

CONCENTRATION OF BIOPETROL FROM PALMITIC ACID

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CONCENTRATION OF BIOPETROL FROM PALMITIC ACID

NOOR ZARIYATI BINTI MOHAMMAD

A thesis submitted in fulfillment of the
requirements for the award of the degree of
Bachelor of Chemical Engineering

Faculty of Chemical and Natural Resources Engineering
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APRIL 2008

DECLARATION

I declare that this thesis entitled “*Concentration of Biopetrol from Palmitic Acid*” 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 other degree.

Signature :
Name : Noor Zariyati Binti Mohammad
Date : APRIL 2008

DEDICATION

To my beloved parents and siblings,

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First of all, I like to express my gratitude to Ilahi because giving me a good health condition during the period of finishing this project. Opportunities doing this project have taught me many new things. There is fun and sad time, but I relieved that there is always people around me when I am in need and I would like to thank them from the bottom of my heart.

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ABSTRACT

Biopetrol is defined as fuel which has the same characteristics with commercial petrol in terms of its molecular formula. The objective of this study is to find the concentration of biopetrol (isooctane) from palmitic acid. Thermal cracking process is used to produce isooctane from palmitic acid. Heat is supplied using hot plate at palmitic acid's melting point within a range of 63°C – 64°C, to melt the solid palmitic acid. After it turns to liquid, the heating is continuous at isooctane's boiling point of 98°C by using heating mantel 250ml to form new arrangements of carbon compounds including isooctane. The heating is continuous and the sample was collected at temperature 200°C, 300°C, 330°C and 350°C. The desired isooctane obtained is around 0.0455% - 0.0743% in the distilled palmitic acid. After the back calculation, the highest concentration of the desired isooctane is 2.92% at temperature 350°C palmitic acid.

ABSTRAK

Biopetrol didefinisikan sebagai bahan bakar yang mempunyai formula molekul yang sama dengan petrol biasa. Tujuan projek ini dijalankan adalah untuk mengenalpasti kepekatan biopetrol (isooktana) di dalam asid palmitik. Kaedah penghuraian haba digunakan untuk mendapatkan isooktana daripada asid palmitik. Pepejal asid palmitik dipanaskan pada suhu di antara 63°C – 64°C , iaitu pada takat lebur asid palmitik. Kemudian proses pemanasan diteruskan sehingga mencapai takat didih isooktana, iaitu 98°C untuk membentuk susunan molekul karbon yang baru. Kemudian pemanasan diteruskan sehingga mencapai suhu 350°C . Sampel diambil pada suhu 98°C , 200°C , 300°C , 330°C dan 350°C . Kepekatan isooktana yang diperolehi di dalam didihan asid palmitik adalah dalam lingkungan 0.0455% - 0.0743%. Kepekatan tertinggi adalah pada suhu 350°C didihan asid palmitik iaitu sebanyak 0.0743%. Selepas mengira semula kepekatan isooktana tanpa pencairan heksana, kepekatan tertinggi adalah pada suhu 350°C iaitu sebanyak 2.92% dan hasil keputusan ini dapat ditingkatkan dengan menggunakan kaedah yang lain seperti penghuraian dengan menggunakan agen pemangkin.

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LIST OF SYMBOLS

P	-	Pressure
m	-	Mass
ΔH	-	Enthalpy change of reaction
ΔS	-	Entropy change of reaction
ΔG	-	Energy change of reaction
T	-	Temperature
ρ	-	Density
μ	-	Viscosity of liquid (Pa.s)
h	-	Heat transfer coefficient
$^{\circ}\text{C}$	-	Degree Celsius
kg	-	Kilogram
K	-	Degree Kelvin
m	-	Meter
n	-	Number of moles
L	-	Liter

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CHAPTER 1

INTRODUCTION

1.0 Introduction

Since the price of petrol increases as well as decreasing of petrol or petroleum supply, more researches are done to find the alternative fuel as substitution of petroleum-based fuel, including biodiesel and biopetrol. Biopetrol is defined as fuel which has the same characteristics with commercial petrol in terms of its molecular formula. Biodiesel, which consists methyl esters has been already developed from vegetable oils and commercialized. However, biodiesel is only suitable for diesel engine.

Producing petrol from the waste of palm oil (palmitic acid) will give an alternative choice to the users, especially for petrol-engine vehicles' owners. In addition, this biopetrol, which is graded 100 for its octane number, burns very smoothly so biopetrol can reduce emissions of some pollutants (Omar, 2005).

This study is to find the concentration of isooctane as the main component of petrol from palmitic acid (palm oil waste). The method that used is cracking method that is applied in petroleum industries.

1.1 Problem Statement

Petroleum price is increasing dramatically year by year and it will burden people especially to the lower working class. This is because of decreasing fuel supply and the sources are unevenly spread. Most petroleum reserves are in the Middle East or West Asia, causing economic and political instabilities.



Figure 1.1 : Malaysia's Looming Energy Crisis (M. Noor, 2008)

Malaysia is the one of the major oil exporters in the world. Malaysia also has the crisis of the declining of these mineral sources. Malaysia's oil production is decreases in 2004 and would then decline by 6.4 percent annually. Figure 1.1 shows the declining Malaysia oil's production by 2004. Forecast, by 2009 to 2010 Malaysia will become a net importer because out of mineral sources (petroleum) and the demand of oil increasing.

Producing petrol from the waste of palm oil (palmitic acid) will give an alternative choice to the users, especially for petrol-engine vehicles' owners. In addition, this biopetrol, which is graded 100 for its octane number, burns very smoothly so biopetrol can reduce emissions of some pollutants (Omar, 2005).

Palmitic acid is the dominative component in palm oil waste. Its disposal into water supply sources causes serious water pollution. Besides that the loss of palmitic acid as a useful industrial component also occurs so that it is not utilized much and always eliminated to improve and upgrade the quality of crude palm oil. Thus, it is disposed as palm oil waste and then pollutes water resources by its spillage.

The challenge of this research is this research will be outstanding at a time when palm-oil prices are going down, production is increase and the energy prices are ruling high.

In this research, the concentration of isooctane that is produced from palmitic acid and also the conversion of fatty acids form desired isooctane in biopetrol will be the objectives.

1.2 Objectives

- To analyze isooctane obtained from palmitic acid
- To find the concentration of biopetrol obtained from palmitic acid

1.3 Scopes

To achieve the objective, scopes have been identified in this research. The scopes of this research are listed as below:-

- ❖ To describe the molecular arrangement in cracking process.
- ❖ To understand the thermal cracking and distillation process.
- ❖ To identify the composition of isooctane using Gas Chromatography method with Gas Chromatographer.
- ❖ To determine the amount of isooctane in sample obtained using Gas Chromatography method as well.

CHAPTER 2

LITERATURE REVIEW

2.0 Definition of fuel

Fuel (from Old French feuaille, from feu fire, ultimately from Latin focus fireplace, hearth) is a substance that may be burned in air (or any other oxidant-containing substance), which so quickly reacts with oxygen that heat and light is emitted in the form of a sustained flame. Oxygen in the air is the basic oxidant for and is readily available from Earth's atmosphere; that is why it is the main oxidizer. Fuels are used as convenient energy stores because of their high specific energy release when burnt with omnipresent ambient air.

2.1 Uses of fuel

Fuel is used as convenient energy stores because of their high specific energy when burnt with omnipresent ambient air. Primary (natural) fuels may be difficult to find in Nature, and secondary (artificial) fuels may be difficult to be manufactured, but, once at hand, fuels are very easy to store, transport and use, with the only nuisance of safety (uncontrolled combustion) and pollution such as toxic emissions during storage and when burnt.

Energy is a basic need to humans and is used for heat generation, for work generation, or for chemical transformations. A common problem to all human needs (except air, in most cases) is that energy is not available at the location and time we desire, and sources must be found (for energy, water, food, minerals) and transportation to a better place must be arranged, as well as storage and end-use details. Storage is sometimes the most cumbersome stage, for example for food (all food is perishable, particularly meat, fish, vegetables and fruits) and for electrical energy.

2.2 Fuel types by period of natural renovation

2.2.1 Fossil fuels

Fossil fuels (coal, crude-oil and natural gas) were formed slowly (during millions of years, mainly at certain remote epochs, not uniformly; for example American oil was formed some 90 million years ago, whereas the rest dates from 150 million years) by high-pressure-decomposition of trapped vegetable and animal matters during extreme global warming. Fossil fuels are found trapped in Earth's crust, up to 10 km depth, although large pressure might stabilise them also at higher depths and temperatures (at 300 km it might be 10 GPa and 1000 °C). They are then non-renewable energy supply at humankind periods, and will eventually be commercially depleted. Table 2.1 below shows the estimated reserves and availability of fossil fuels.

Table 2.1 : Estimated reserves and availability of fossil fuels.

	Commercial reserve-2000	Reserve/Consumption-2000
Coal	$1000 \cdot 10^{12}$ kg	250 yr
Crude oil	$100 \cdot 10^{12}$ kg	40 yr
Natural gas	$150 \cdot 10^{12}$ kg.	70 yr

2.2.2 Petroleum fuel

More than 50% of world's primary energy comes nowadays from petroleum that is all vehicle fuels, and small and medium stationary applications fuels are petroleum derivatives, obtained by fractional distillation and reforming. Main commercial fuels and their physical data are presented in Table 2.2

Table 2.2 : Main commercial fuels derivatives from crude-oil, and their main averaged properties.

	Boiling range T_b [K]	Boiling range T_b [°C]	Carbon chain range	Density (liquid at 15 °C) ρ [kg/m ³]	Viscosity at 40 °C $\nu \cdot 10^6$ [m ² /s]	Flash point T_{flash} [°C]	Main use
Liquefied petroleum gases (LPG)	<300	<30	1-4	580	0.5	−100	domestic heating, cars
Gasoline	300-500	30-200	4-12	730-760	0.5	−30	cars
Kerosene	450-650	150-350	10-14	780-850	3	40	aircrafts
Diesel	500-600	200-300	10-20	820-880	3	40	cars, lorries, boats
Fuel oil distillate	600-800	300-500	15-30	840-930	10	60	industry, ships

2.2.3 Renewable fuel

Renewable resources include energy from sun, wind, flowing water, the earth's internal heat, and biomass. For example,

- Passive solar heating captures sunlight directly within a structure and converts it into low temperature heat for heating.
- Hydroelectric power supplies 20% of the world's power and 6 % of the total commercial energy.

Wind and solar power represent an ultimate in environmental sustainability. But the problem is the sun does not always shine and the wind may not blow when needed. Thus, the alternative renewable and environmental friendly sources of energy are biomass.

Biomass is organic material from living organisms, such as plant matter including trees, grasses, and agricultural crops that can be burned or converted to liquid or gaseous fuels for energy (Lim, 2006).

Biomass is formed in a year or a few years basis. Synthetic fuels may come from fossil or from renewable sources such as:

- Gas: biogas from anaerobic fermentation or flue gas from pyrolysis of biomass.
- Liquid: alcohols, ethers, liquid paraffins (biopetrol), esters (biodiesel).
- Solid: wood, charcoal, fuel pellets (from wood or vegetable residues), agricultural residues, cattle manure, urban waste.

2.3 Biological fuel

The terms of biofuels, biomass fuels and renewable fuels, may be used indistinctly if they refer to natural or artificial fuels obtained from renewable sources, although the other times distinctions are introduced and then biofuels may refer to biomass derivatives directly substituting fossil fuels for the same combustor, biomass may be restricted to unprocessed biomass (forest waste, crops and agriculture waste, animal waste, domestic waste), and renewable may include fuels like hydrogen obtained by electrolysis and not from biomass.

A 1999 biofuel life cycle study concluded that biofuel reduces net CO₂ emissions by 78% compared to petroleum fuel from biofuel's closed carbon cycle. The CO₂ released into the atmosphere from the combusted biofuel is recycled and reused by growing plants, which are later processed into fuel (Lee, 2006).

Scientific research confirms that biofuel has a less harmful effect on human health than petroleum fuel. Biofuel emissions have decreased levels of polycyclic aromatic hydrocarbons (PAHs) and nitrated PAH compounds (nPAH), which have been identified as carcinogenic (cancer-causing agent) compounds. The test results indicate that PAH compounds were reduced by 50 - 85%. Biofuel is nontoxic and biodegradable. Otherwise, the flashpoint (the lowest temperature at which it can form an ignitable mix with air) is 300 °F while petroleum fuel's flashpoint of 125 °F (Lee, 2006).

But the complete utilization movement to biofuels is not based on their short-term advantage over fossil fuels but on the long-term need to have fuels of any kind. And for the time being, living matter and their residues are a handy alternative to recover the non-renewable fossil fuels.

2.3.1 Classes of Biofuels

2.3.1.1 Solid Biofuels

There are many forms of solid biomass that are combustible as a fuel such as:

- Wood
- Straw and other dried plants
- Animal waste such as poultry droppings or cattle dung
- Crops such as maize, rice, soybean, peanut and cotton (usually just the husks or shells) & sugarcane- or agave-derived bagasse.

2.3.1.2 Liquid Biofuels

There are also a number of liquid forms of biomass that can be used as a fuel:

- Bioalcohols
 - Ethanol – usually produced from sugarcane, also from corn
 - Methanol, which is currently produced from natural gas, can also be produced from biomass. The methanol economy is an interesting alternative to the hydrogen economy
 - Butanol, formed by A.B.E. fermentation (Acetone, Butanol Ethanol) and experimental modifications of the ABE process show potentially high net energy gains. Butanol can be burned "straight" in existing gasoline engines (without modification to the engine or car), produces more energy and is less corrosive and less water soluble than ethanol, and can be distributed via existing infrastructures.

- Biologically produced oils (bio-oils) can be used in diesel engines
 - Straight vegetable oil (SVO)
 - Waste vegetable oil (WVO)
 - Biodiesel obtained from transesterification of animal fats and vegetable oil, directly usable in petroleum diesel engines
- Oils produced from various wastes
 - Thermal depolymerization from waste materials can extract methane and oil similar to petroleum
 - Methane and oils are being extracted from landfill wells and leachate in test sites

2.3.1.3 Gaseous Biofuels

- Bio-methane produced by the natural decay of garbage or agricultural manure can be collected for use as fuel
 - It is also possible to estimate the number of animals needed for desirable size of biogas driven engine with Biogas Calculator
- Wood gas can be extracted from wood and used in petrol engines.
- Hydrogen can be produced in water electrolysis or, less ecologically, by cracking any hydrocarbon fuel in a reformer, some fermentation processes also produce hydrogen, such as A.B.E. fermentation
- Gasification, that produces carbon monoxide.

2.3.2 Biofuel From Palm Oil.

Palm oil is a superior biofuel sources compared to other vegetable oils. This is due to its availability, and the fact that is able to be produced on a positive energy balance, compared to other competing vegetable oils.

Palm oil is called as a very energy-efficient raw material. The energy output and input ratio is nine to one, compared to three to one for corn, soy, and rapeseed. Palm oil is a real energy factory, whereas these other crops have a very low output to input energy ratio.

2.3.2.1 Price of Palm Oil

DBS Vickers Research has raised its crude palm oil (CPO) price forecast for 2008 to RM 2,650 per tonne. This is higher than the previous RM 2,500 forecast and is said to be due to a potential supply shortage. DBS Vickers Research has raised its crude palm oil (CPO) price forecast for 2008 to RM 2,650 per tonne. This is higher than the previous RM 2,500 forecast and is said to be due to a potential supply shortage.

