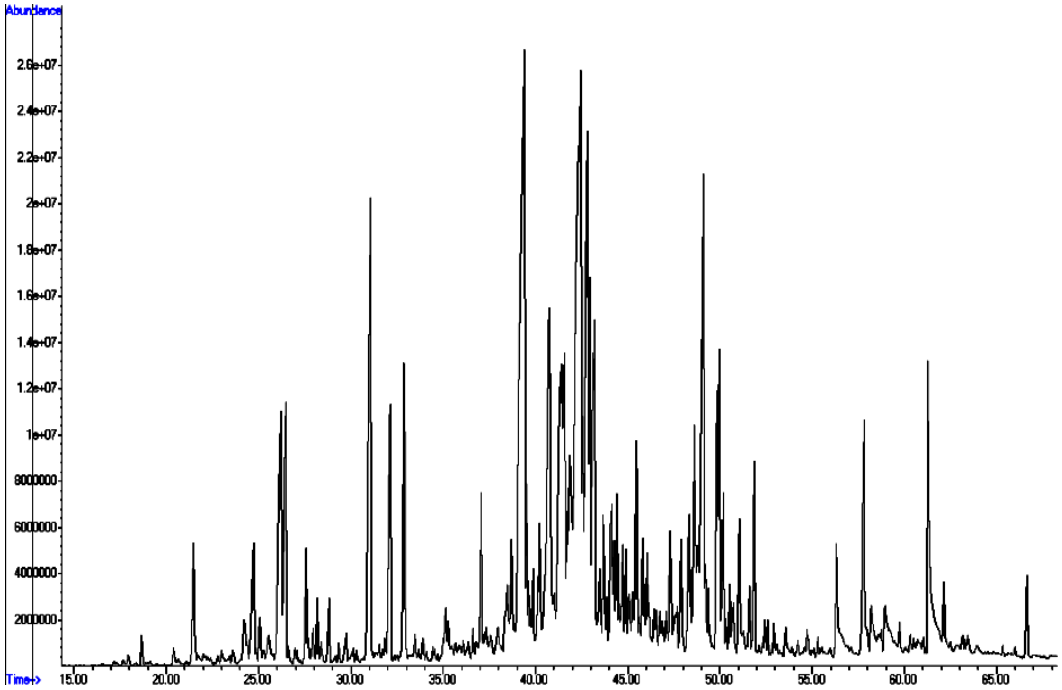

Figure B.5: One dimensional total ion current chromatogram for sample extracted via industrial scale hydrodistillation (Kelantan)

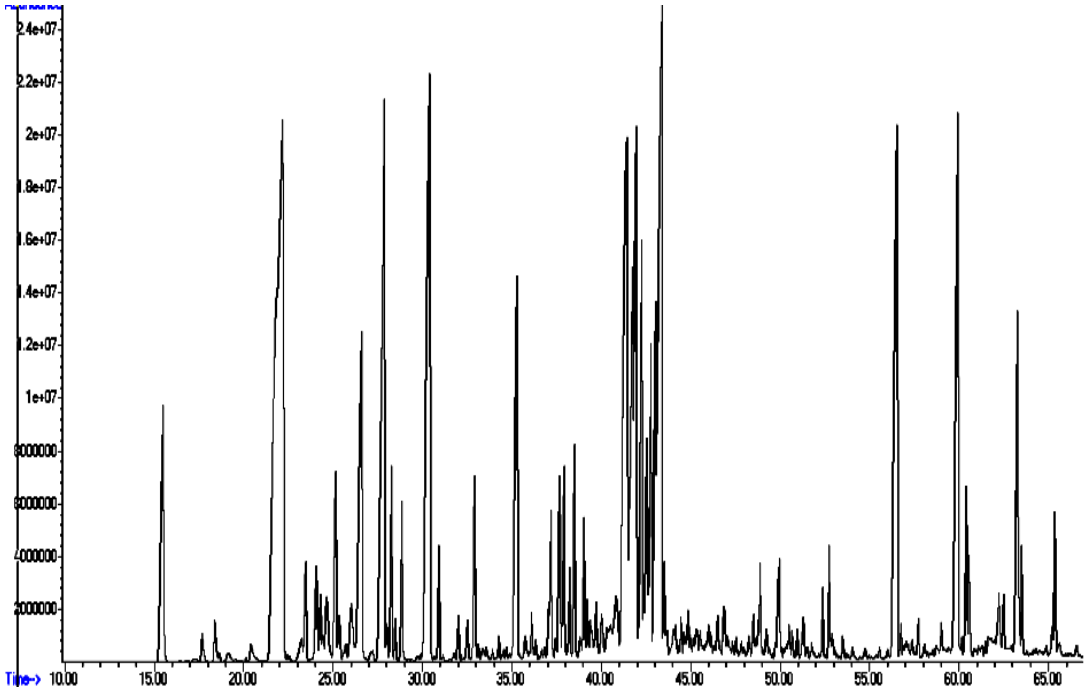

Figure B.6: One dimensional total ion current chromatogram for sample extracted via industrial scale hydrodistillation (MAHA)