Ben Santoso, DBS Vickers' plantation analyst in Indonesia said that crude palm oil prices will remain buoyant through the first half of next year as much of the global oil seeds output has been adversely affected by the drought in many oilseeds producing countries.

Oil World, an independent agency offering analyses and forecasts of supply, demand and price for oil seeds industries indicated that production deficits will most likely put pressure on prices next year.

Malaysia, the world's leading palm oil producer had already estimated lower output this year although it expected export revenue to be a record RM 40 billion this year due to rising product prices.

Demand for CPO is expected to rise as rising crude oil prices and environmental concerns prompt consumers to make the switch to greener energy such as biodiesel.

2.3.2.2 Palm Oil Waste

Large quantities of palm waste called Empty Fruit Bunches (EFB) are available from plantations where palm oil is produced. In its raw state, EFB is both very fibrous and wet. EFB is a solid waste produce from oil palm milling process and has high moisture content. The treated empty bunches are mechanically crushed (de-watered and de-oiled) in the process. EFB is rich nutrients and contained reasonable amounts of trace elements. EFB have a value when returned to the field to be applied as mulch for the enrichment of soil. However, it was noted that over application of the effluent must be avoided as it may result anaerobic conditions in the soil by formation of an impervious coat of organic matter on the soil surface (Mansur, 2005). Thus, used of EFB to become biofuel can reduce the amount of waste, lower cost and can reduce the pollution.

2.4 Biofuel production methods

In Japan, bacteria has been bred which produces ethanol from paper or rice-straw without any pre-treatment. There are some methods to produce biofuel:

- Methane (actually a biogas mixture) by anaerobic digestion of biomass waste (manure, straw, sewage, municipal solid waste (MSW)).

- Oils (biodiesel) by reforming oleaginous plant seeds (e.g. colza, sunflower, soy). The marine microscopic algae *Botryococcus Braunii* has been shown to accumulate a quantity of hydrocarbons amounting to 75% of their dry weight.
- Methanol from wood-waste distillation.

For mobile applications, because of higher energy density and simpler infrastructure, liquid biofuels are preferred (ethanol and biodiesel), gaseous biofuels being restricted to stationary applications. As an aid in transition from fossil fuels to biofuels, mixtures of both fuels and biofuels are being progressively put on the market for old engines and combustors, and new engines and combustors are progressively developed to run on 'biofuel prototypes' derived from current fossil fuels.

2.4.1 Biodiesel

Biodiesel refers to any diesel-equivalent biofuel made from renewable biological materials such as vegetable oils or animal fats. While there are numerous interpretations being applied to the term biodiesel, the term biodiesel usually refers to an ester, or oxygenate, made from the oil and methanol (in other words, the name "biodiesel" can be applied to any transesterified vegetable oil that makes it suitable for use as a diesel fuel).

Technically, as mentioned earlier, biodiesel is vegetable oil methyl ester, or in general one could say that biodiesel consists what are called mono alkyl-esters. It is usually produced by a transesterification and esterification reaction of vegetable or waste oil respectively with a low molecular weight alcohol, such as ethanol and methanol. During this process, the triglyceride molecule from vegetable oil is removed in the form of glycerin (soap). Once the glycerin is removed from the oil, the remaining molecules are, to a diesel engine, somewhat similar to those of petroleum diesel fuel. There are some notable differences though. While the petroleum and other fossil fuels contain sulfur, ring molecules & aromatics, the biodiesel molecules are very simple hydrocarbon

chains, containing no sulfur, ring molecules or aromatics. Biodiesel is thus essentially free of sulfur and aromatics. Biodiesel is made up of almost 10% oxygen, making it a naturally "oxygenated" fuel.

The concept of using vegetable oil as a fuel dates back to 1895 when Dr. Rudolf Diesel developed the first diesel engine to run on vegetable oil. Diesel demonstrated his engine at the World Exhibition in Paris in 1900 using peanut oil as fuel.

Bio-diesel can be used in diesel engines either as a standalone or blended with petro diesel. Much of the world uses a system known as the "B" factor to state the amount of biodiesel in any fuel mix. For example, fuel containing 20 % biodiesel is labeled B20. Pure biodiesel is referred to as B100.

2.4.2 Biopetrol

Gasoline or petrol is a complex mixture of hydrocarbons which consists a mixture of C_4 to C_{10} alkanes. However isooctane (C_8H_{18}) as dominative component in petrol is assigned an octane number of 100. Isooctane or 2, 2, 4-trimethylpentane ($CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$) is burns smoothly with a little knock in petrol engine. It is the highest quality of petrol (Mansur, 2005).

The other alternative to produce petrol is by using biopetrol. Biopetrol is defined as fuel which has the same characteristics with the commercial petrol in terms of its molecular formula.

2.4.2.1 Biopetrol in The Future

Biopetrol is an alternative fuel that is a renewable energy with a lower cost rather than petrol itself. Biopetrol from palm oil is biodegradable and non-toxic. From the environmental point view, all the fuel from vegetable sources is environmentally friendly.

From the technical point of view, biofuel (biopetrol) is technically compatible with current internal combustion engine. Slight modification might be required to enhance the power. Biopetrol can be the solution for the future air emission control.

The application of existing biodiesel from palm oil in motor vehicle (diesel engine) has been proven successful. However its commercial viability requires further in depth study (Mansur, 2005).

There are four primary reasons for encouraging the development of biopetrol in Malaysia:

- Provides market for excess production of palm oil.
- The prices of petroleum are increasing.
- Decreases the total import of petroleum.
- Fuel (biopetrol) from vegetable oil is renewable and environmental friendly.

2.4.2.2 Biopetrol from Palmitic Acid

Palmitic acid or hexadecanoic acid ($\text{CH}_3 (\text{CH}_2)_{14}\text{COOH}$) is a fatty acid which is found in animal fats and vegetable oils.

To produce isooctane from palmitic acid, thermal cracking process is needed. Heat is supplied at palmitic acid's melting point within a range of 63°C – 64°C to melt the solid palmitic acid. After it turns to the liquid, the heating must be continuous until the isooctane's boiling point of 98°C by using heating mantle to form new arrangements of carbon compounds including isooctane.

The sample produced will have lots of hydrocarbon chains because of the heat that breaks the carbon chain randomly. Although alkanes from C_5 until C_9 are categorized as gasoline, C_8 will be the major component in this study.

2.5 Overview on petroleum refining process

Petroleum is a complex mixture of organic compounds, most of which are alkanes and aromatic hydrocarbons. It also contains small amounts of oxygen (O), nitrogen (N), and sulfur (S). Mixtures of alkanes are perfectly suitable for uses in fuels, solvents and lubricants.

As we learned from history, alchemists of the middle Ages attempted to change base metals into gold by practicing wizardry. In a sense, refiners could be regarded as the modern day heirs apparent to these medieval sorcerers by transforming crude oil into a variety of useful and valuable products. Instead of using magic, however, refiners employ chemical science and processing technology to perform their unique brand of metamorphosis. Spread out over a number of acres, a refinery is a remarkable maze of metal, machinery and manpower. Towers, tanks, process vessels, pipelines, pumps, heat exchangers and compressors are just some of the components of a modern refinery. Operators, engineers, researchers, technicians, craftsmen and maintenance personnel are among those needed to keep a refinery running round-the-clock. A refinery consists of a number of different units, each with a specific purpose, integrated into a processing sequence.

The petroleum industry refines crude oil to obtain useful products. Refineries and chemical plants account for about a fifth of the industry's total investment in property and equipment. The United States has about 300 refineries that range in capacity from 40 to 365,000 barrels of oil a day. The world's largest refinery is in Abadan, Iran. It can process 412,000 barrels daily when running at full capacity. Hydrocarbons contain a lot of energy. Many of the things derived from crude oil like gasoline, diesel fuel, paraffin wax and so on take advantage of this energy.

Hydrocarbons can take on many different forms. The smallest hydrocarbon is methane (CH_4), which is a gas that is lighter than air. Longer chains with 5 or more carbons are liquids. Very long chains are solids like wax or tar. By chemically cross-linking hydrocarbon chains can be everything from synthetic rubber to nylon to the plastic in Tupperware. The major classes of hydrocarbons in crude oils include Paraffin, Aromatics, Napthenes or Cycloalkanes, and other hydrocarbons.

Distillation, or fractioning, is the first step in the refining process. It separates the various fractions of crude oil. The fact that different hydrocarbons vaporize (boil) at different temperatures makes possible the process of distillation. Table 2.3 below shows the boiling pint differences for hydrocarbon cracking.

Table 2.3 : Boiling point differences for hydrocarbon cracking (Solomons, 1997)

Boiling Range of Fraction	Number of Carbon Atoms per Molecule	Use
Below 20	C1 – C4	Natural Gas, bottled gas, petrochemicals
20 – 60	C5 – C6	Petroleum ether, solvents
60 – 100	C6 – C7	Ligroin, solvents
40 – 200	C5 – C10	Gasoline (straight run gasoline)
175 – 325	C12 – C18	Kerosene and jet fuel
250 – 400	C12 and higher	Gas oil, fuel oil, and diesel oil

Distillation is the evaporation and subsequent collection of a liquid that is a component in a mixture. Fractional distillation is the evaporation of two or more liquids from a parent mixture by using the differences in their boiling points. Both processes may be used for purification or separation.

A typical example of fraction distillation is in the separation of various hydrocarbons, for instance, butane, pentane from a hydrocarbon mixture that result from some process in the overall refining process. In this example, a refinery fractional distillation apparatus is commonly termed a fractional distillation column or a fractionating column and can be several hundred feet high, depending on the refinery throughput (Soares, 2001).

In the petroleum refining, this distillation process is started by running crude oil into pipes that pass through a furnace. As the oil is heated, the fractionated gasoline vaporizes first, followed by kerosene. At higher temperatures, such oil fractions as diesel oil and lubricant stocks boil. The mixture of hot vapors and liquid goes into a fractionating tower, which consisting bubble-cap trays. The vapor rises through the tower, which separates the fractions in a continuous process.

This separation of petroleum into its various fractions takes place in a crude distillation tower. Crude oil is first heated in a furnace. The resulting mixture of hot vapors and liquid is pumped into the closed, vertical distillation tower, which is sometimes as high as 100 feet. As the vapors rising, they are cooled and condensed at various levels and temperatures where they are trapped by a number of horizontal bubble-cap trays. The trays on the upper levels collect the lighter petroleum fractions such as naphtha (straight-run gasoline) and kerosene. Middle trays collect components such as light heating oil and diesel fuel. Heavy fuel oils asphalt and pitch fractions settle on lower trays. For example, heavy fuel oils condense at the bottom of the tower, and gasoline condenses at the top.

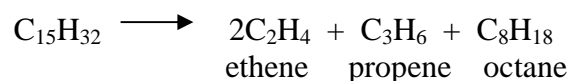
2.6 Conversion oil refining

2.6.1 Cracking

Cracking is a petroleum refining process in which heavy-molecular weight hydrocarbons are broken up into light hydrocarbon molecules by the application of heat and pressure, with or without the use of catalysts, to derive a variety of fuel products. Cracking is one of the principal ways in which crude oil is converted into useful fuels such as motor gasoline, jet fuel, and home heating oil. There are two type of cracking process which are thermal cracking and catalytic cracking.

The source of the large hydrocarbon molecules is often the naphtha fraction or the gas oil fraction from the fractional distillation of crude oil (petroleum). These fractions are obtained from the distillation process as liquids, but are re-vaporized before cracking.

There is not any single unique reaction happening in the cracker. The hydrocarbon molecules are broken up in a fairly random way to produce mixtures of smaller hydrocarbons, some of which have carbon-carbon double bonds. One possible reaction involving the hydrocarbon $C_{15}H_{32}$ might be:



Or, showing more clearly what happens to the various atoms and bonds as shown in Figure 2.1:

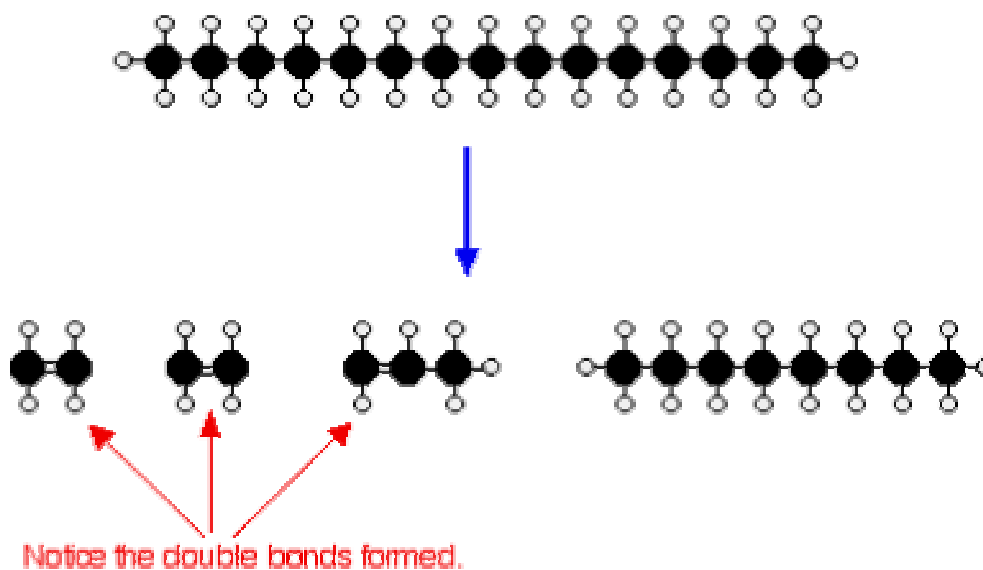


Figure 2.1 : Hydrocarbon Break Up Structure (Clark, 2003).

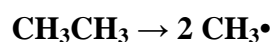
This is only one way in which this particular molecule might break up. The ethene and propene are important materials for making plastics or producing other organic chemicals. The octane is one of the molecules found in petrol (gasoline).

2.6.1.1 Thermal cracking

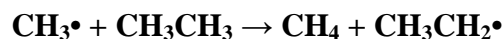
Thermal cracking is a refining process in which heat ($\sim 800\text{ }^{\circ}\text{C}$) and pressure ($\sim 700\text{ kPa}$) are used to break down, rearrange, or combine hydrocarbon molecules. The first thermal cracking process was developed around 1913. Distillate fuels and heavy oils were heated under pressure in large drums until they cracked into smaller molecules with better antiknock characteristics. However, this method produced large amounts of solid, unwanted coke.

The main reactions of thermal cracking include:

1. Initiation reactions, where a single molecule breaks apart into two free radicals. Only a small fraction of the feed molecules actually undergo initiation, but these reactions are necessary to produce the free radicals that drive the rest of the reactions. In steam cracking, initiation usually involves breaking a chemical bond between two carbon atoms, rather than the bond between a carbon and a hydrogen atom.



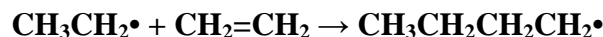
2. Hydrogen abstraction, where a free radical removes a hydrogen atom from another molecule, turning the second molecule into a free radical.



3. Radical decomposition, where a free radical breaks apart into two molecules, one an alkene, the other a free radical. This is the process that results in the alkene products of steam cracking.

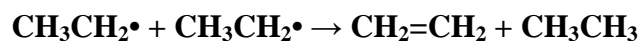
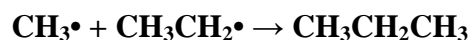


4. Radical addition, the reverse of radical decomposition, in which a radical reacts with an alkene to form a single, larger free radical. These processes are involved in forming the aromatic products that result when heavier feedstocks are used.



5. Termination reactions, which happen when two free radicals react with each other to produce products that are not free radicals. Two common forms of termination are recombination, where the two radicals combine to form one

larger molecule, and disproportionation, where one radical transfers a hydrogen atom to the other, giving an alkene and an alkane.



Thermal cracking is an example of a reaction in which energies are dominated by entropy (ΔS°) rather than by enthalpy (ΔH°) in the free equation $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$. Although the bond dissociation energy D for a carbon-carbon single bond is relatively high (about 375 kJ/mol) and cracking is highly endothermic, the large positive entropy change resulting from the fragmentation of one large molecule into several smaller pieces, together with the extremely high temperature, makes $T\Delta S^\circ$ term larger than the ΔH° term, thereby favoring the cracking reaction.

Thermal cracking doesn't go via ionic intermediates like catalytic cracking. Instead, carbon-carbon bonds are broken so that each carbon atom ends up with a single electron. In other words, free radicals are formed as shown in Figure 2.2.

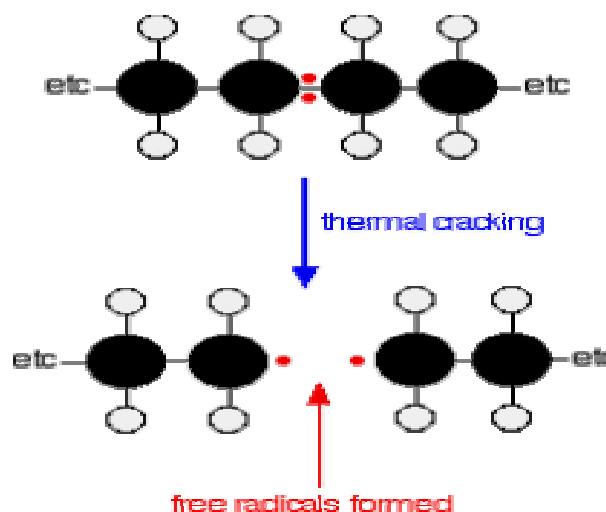


Figure 2.2 : Thermal Cracking Break Up Structure (Clark, 2003)

Reactions of the free radicals lead to the various products.

2.6.1.2 Catalytic cracking

Catalytic cracking breaks complex hydrocarbons into simpler molecules in order to increase the quality and quantity of lighter, more desirable products and decrease the amount of residuals. This process rearranges the molecular structure of hydrocarbon compounds to convert heavy hydrocarbon feedstock into lighter fractions such as kerosene, gasoline, liquified petroleum gas (LPG), heating oil, and petrochemical feedstock.

Catalytic cracking is similar to thermal cracking except that the additional catalysts facilitate the conversion of the heavier molecules into smaller molecules of desirable products. Use of a catalyst (a material that assists a chemical reaction but does not take part in it) in the cracking reaction increases the yield of improved-quality products under much less severe operating conditions than in thermal cracking.

Typical temperatures are from 450°-510°C at much lower pressures of 10-20 psi to aid the process of breaking down large hydrocarbon molecules into smaller ones. During this process, less reactive, and therefore more stable and longer lived intermediate cations accumulate on the catalysts' active sites generating deposits of carbonaceous products generally known as coke. Such deposits need to be removed (usually by controlled burning) in order to restore catalyst activity.

The catalysts used in refinery cracking units are typically solid materials (zeolite, aluminum hydrosilicate, treated bentonite clay, fuller's earth, bauxite, and silica-alumina) that come in the form of powders, beads, pellets or shaped materials called extrudites.

The zeolites used in catalytic cracking are chosen to give high percentages of hydrocarbons with between 5 and 10 carbon atoms - particularly useful for petrol (gasoline). It also produces high proportions of branched alkanes and aromatic hydrocarbons like benzene.

The zeolite catalyst has sites which can remove hydrogen from an alkane together with the two electrons which bound it to the carbon. That leaves the carbon atom with a positive charge. Ions like this are called carbonium ions (or carbocations). Reorganisation of these leads to the various products of the reaction.

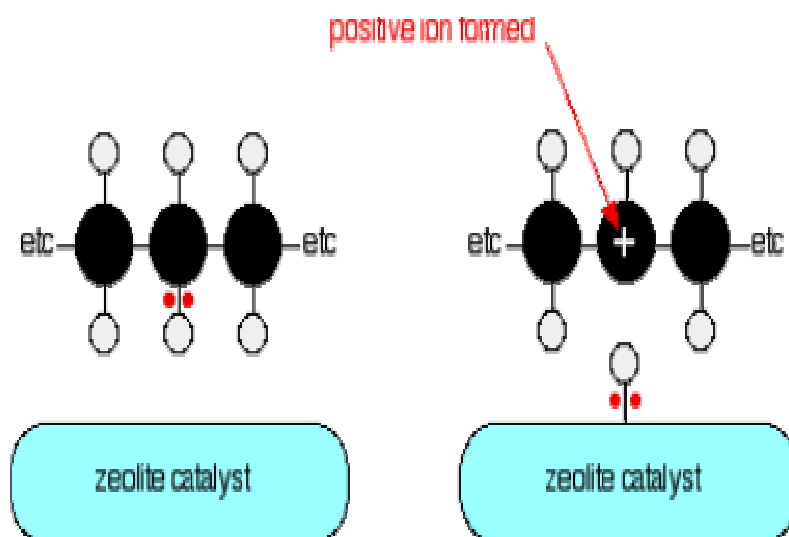


Figure 2.3 : Catalytic Cracking Break Up Structure (Clark, 2003)

There are three basic functions in the catalytic cracking process:

1. **Reaction:** Feedstock reacts with catalyst and cracks into different hydrocarbons;
2. **Regeneration:** Catalyst is reactivated by burning off coke.
3. **Fractionation:** Cracked hydrocarbon stream is separated into various products.

2.7 Chemicals

2.7.1 Palmitic acid

Figure 2.4 below shows the structure of palmitic acid.

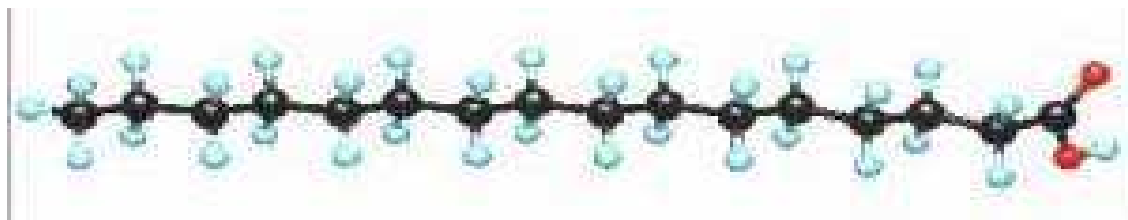


Figure 2.4 : Palmitic Acid Structure

Palmitic acid is a kind of carboxylic acids, with carboxyl (-COOH) molecule as functional group. The IUPAC name is hexadecanoic acid with the molecular formula ($\text{CH}_3 (\text{CH}_2)_{14}\text{COOH}$). As its name indicates, it is a major component of the oil from palm oil trees and palm kernel oil trees.

Palmitic acid constitutes between 20 and 30 percent of most animal fats and is also an important constituent of most vegetable fats (35 – 45 percent of palm oil). Palmitic acid consists 44% of wrung crude palm oil and 55% of empty palm fruit bunch. At room temperature it forms in white crystalline solid. Palmitic acid is used in industries of rubber latex, plastics, lubricants, grease, pharmaceuticals, cosmetics, food additives and toiletries.

Palmitic acid is stable but it is combustible and incompatible with bases, oxidizing or reducing agents. Palmitic acid may cause irritation to the eyes, skins and also to the respiratory tract. Thus, for the personal protection we must wear safety glasses. For transport information, it is non-hazardous for air, sea and road freight. Table 2.4 below shows the physical and chemical properties of palmitic acid and Figure 2.5

below indicates the skeleton structure of palmitic acid while Figure 2.6 indicates the structure of palmitic acid.

Table 2.4 : Physical and Chemical properties of Palmitic acid

Other names	cetylic acid, hexadecylic acid, hexadecanoic acid
Appearance	White chips, crystal or powder
Molecular formula	$C_{16}H_{32}O_2$
Molecular weight	256.42 g/mol
Melting point $^{\circ}C$	61 – 64 $^{\circ}C$
Boiling point $^{\circ}C$	352 $^{\circ}C$
Density	0.853 g/cm ³ at 62 $^{\circ}C$
Solubility	Insoluble in water

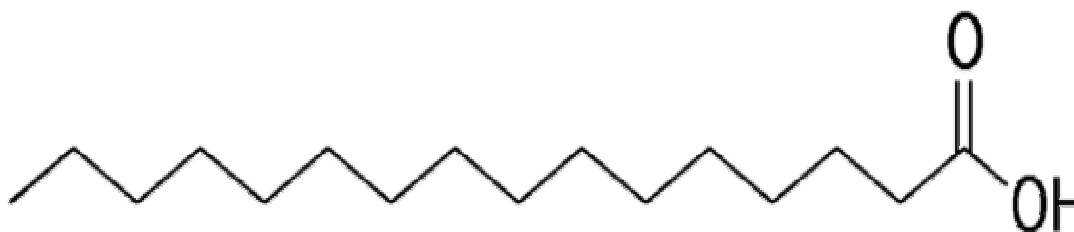


Figure 2.5 : Skeleton Structure of Palmitic acid (Palmitic acid, n.d)

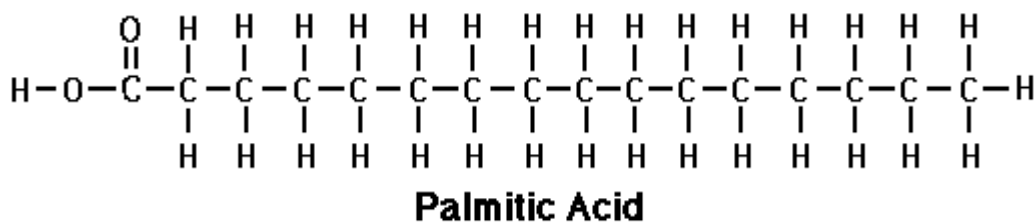


Figure 2.6 : Structure of Palmitic Acid

2.7.2 Isooctane

Figure 2.7 below indicates the structure of isooctane. Isooctane is one of the compounds in petrol and exists in palmitic acid.

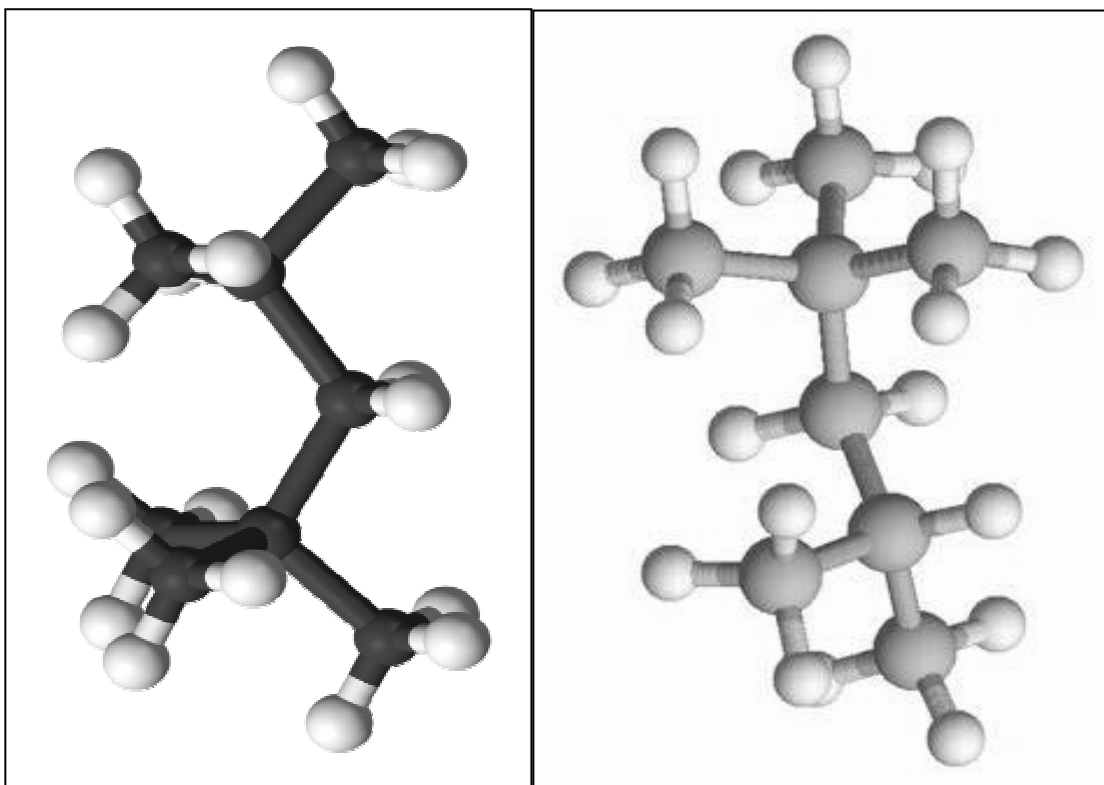


Figure 2.7 : Isooctane Structure

Isooctane, also known as 2,2,4-Trimethylpentane, is an octane isomer which defines the 100 point on the octane rating scale.

Isooctane 100 is a mixture of C₈ isoparaffins which contains virtually no aromatics or sulphur compounds. It is one of the compounds in petrol/gasoline and has an enthalpy of combustion of -48 kJ/g or -33 kJ/cm³. Isooctane 100 has a range of properties including low toxicity, lack of colour, high colour stability, low odour and rapid evaporation or drying which makes it an excellent solvent for a variety of surface applications. It has found particular use in the extraction of fats.

Isooctane, usually as a mixture with related hydrocarbons, is produced on a massive scale in the petrol industry. A major use is as a reference fuel, used in the development of new petrol (gasoline) blends. The fuel 'octane' number, familiar from the garage forecourt, is based on the 2, 2, 4-trimethylpentane standard.

Isooctane is very flammable and incompatible with oxidizing agents or reducing agents. It is harmful if inhaled or ingested and may be harmful through skin contact because it can cause irritation of eye tissue, irritation of the respiratory tract and skin irritant. Thus, for the personal protection we must wear safety glasses, handle it with good ventilation and keep away from sources of ignition. Isooctane is very toxic to aquatic organisms and may cause long-term damage to the environment. Table 2.5 below indicates the physical and chemical properties of isooctane and Figure 2.8 below indicates the skeleton structure of isooctane while Figure 2.9 indicates the structure of isooctane.

Table 2.5 : Physical and Chemical properties of Isooctane (Safety data for 2,2,4-trimethylpentane, 2005)

Synonyms	Isobutyltrimethylpentane, 2,2,4-Trimethylpentane
Appearance	colourless liquid
Molecular formula	C_8H_{18} or $CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$
Molecular weight	114.22 g/mol
Melting point $^{\circ}C$	-107.38 $^{\circ}C$
Boiling point $^{\circ}C$	99.3 $^{\circ}C$
Density	0.688 g/ml
Specific gravity	0.692
Solubility in water	Immiscible



Figure 2.8 : Skeleton Structure of Isooctane

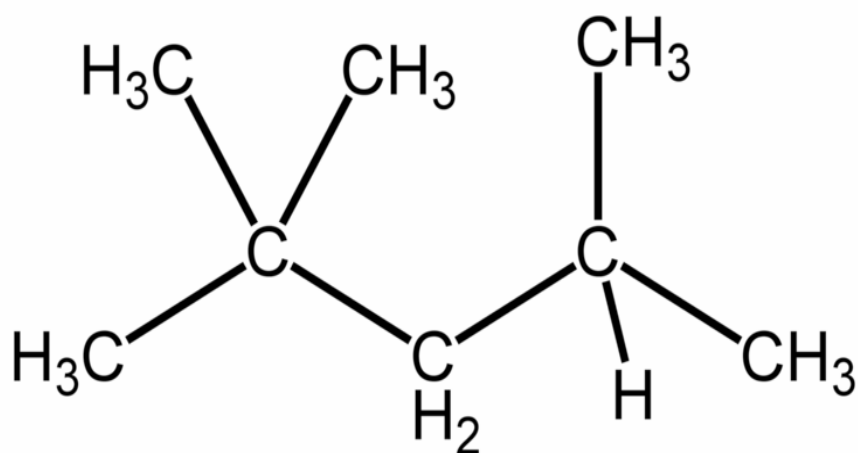


Figure 2.9 : Structure of Isooctane

CHAPTER 3

METHODOLOGY

3.1 Chemical Substances

The chemical substances used in this research are palmitic acid as the raw material, hexane as the dilution agent and isooctane as the standard substance for analysis.

3.2 Apparatus

Apparatus used in this research is the heating mantel 250mL, condenser, thermometer 360°C, round-bottom flask 50mL and heating plate. Figure 3.1 indicated set up of the apparatus.



Figure 3.1 : Set Up of the Apparatus

3.3 Experimental Works

The related experimental works involved in order to achieve isooctane production from the samples are divided into four major sections:

- i. Preparation of calibration curve for standard pure isooctane
- ii. Sample preparation (palmitic acid distillate)
- iii. Analysis the sample using Gas Chromatography Method
- iv. Determination of isooctane concentration obtained from palmitic acid distillate

3.4 Preparation of Calibration Curve for Isooctane

Four calibration isooctane-hexane mixtures (Table 3.1) are prepared, injected into several vials, labeled and analyzed using gas chromatography method to find the peak area of hexane and isooctane for each calibration isooctane-hexane mixture.

Table 3.1 : Sample of Isooctane-Hexane Mixture

Vial	Composition (%)	
	Isooctane (mL)	Hexane(mL)
1	10% (1.0mL)	90% (9.0mL)
2	5% (0.5mL)	95% (9.5mL)
3	1% (0.1mL)	99% (9.9mL)
4	0% (0.0mL)	100% (10mL)

3.5 Sample Preparation

3.5.1 Experiment 1: Palmitic Acid Heating until 98°C

The palmitic acid is heated using combination hotplate-magnetic stirrer equipment until it reaches its melting point at 64°C. At this temperature, palmitic acid will change its phase from solid to liquid. After that, the heating process continues until 98°C, which is at isooctane's boiling point. The hydrocarbon chain in palmitic acid will break down forming several new compounds. A portion of distillate at this stage is withdrawn using a syringe, which then injected into a vial specified for 98°C distillate. Figure 3.2 below indicates the flow diagram of the preparation method used.

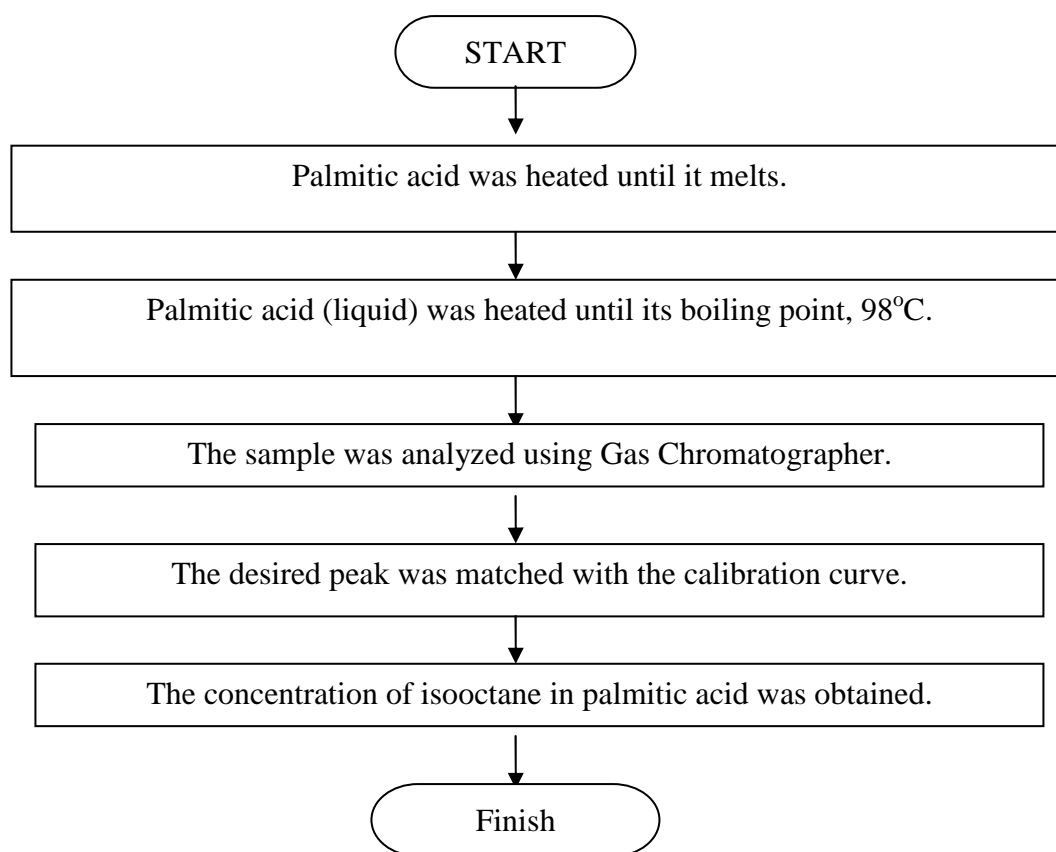


Figure 3.2 : Flow Diagram of Experiment 1

3.5.2 Experiment 2: Palmitic Acid Heating until 200°C

The liquid palmitic acid at 98°C is continuously heated until 200°C. The hydrocarbon chain in palmitic acid will continuously break down forming several new compounds. A portion of distillate at this stage is withdrawn using a syringe, which then injected into a vial specified for 200°C distillate. Figure 3.3 below indicates the flow diagram of the method to use.

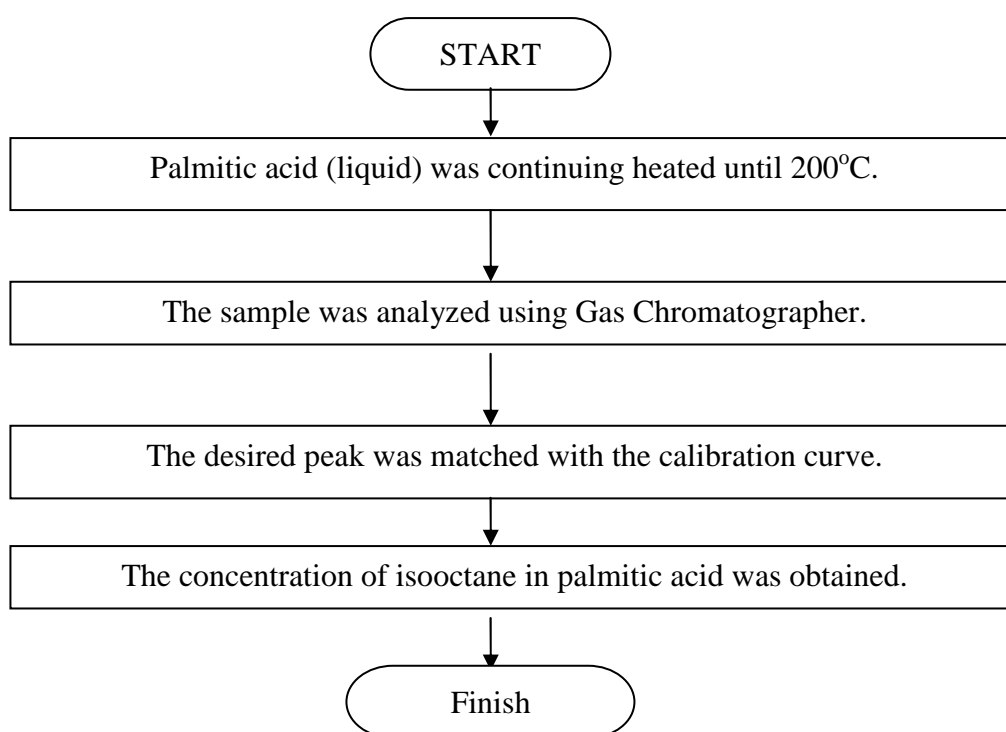


Figure 3.3: Flow Diagram of Experiment 2

3.5.3 Experiment 3: Palmitic Acid Heating until 300°C

The liquid palmitic acid at 200°C is continuously heated until 300°C. The hydrocarbon chain in palmitic acid will continuously break down forming several new compounds. A portion of distillate at this stage is withdrawn using a syringe, which then injected into a vial specified for 300°C distillate. Figure 3.4 below indicates the flow diagram of the method to use.

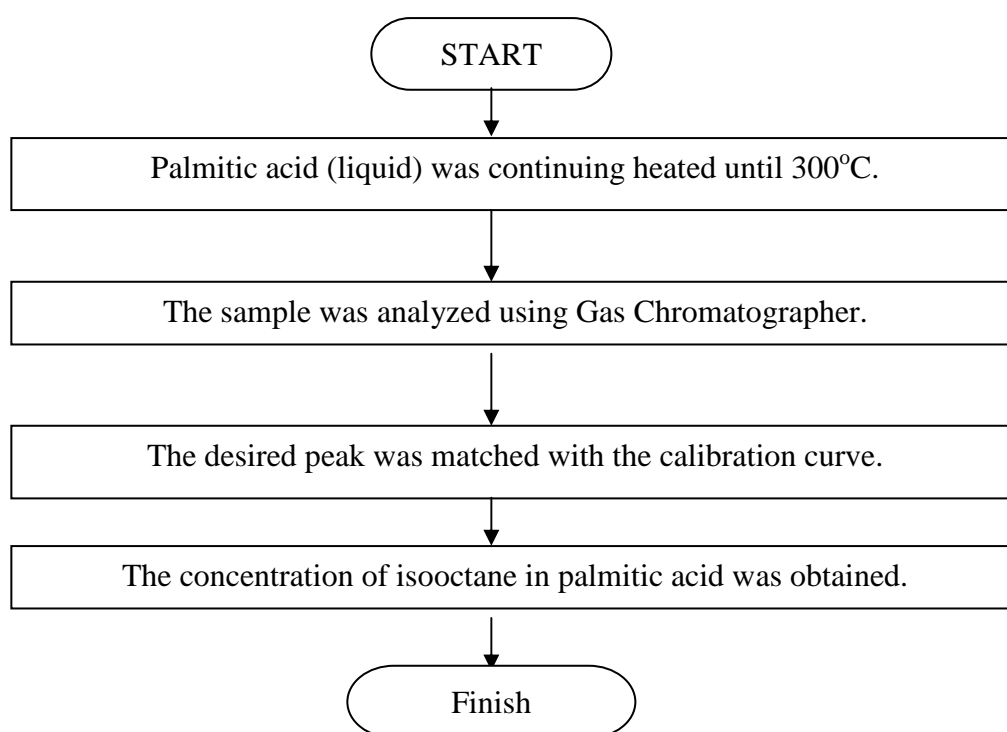


Figure 3.4 : Flow Diagram of Experiment 3

3.5.4 Experiment 4: Palmitic Acid Heating until 330°C

The liquid palmitic acid at 300°C is continuously heated until 330°C. The hydrocarbon chain in palmitic acid will continuously break down forming several new compounds. A portion of distillate at this stage is withdrawn using a syringe, which then injected into a vial specified for 330°C distillate. Figure 3.5 below indicates the flow diagram of the method to use.

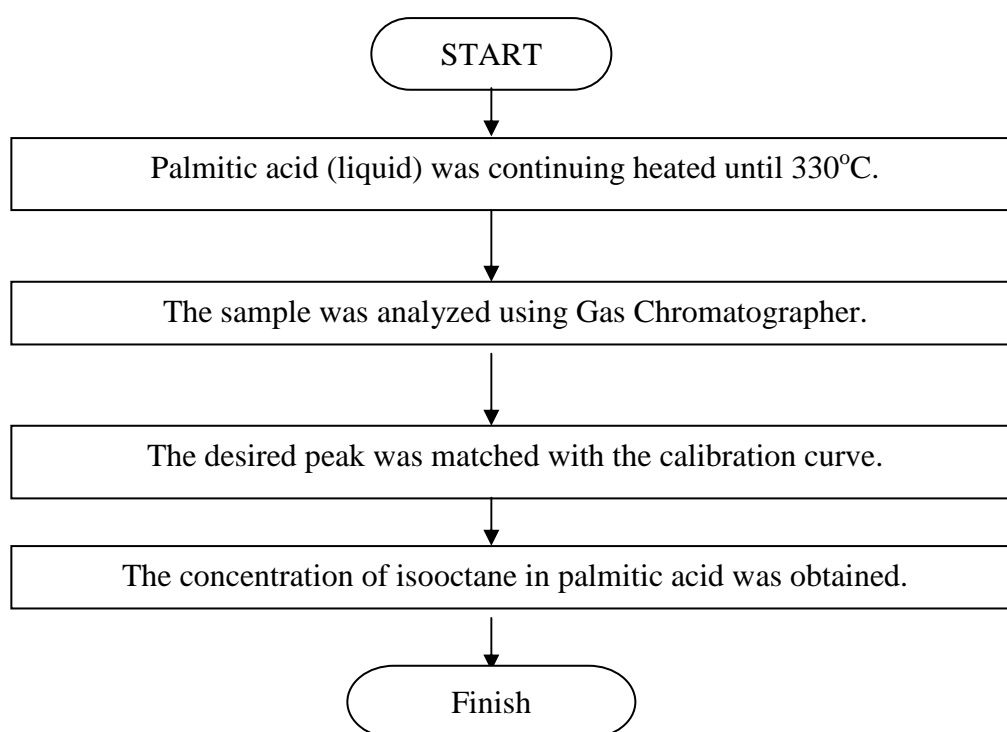


Figure 3.5 : Flow Diagram of Experiment 4

3.5.5 Experiment 5: Palmitic Acid Heating until 350°C

The liquid palmitic acid at 330°C is continuously heated until 350°C. The hydrocarbon chain in palmitic acid will continuously break down forming several new compounds. A portion of distillate at this stage is withdrawn using a syringe, which then injected into a vial specified for 350°C distillate. Figure 3.6 below indicates the flow diagram of the method to use.

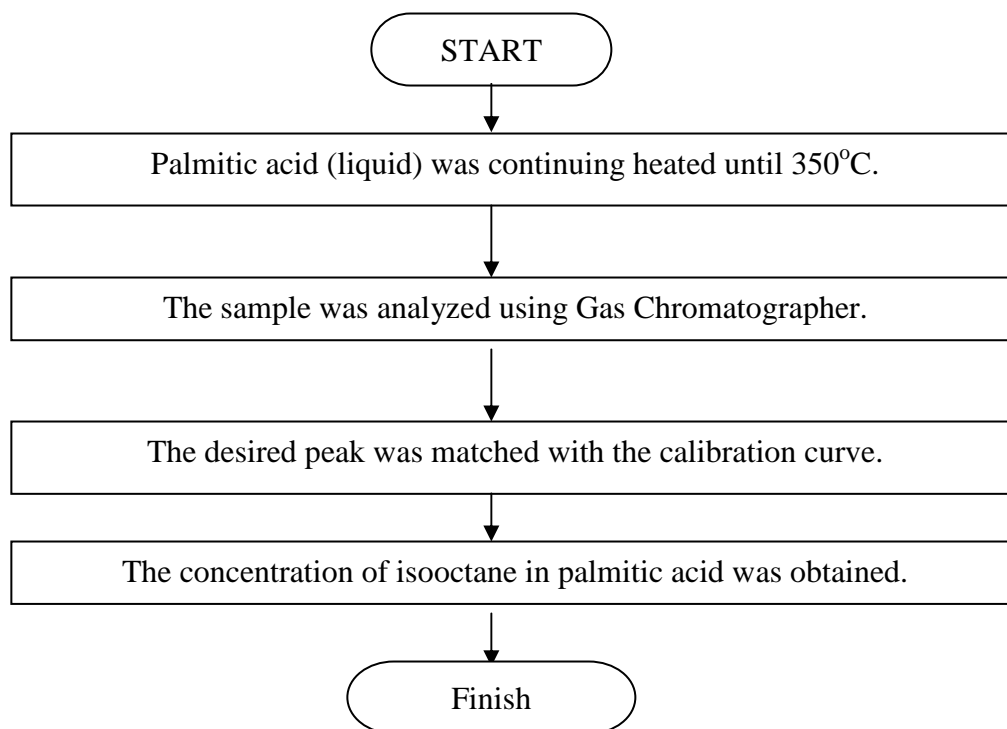


Figure 3.6 : Flow Diagram of Experiment 5

3.6 Analysis with Gas Chromatographer (GC)

Figure 3.7 below shows the picture of GC used.



Figure 3.7 : Gas Chromatographer

3.6.1 GC Condition

Because the gas chromatography method is widely used in measuring the presence and the purity of organic compounds, so the analysis of isooctane standard mixtures and palmitic acid distillates is carried out using the same method. The following conditions stated in Table 3.2 are set at gas chromatographer.

Table 3.2 : Gas Chromatographer FID Data Condition (Omar, 2006)

Temperature Column	Initial 50°C, hold 3 minutes, program at 8°C/min to 185°C, hold 5 minutes
Injector Temperature	225°C
Detector Temperature	25°C
Injection size	1.0µL (10:1 split)
Hydrogen flow	35mL/min
Air flow	450mL/min
Nitrogen make up	35mL/min
Carrier gas	Helium, Compress Air, H ₂ , N ₂

3.6.2 Analysis Method

For analysis, there are 5 samples and 4 standards that were analyzed.

1. Standards Isooctane

- Vial 1 for 10% isooctane
- Vial 2 for 5% isooctane
- Vial 3 for 1% isooctane
- Vial 4 for 100% hexane

All the standards isooctane in all vials (1, 2, 3, and 4) which contain the mixture of hexane and isooctane were placed in the gas chromatography's tube rack. GC was set up according to the GC condition in Table 3.2. All standards isooctane are then being analyzed to measure the peak area. Each of the standards isooctane takes about 20 minutes to be analyzed including 5 minutes time to cool it down before another standard isooctane can be analyze.

Figures 3.8, 3.9, 3.10 and 3.11 showed the picture of standards in vials that are used for analysis.

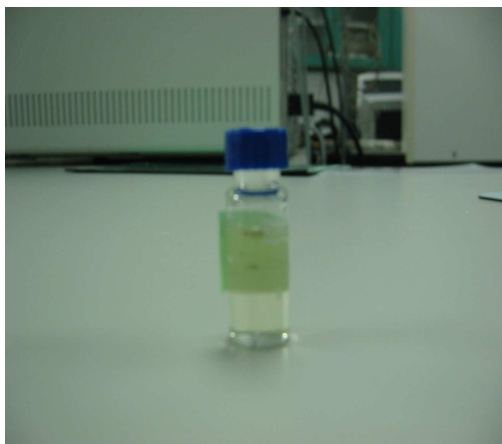


Figure 3.8 : Standard for Analysis (Vial 1)



Figure 3.9 :Standard for Analysis (Vial 2)

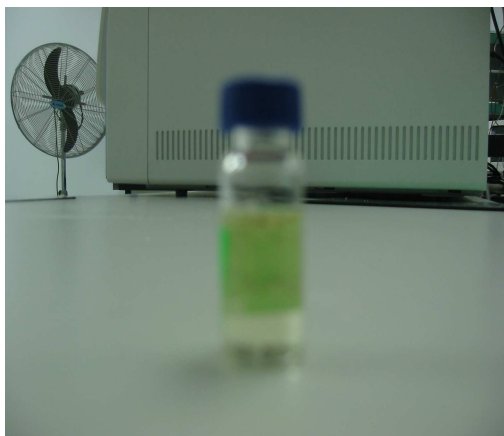


Figure 3.10 : Standard for Analysis (vial 3)



Figure 3.11 : Standard for Analysis (Vial 4)

2. Samples

- Vial 1 for 98°C distillate palmitic acid
- Vial 2 for 200°C distillate palmitic acid
- Vial 3 for 300°C distillate palmitic acid
- Vial 4 for 330°C distillate palmitic acid
- Vial 5 for 350°C distillate palmitic acid

All the samples in all vials (1, 2, 3, 4 and 5) which contain the mixture of hexane and distillate palmitic acid were placed in the gas chromatography's tube rack. GC was set up according to the GC condition in Table 3.2. All samples are then being analyzed to measure the peak area. Each of the sample takes about 20 minutes to be analyzed including 5 minutes time to cool it down before another samples can be analyze.

CHAPTER 4

RESULT AND DISCUSSION

4.1 Observation

4.1.1 Palmitic acid heated at 98°C

At room temperature, palmitic acid was in white solid form. When the heat was supplied, the palmitic acid started melting and at 64°C which is the palmitic acid's melting point, all of the solid palmitic acid melts and becomes colorless liquid. At the temperature 98°C, the liquid palmitic acid becomes light white color.

4.1.2 Palmitic acid heated at 200°C

At the initial condition, the liquid of palmitic acid was in the light white color. The liquid was continuously heated using heating mantel until it reaches temperature 200°C. At this temperature, the heated liquid becomes bright white color.

4.1.3 Palmitic acid heated at 300°C

At the initial condition, the liquid of the palmitic acid was in the dark white color. At the temperature 230°C – 250°C, the palmitic acid starts vaporizing. A small explosion occurred in the round bottom flask because some of the vapor does not enter the condenser. On the other hand, it condenses into liquid at the top of internal vessel and drops back into the boiled palmitic acid. The liquid was continuously heated until 300°C and the small explosion still occurs. At the same time, the liquid color changes into yellowish liquid.

4.1.4 Palmitic acid heated at 330°C

The heated liquid at the initial condition was in yellow color and the small explosion occurs because of the return dripping of the condensed vapor into the boiled palmitic acid. At temperature 330°C, the color of the heated liquid changes into darkish yellow.

4.1.5 Palmitic acid heated at 350°C

The darkish yellow liquid at the initial condition was continuously heated using heating mantel until 350°C. The small explosion still occurs and it is needed to be handled more carefully when collecting the sample distillate. The color of the heated liquid in this process changes into brown. The sample solidifies in the short time when it is cooled.

Figure 4.1 below shows the picture of samples.

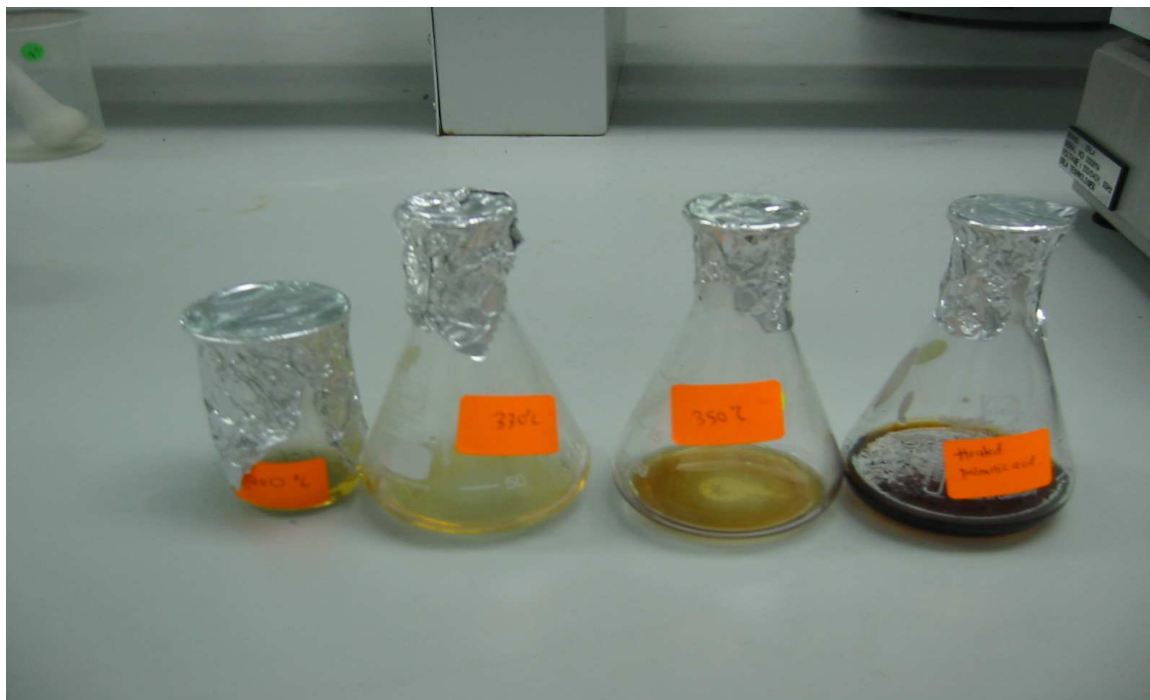


Figure 4.1 : Samples of Distillate Palmitic Acid

4.2 Results for Standard Isooctane

The standard mixtures contained pure isooctane and the hexane with the amount recorded in Table 3.1 were analyzed using Gas Chromatography method. For the vial 1 which is 10% isooctane, the value of the peak area was 1.44×10^5 pA.s with the retention time at 2.149 min. The peak area was 7.12×10^4 and retention time at 2.139 min for 5% isooctane in vial 2. For 1% isooctane in vial 3, the peak area was 5.14×10^4 at the retention time 2.130 min. All the obtained results of the standards were recorded in Table 4.1.

Table 4.1 : Retention Time and Area for Standard Isooctane

Concentration of Isooctane (%)	Retention Time (min)	Peak Area (pA*s)
0	0	0.00
1	2.13	2.14×10^4
5	2.139	7.12×10^4
10	2.149	1.44×10^5

The Table 4.1 describes the time where the compound exist and also its peak area. The result shows that the peak area of isooctane is increasing with the amount of the concentration of isooctane in percent. The time in minutes indicates where the compound is existing is between 2.13 minutes and 2.149 minutes. The other peaks that exist outside from the range are considered as the non-desired product. All of the standard results were plotted to obtain a standard calibration curve as shown in Figure 4.2.

This calibration curve then is used to determine the exact concentration of isooctane obtained in the 98°C distilled palmitic acid, 200°C distilled palmitic acid, 300°C distilled palmitic acid, 330°C distilled palmitic acid and 350°C distilled palmitic acid according to their individual peak areas.

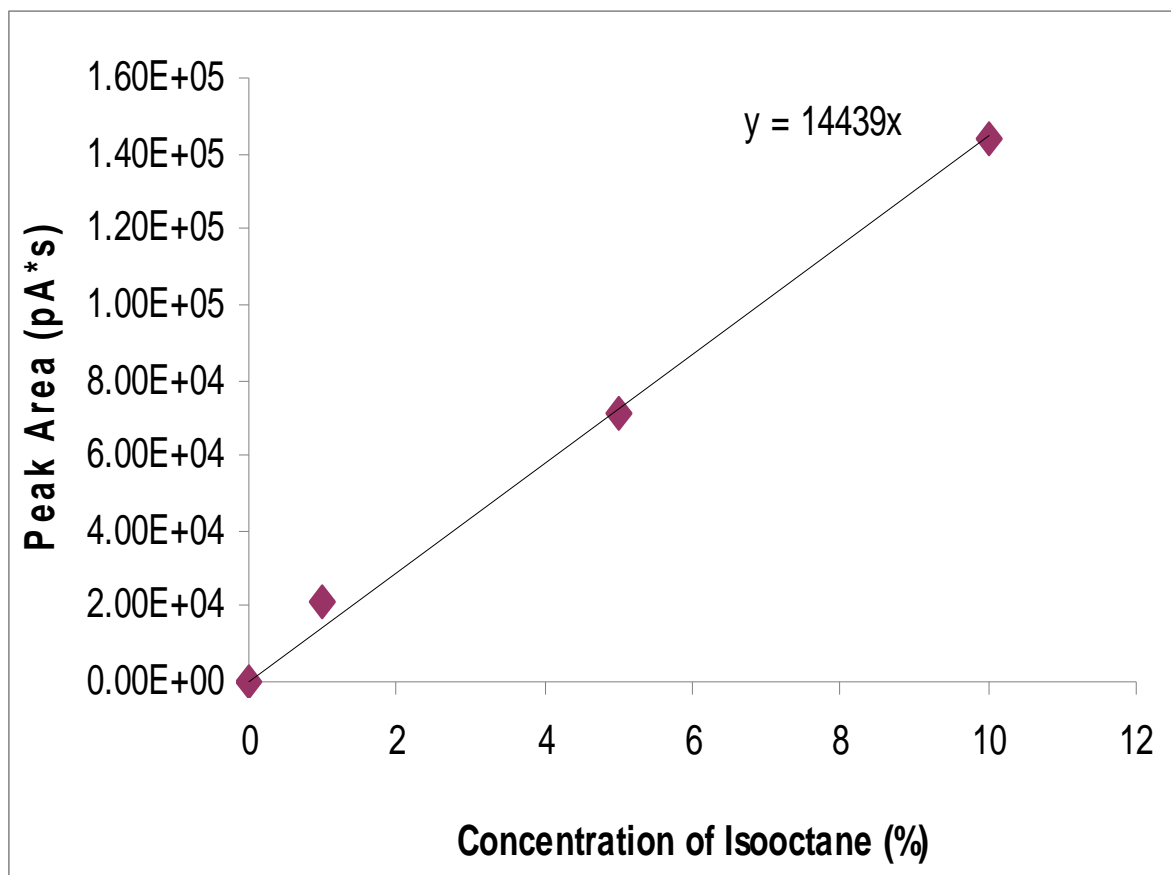


Figure 4.2 : Standard Calibration Curve

Figure 4.3, 4.4, 4.5 and 4.6 below show the chromatogram of the isooctane standards those consisting 10% isooctane, 5% isooctane, 1% isooctane and 0% isooctane (100% hexane) that are analyzed by using Gas Chromatographer.

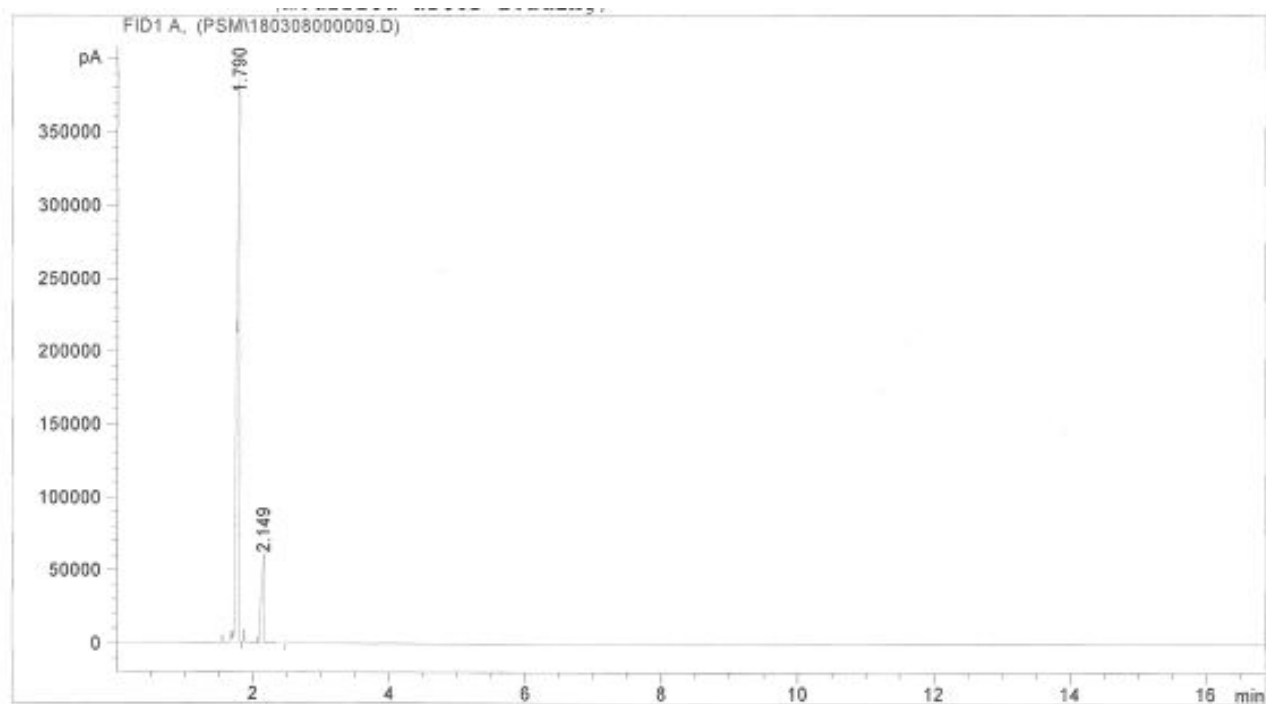


Figure 4.3 : Chromatogram of Isooctane Standard for 10% Isooctane

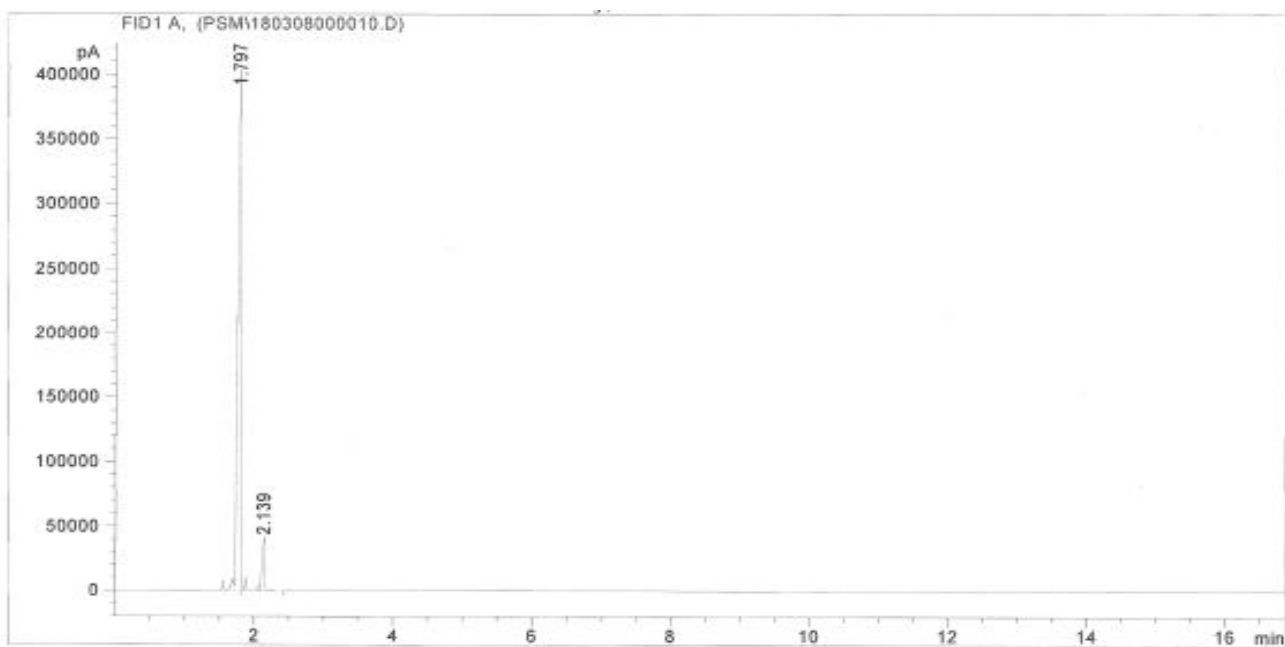


Figure 4.4 : Chromatogram of Isooctane Standard for 5% Isooctane

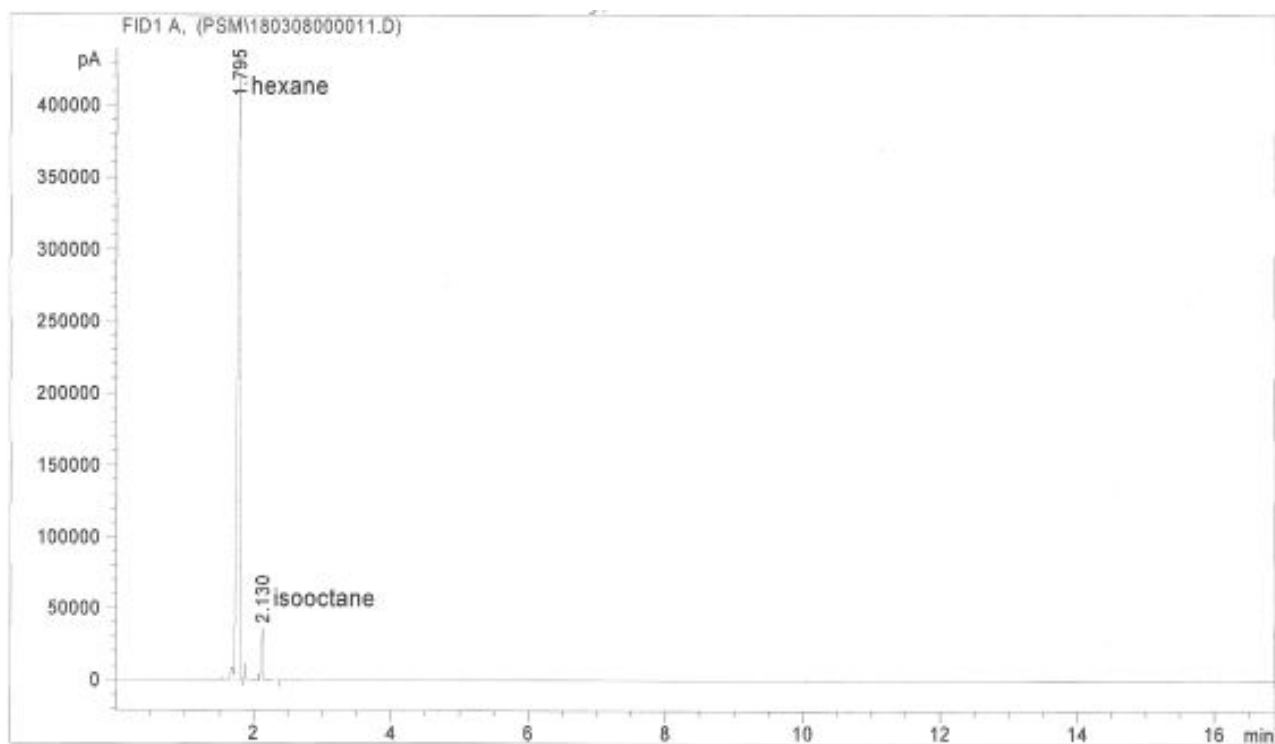


Figure 4.5 : Chromatogram of Isooctane Standard for 1% Isooctane

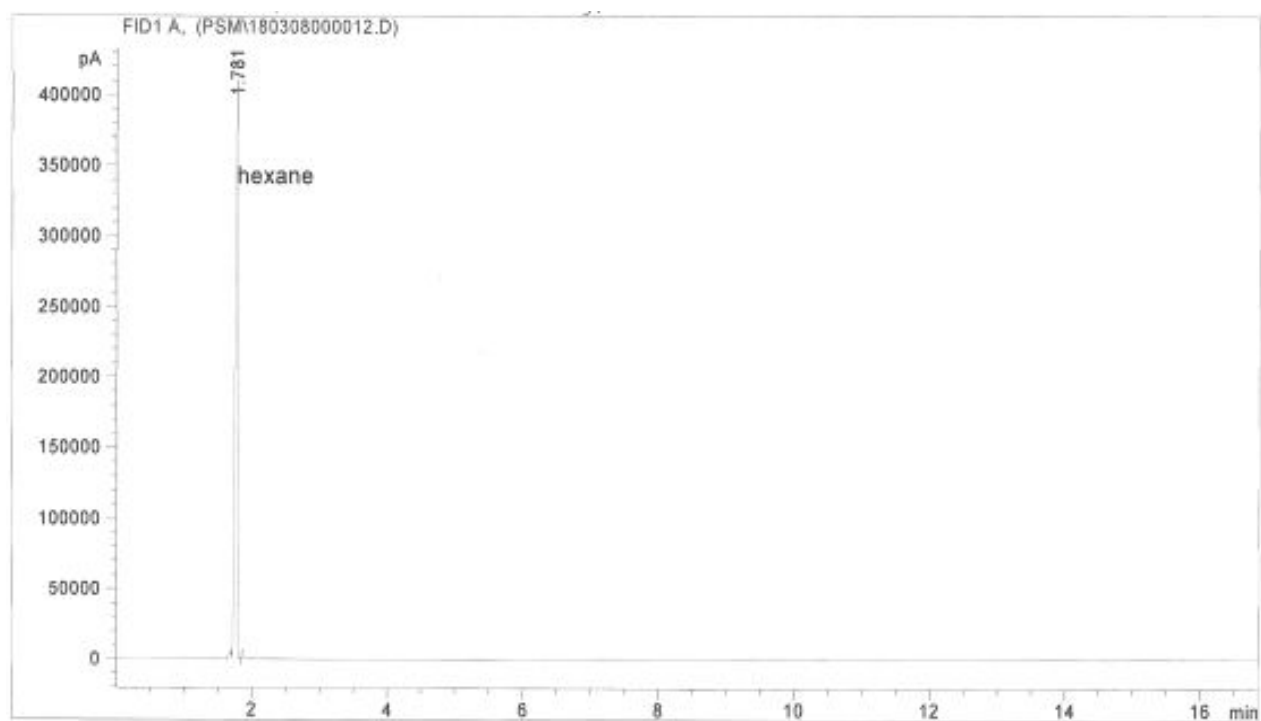


Figure 4.6 : Chromatogram of Isooctane Standard for 100% Hexane

4.3 Result for samples (palmitic acid)

4.3.1 Result for 98°C Distilled Palmitic Acid

The sample of 98°C distilled palmitic acid was analyzed using Gas Chromatographer and the retention time and area is shown in Table 4.2 while the chromatogram is shown in Figure 4.7 (for more detail refer appendix G). The nearest retention time in sample with standard isooctane retention time in range 2.130 min to 2.159 min is considered as desired isooctane in the sample.

Table 4.2 : Retention Time and Area of 98°C Distilled Palmitic Acid

Peak	Retention Time (min)	Area (pA*s)	Area (%)
1	1.477	3.73417	0.00047
2	1.559	227.13031	0.02868
3	1.611	96.27958	0.01216
4	1.658	1.50068e4	1.89475
5	1.768	7.69967e5	97.21544
6	1.850	6012.63037	0.75915
7	1.980	32.08628	0.00405
8	2.068	17.38913	0.00220
*9	2.130	657.23083	0.08298
10	2.299	1.03004	0.00013

* Desired isooctane in sample

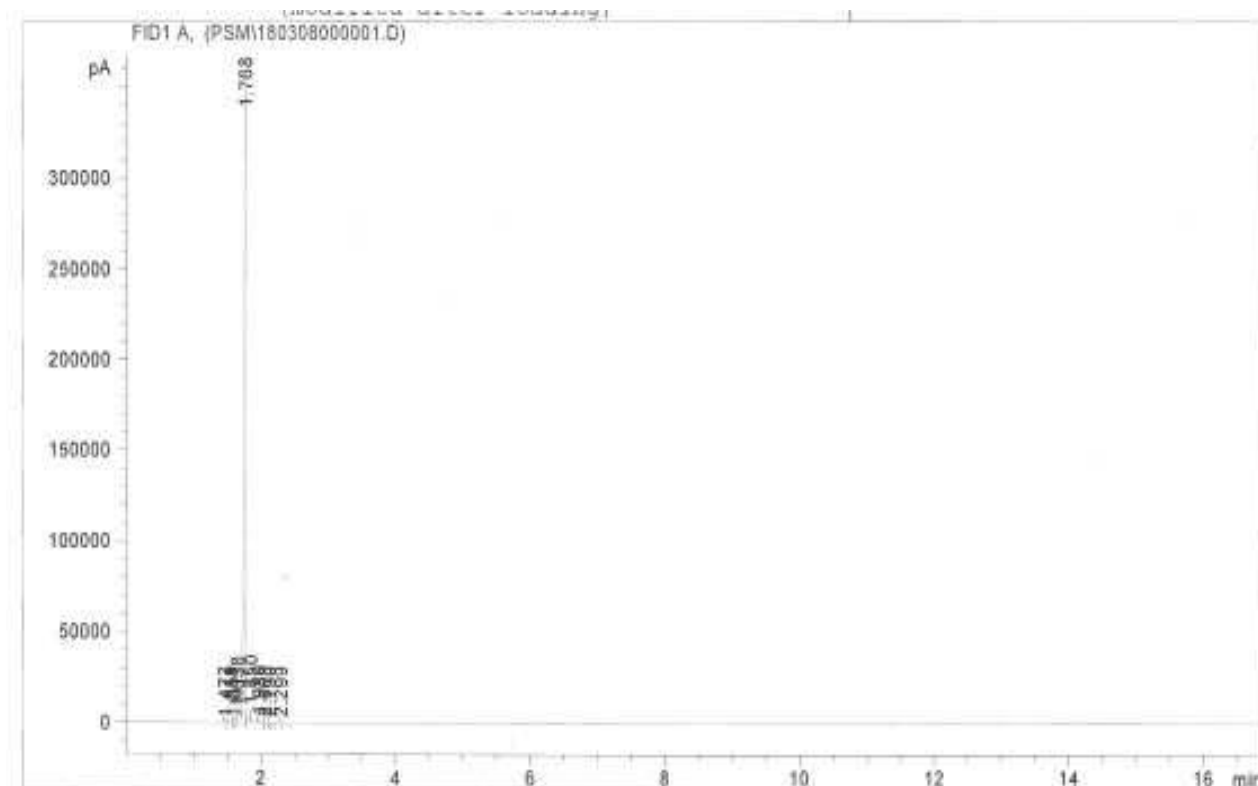


Figure 4.7 : Chromatogram of 98°C Palmitic Acid

4.3.2 Result for 200°C Distilled Palmitic Acid

The sample of 200°C distilled palmitic acid was analyzed using Gas Chromatographer and the retention time and resulting peak area are shown in Table 4.3, while the related chromatogram is shown in Figure 4.8 (for more detail refer appendix G). The nearest retention time in sample with standard isooctane retention time in range 2.130 min to 2.159 min is considered as desired isooctane in the sample.

Table 4.3 : Retention Time and Area of 200°C Distilled Palmitic Acid

Peak	Retention Time (min)	Area (pA*s)	Area (%)
1	1.472	4.46343	0.00037
2	1.529	99.57352	0.00826
3	1.555	190.94455	0.01583
4	1.608	132.09825	0.01095
5	1.678	1.92801e4	1.59878
6	1.780	1.17697e6	97.59833
7	1.860	8131.28711	0.67428
8	1.989	44.45758	0.00369
9	2.022	69.13501	0.00573
10	2.077	29.82965	0.00247
*11	2.138	978.80133	0.08117
12	2.307	1.69924	0.00014

* Desired isooctane in sample

**Figure 4.8** : Chromatogram of 200°C Palmitic Acid

4.3.3 Result for 300°C Distilled Palmitic Acid

The sample of 300°C distilled palmitic acid was analyzed using Gas Chromatographer and the retention time and resulting peak area are shown in Table 4.4, while the related chromatogram is shown in Figure 4.9 (for more detail refer appendix G). The nearest retention time in sample with standard isooctane retention time in range 2.130 min to 2.159 min is considered as desired isooctane in the sample.

Table 4.4 : Retention Time and Area of 300°C Distilled Palmitic Acid

Peak	Retention Time (min)	Area (pA*s)	Area (%)
1	1.471	4.23257	0.00039
2	1.554	261.21362	0.02405
3	1.608	117.98956	0.01086
4	1.681	1.79983e4	1.65734
5	1.773	1.05901e6	97.51717
6	1.856	17529.75830	0.69336
7	1.987	52.57343	0.00484
8	2.021	60.76396	0.00560
9	2.078	30.01020	0.00276
*10	2.138	894.45276	0.08236
11	2.308	1.55715	0.00014
12	2.796	5.69365	0.00052
13	2.876	6.35030	0.00058

* Desired isooctane in sample

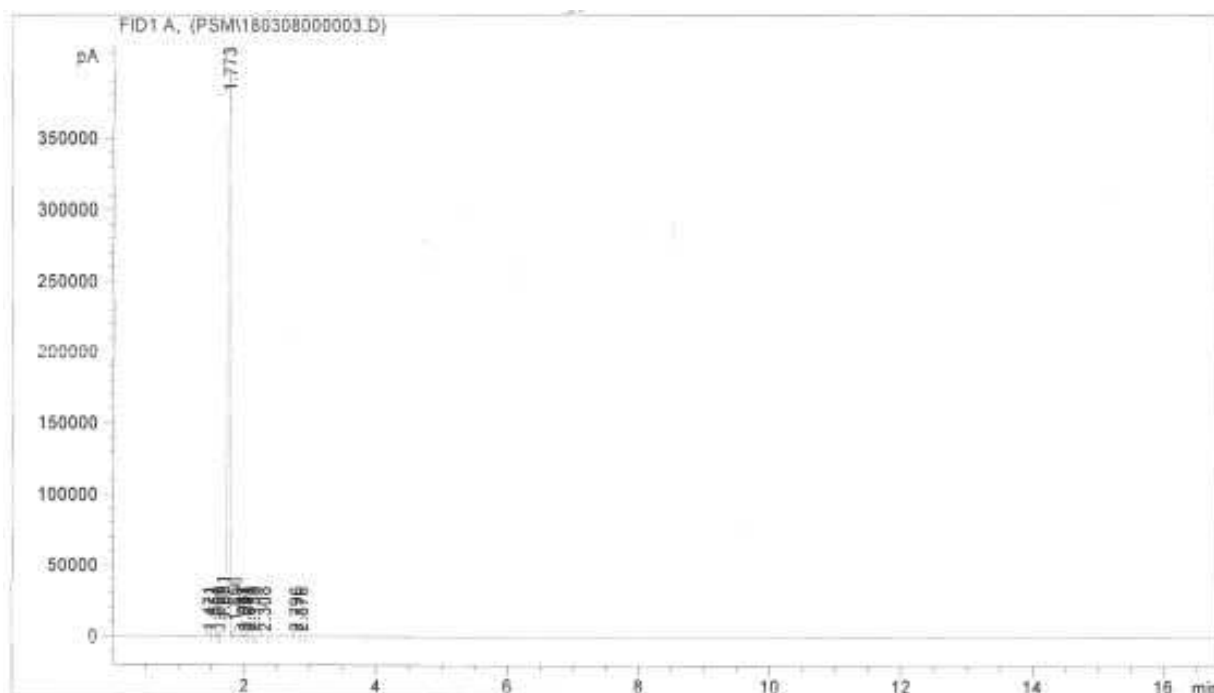


Figure 4.9 : Chromatogram of 300°C Palmitic Acid

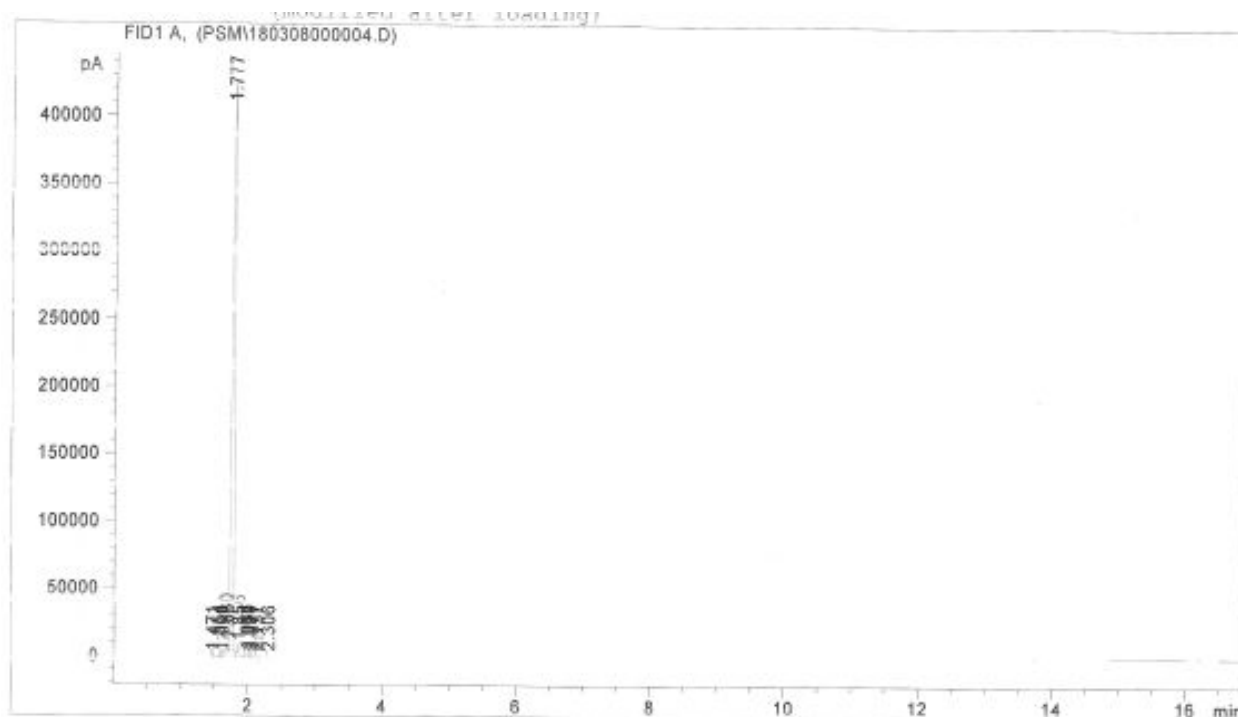
4.3.4 Result for 330°C Distilled Palmitic Acid

The sample of 330°C distilled palmitic acid was analyzed using Gas Chromatographer and the retention time and resulting peak area are shown in Table 4.5, while the related chromatogram is shown in Figure 4.10 (for more detail refer appendix G). The nearest retention time in sample with standard isooctane retention time in range 2.130 min to 2.159 min is considered as desired isooctane in the sample.

Table 4.5 : Retention Time and Area of 330°C Distilled Palmitic Acid

Peak	Retention Time (min)	Area (pA*s)	Area (%)
1	1.471	4.10852	0.00035
2	1.554	277.70157	0.02374
3	1.608	127.43944	0.01089
4	1.680	1.92941e4	1.64921
5	1.777	1.14090e6	97.52126
6	1.856	8182.32813	0.69940
7	1.987	44.14463	0.00377
8	2.020	68.24841	0.00583
9	2.077	33.27420	0.00284
*10	2.137	965.77350	0.08255
11	2.306	1.73327	0.00015

* Desired isooctane in sample

**Figure 4.10** : Chromatogram of 330°C Palmitic Acid

4.3.5 Result for 350°C Distilled Palmitic Acid

The sample of 350°C distilled palmitic acid was analyzed using Gas Chromatographer and the retention time and resulting peak area are shown in Table 4.6, while the related chromatogram is shown in Figure 4.11 (for more detail refer appendix G). The nearest retention time in sample with standard isooctane retention time in range 2.130 min to 2.159 min is considered as desired isooctane in the sample.

Table 4.6 : Retention Time and Area of 350°C Distilled Palmitic Acid

Peak	Retention Time (min)	Area (pA*s)	Area (%)
1	1.471	5.24573	0.00040
2	1.527	106.81397	0.00806
3	1.554	220.89143	0.01667
4	1.607	145.34619	0.01097
5	1.677	2.11993e4	1.59988
6	1.784	1.29134e6	97.45585
7	1.862	8969.66309	0.67693
8	1.990	52.67149	0.00398
9	2.023	76.27290	0.00576
10	2.088	1860.12720	0.14038
*11	2.139	1073.29834	0.08100
12	2.308	1.70571	0.00013

* Desired isooctane in sample

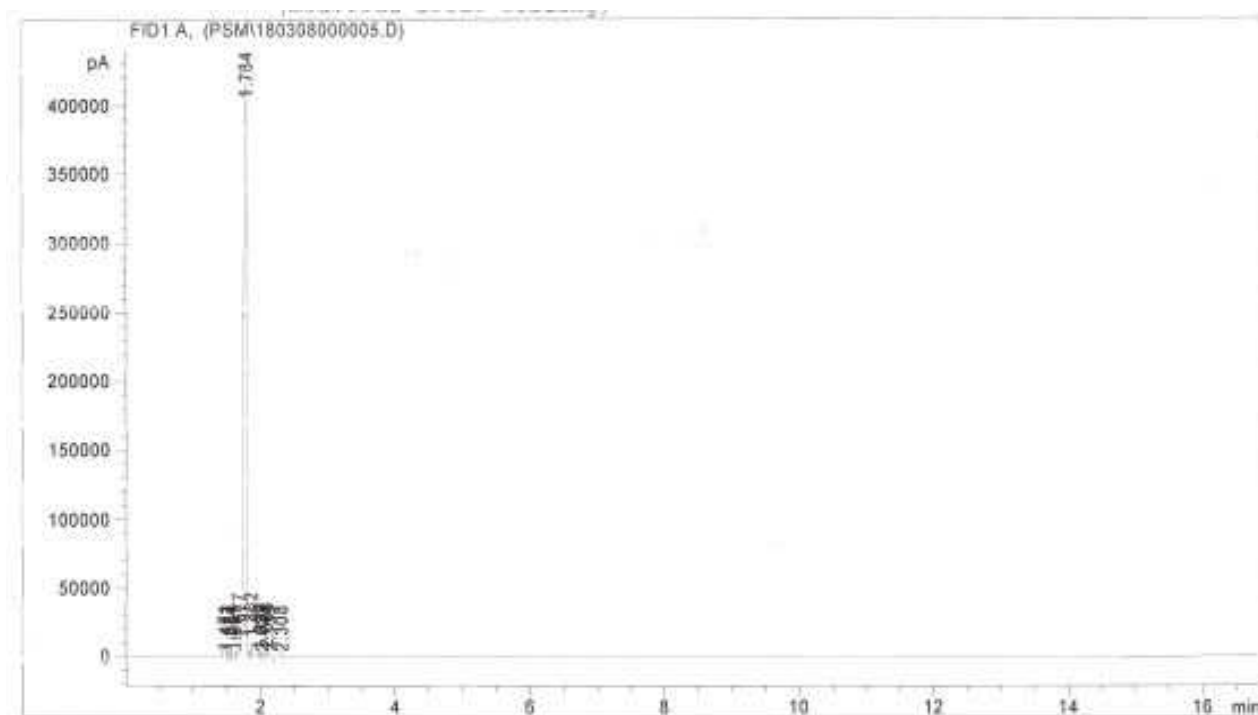


Figure 4.11 : Chromatogram of 350°C Palmitic Acid

4.4 Concentration of Desired Isooctane in All Samples.

The samples were analyzed using the Gas Chromatography method and the obtained results were recorded in Table 4.7. The value of concentration of each sample was calculated from formula shown in the standard calibration curve ($Y=14439X$).

Table 4.7 : Peak Area, Retention Time and Concentration of All Samples

Samples (°C)	Peak Area (pA*s)	Time (min)	Concentration (%)
98	657.23083	2.130	0.0455
200	978.80133	2.138	0.0678
300	894.45276	2.138	0.0619
330	965.77350	2.137	0.0663
350	1073.29834	2.139	0.0743

4.5 Discussion

Cracking method is used to breaking up large hydrocarbon molecules into smaller and more useful bits of hydrocarbon compounds. The long-chain hydrocarbon molecules are at first broken up in a fairly random way to produce mixtures of various smaller hydrocarbon radicals, and then these radicals recombine in different arrangement through isomerization process. The desired isooctane molecules are formed through this process. Some of the rest hydrocarbon compounds have carbon-carbon double bonds.

From the obtained result, the percentage concentration of isooctane obtained in 98°C palmitic acid distillate is 0.0455%, the percentage concentration of isooctane obtained in 200°C distillate is 0.0678%, for 300°C distillate the concentration is 0.0619%, for 330°C distillate the concentration is 0.0663% and at 350°C palmitic acid distillate the concentration is 0.0743%. These values are fluctuating. The highest concentration of desired isooctane is 0.0743% which is at 350°C distillate palmitic acid. This result means that the temperatures can be the factor to get the maximum concentration of desired isooctane but this factor does not effect too much. This is because the energy of heat supply randomly attacks any of the C-C bonds in the palmitic acid, which make hydrocarbon bonds fairly break in the random way. High temperature can only supply more energy to break up the hydrocarbon bonds but it cannot select specific desired molecules as expected.

The concentrations of all heated palmitic acid are obtained only in the small amounts. This is because before analyzing the samples using Gas Chromatographer, the samples were diluted twice with hexane as the dilution agent. The dilution is required because only colorless and non-particle liquid sample can be injected and run using the Gas Chromatographer, to avoid the blocking occurrence in the gas chromatography column by the solid particles. This dilution makes the concentration of the heated palmitic acid decreases and at the same time makes the concentration of obtained isooctane decreases too.

In order to determine the real concentration of isooctane produced in the sample, back calculation of the isooctane concentration determination is required. By using back calculation technique, hexane as dilution agent is eliminated as the main assumption. The rest of the sample is recalculated to get the actual concentration of the desired isooctane, which assumes that the samples are injected directly into the gas chromatographer, without require any dilution. The actual concentrations of isooctane in all samples are recorded in the Table 4.8 and in Figure 4.12.

Table 4.8 : Actual Concentration of Isooctane in Samples

Samples (°C)	Actual Peak Area (%)	Actual Peak Area (pA*s)	Actual Concentration Of Desired Isooctane (%)
98	2.980004	23602.68	1.634648
200	3.379732	40755.03	2.822566
300	3.317182	36025.53	2.495016
330	3.330321	38599.19	2.673259
350	3.183775	42186.91	2.921734

All of the calculations are shown in appendix A at the back.

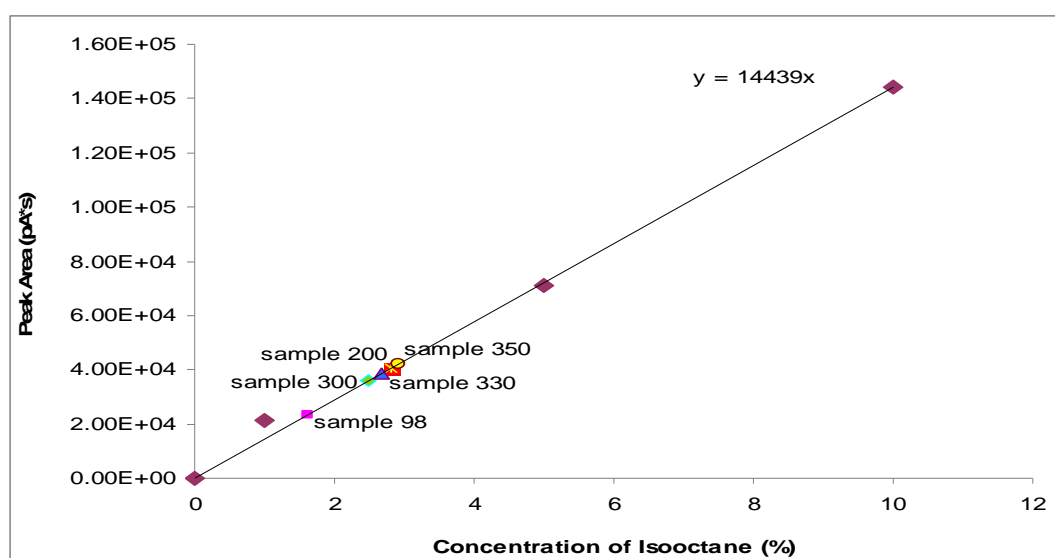


Figure 4.12 : Concentration of Actual Desired Isooctane in the Samples

CHAPTER 5

CONCLUSION

5.0 Conclusion

The purpose of this project is to investigate the highest concentration of biopetrol (isooctane) in palmitic acid.

From the obtained result, the percentage concentration of isooctane obtained in 98°C palmitic acid distillate is 0.0455%, the percentage concentration of isooctane obtained in 200°C distillate palmitic acid is 0.0678%, for 300°C distillate palmitic acid, the concentration of desired isooctane is 0.0619%, for 330°C distillate palmitic acid, the concentration of desired isooctane is 0.0663% and at 350°C palmitic acid distillate the concentration of desired isooctane is 0.0743%.

Thus, the highest concentration of biopetrol (isooctane) obtained is 0.0743% which is at 350°C distillate palmitic acid and after the back calculation without dilution agent (hexane) the highest concentration is 2.92% at temperature 350°C palmitic acid.

Biopetrol from vegetable oil is biodegradable, non-toxic and environmental friendly substance. So by producing biopetrol from palmitic acid, it can help to recover the decrease of fossil fuel, reduces water and air pollution and also reduces the amounts of wastes disposed among vegetable oil productions.

5.1 Recommendation

This research was extended to understand the fundamental of cracking hydrocarbon. To further establish this method of cracking, it is necessary to develop advanced analytical method for the qualitative and quantitative analysis of palmitic acid in producing biopetrol. The development of real-time techniques such as spectroscopy is useful in confirmation of identification of the biopetrol in palmitic acid and should be considered in future.

In order to increase the concentration of biopetrol (isooctane) in palmitic acid, it is recommended to use catalytic cracking method, which means the cracking process using solid catalyst instead of thermal cracking. This is because the catalytic cracking using certain heterogeneous solid catalysts is more effective and it is already practiced in all petroleum refineries.

Before starting the cracking process, the whole vessel should be evacuated to prevent oxygen from involving reaction during cracking process, in order to avoid oxidation. Optionally, the whole vessel should be filled first with either nitrogen (N_2) or inert gas to ensure the cracking process is effective and the desired product amount will increase more than this current process.

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APPENDIX A

Example of Calculation

For 98°C heated palmitic acid,

$$\begin{aligned}\text{Actual peak area isooctane (\%)} &= [\text{peak area isooctane (\%)} / [100 - \text{peak area hexane} \\ &\quad (\%)] * 100 \\ &= [0.08298 / (100 - 97.21544)] * 100 \\ &= 2.98\%\end{aligned}$$

$$\begin{aligned}\text{Actual peak area (pA*s)} &= [\text{peak area isooctane (pA*s)} / \text{peak area isooctane (\%)}] * \text{actual} \\ &\quad \text{peak area of isooctane (\%)} \\ &= [657.23083 / 0.08298] * 2.98 \\ &= 23602.68 \text{ pA*s}\end{aligned}$$

From the equation shown in standard calibration curve (Figure 4.2):

$$Y = 14439X$$

$$\begin{aligned}\text{Actual concentration of Isooctane (\%)} &= \text{actual peak area (pA*s)} / 14439 \\ &= 23602.68 / 14439 \\ &= 1.634648 \%\end{aligned}$$

The others calculations are using same method and recorded in table below.

Samples (°C)	Peak Area Desired Isooctane (%)	Peak Area Hexane (%)	Area (pA*s)	Actual Peak Area (%)	Actual Peak Area (pA*s)	Actual Concentration Of Desired Isooctane (%)
98	0.08298	97.21544	657.2308	2.980004	23602.68	1.634648
200	0.08117	97.59833	978.8013	3.379732	40755.03	2.822566
300	0.08236	97.51717	894.4528	3.317182	36025.53	2.495016
330	0.08255	97.52126	956.7735	3.330321	38599.19	2.673259
350	0.081	97.45585	1073.2983	3.183775	42186.91	2.921734

APPENDIX B

Material Safety Data Sheet

Safety Data for Palmitic Acid

General

Synonyms: cetylic acid, hexadecylic acid, hexadecanoic acid

Molecular formula: $C_{16}H_{32}O_2$

CAS No: 57-10-3

EINECS No: 200-312-9

Physical data

Appearance: white chips, crystals or powder

Melting point: 61 - 64 C

Boiling point: 352 C

Vapour pressure: 10 mm Hg at 210 C

Density ($g\ cm^{-3}$): 0.84

Stability

Stable. Combustible. Incompatible with bases, oxidizing agents, reducing agents.

Toxicology

Skin, eye and respiratory irritant.

Toxicity data

(Refer appendix C)

ORL-RAT LD50 > 10000 mg kg^{-1}

IVN-MUS LD50 57 mg kg^{-1}

Risk phrases

(The meaning of any risk phrases which appear in this section is given in appendix D)

R36 R37 R38.

Transport information

Non-hazardous for air, sea and road freight.

Personal protection

Safety glasses.

Safety phrases

(The meaning of any safety phrases which appear in this section is given in appendix E)

S26 S36.

Safety Data For 2,2,4-Trimethylpentane



General

Synonyms: isobutyltrimethylpentane, isooctane

Molecular formula: $(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2$

CAS No: 540-84-1

EC No: 208-759-1

Annex I Index No: 601-009-00-8

Physical data

Appearance: colourless liquid

Melting point: -107 C

Boiling point: 98 C

Vapour density: 3.9

Vapour pressure: 41 mm Hg at 21 C

Specific gravity: 0.692

Flash point: -7 C (closed cup)

Explosion limits: 1 - 6%

Autoignition temperature: 396 C

Stability

Stable. Highly flammable. Incompatible with oxidizing agents, reducing agents.

Toxicology

Harmful if inhaled or ingested. May be harmful through skin contact. Eye, respiratory and skin irritant.

Risk phrases

(The meaning of any risk phrases which appear in this section is given in appendix D)

R11 R20 R22 R36 R37 R38 R50 R53 R65 R67.

Environmental information

Very toxic to aquatic organisms - may cause long-term damage to the environment.

Transport information

(The meaning of any UN hazard codes which appear in this section is given appendix F)

UN No 1262. Hazard class 3.0. Packing group II.

Personal protection

Safety glasses, good ventilation, keep away from sources of ignition.

Safety phrases

(The meaning of any safety phrases which appear in this section is given appendix F)

S16 S26 S33 S36 S37 S39.

APPENDIX C

Abbreviations used in Toxicity data

dom	domestic animal (goat, sheep)
dpo	<i>Drcsophila pseudo-obscura</i>
emb	embryo
esc	<i>Escherichia coli</i>
eug	<i>Euglena gracilis</i>
eye	administration into eye (irritant)
ice	intracerebral
icv	intracervical
idr	intradermal
idu	intraduodenal
ihl	inhalation
isp	intrapinal
itr	intratracheal
itt	intratesticular
iu	international unit
iut	intrauterine
ivg	intravaginal
ivn	intravenous
kdy	kidney
LC50	lethal concentration 50 percent kill
LCLo	lowest published lethal concentration
LD50	lethal dose 50 percent kill
LDlo	lowest published lethal dose
leu	leukocyte
Liq	liquid
lng	lung
lvr	liver
MOD	moderate irritation effects
mol	mole
mppcf	million particles per cubic foot

mrc	gene conversion and mitotic recombination
msc	mutation in mammalian somatic cells
mul	multiple routes
mus	mouse
orl	oral
ORM	Other Regulated Material (DoT)
oth	other cell types
otr	oncogenic transformation
ovr	ovary
par	parenteral
pg	picogram
pgn	pigeon
pic	phage inhibition capacity
pig	pig
Pk	peak concentration
pmol	picomole
post	after birth
ppb	parts per billion (v/v)
pph	parts per hundred (v/v) (percent)
ppm	parts per million (v/v)
ppt	parts per trillion (v/v)
preg	pregnant
qal	quail
rat	rat
STEL	short term exposure limit
TC	toxic concentration (other than lowest concentration)
TCLo	lowest published toxic concentration
TD	toxic dose (other than lowest toxic dose)
TDLo	lowest published toxic dose
Y	year

APPENDIX D

Risk Phrases

- R1 Explosive when dry.
- R2 Risk of explosion by shock, friction, fire or other source of ignition.
- R3 Extreme risk of explosion by shock, friction, fire or other sources of ignition.
- R4 Forms very sensitive explosive metallic compounds.
- R5 Heating may cause an explosion.
- R6 Explosive with or without contact with air.
- R7 May cause fire.
- R8 Contact with combustible material may cause fire.
- R9 Explosive when mixed with combustible material.
- R10 Flammable.
- **R11 Highly flammable.**
- R12 Extremely flammable.
- R13 Extremely flammable liquefied gas
- R14 Reacts violently with water.
- R15 Contact with water liberates extremely flammable gases.
- R16 Explosive when mixed with oxidizing substances.
- R17 Spontaneously flammable in air.
- R18 In use, may form inflammable/explosive vapour-air mixture.
- R19 May form explosive peroxides.
- **R20 Harmful by inhalation.**
- R21 Harmful in contact with skin.
- **R22 Harmful if swallowed.**
- R23 Toxic by inhalation.
- R24 Toxic in contact with skin.
- R25 Toxic if swallowed.
- R26 Very toxic by inhalation.
- R27 Very toxic in contact with skin.
- R28 Very toxic if swallowed.
- R29 Contact with water liberates toxic gas.
- R30 Can become highly flammable in use.
- R31 Contact with acids liberates toxic gas.
- R32 Contact with acid liberates very toxic gas.
- R33 Danger of cumulative effects.
- R34 Causes burns.
- R35 Causes severe burns.
- **R36 Irritating to eyes.**

- **R37 Irritating to respiratory system.**
- **R38 Irritating to skin.**
- R39 Danger of very serious irreversible effects.
- R40 Limited evidence of a carcinogenic effect.
- R41 Risk of serious damage to the eyes.
- R42 May cause sensitization by inhalation.
- R43 May cause sensitization by skin contact.
- R44 Risk of explosion if heated under confinement.
- R45 May cause cancer.
- R46 May cause heritable genetic damage.
- R47 May cause birth defects
- R48 Danger of serious damage to health by prolonged exposure.
- R49 May cause cancer by inhalation.
- **R50 Very toxic to aquatic organisms.**
- R51 Toxic to aquatic organisms.
- R52 Harmful to aquatic organisms.
- **R53 May cause long-term adverse effects in the aquatic environment.**
- R54 Toxic to flora.
- R55 Toxic to fauna.
- R56 Toxic to soil organisms.
- R57 Toxic to bees.
- R58 May cause long-term adverse effects in the environment.
- R59 Dangerous to the ozone layer.
- R60 May impair fertility.
- R61 May cause harm to the unborn child.
- R62 Risk of impaired fertility.
- R63 Possible risk of harm to the unborn child.
- R64 May cause harm to breastfed babies.
- **R65 Harmful: may cause lung damage if swallowed.**
- R66 Repeated exposure may cause skin dryness or cracking.
- **R67 Vapours may cause drowsiness and dizziness.**
- R68 Possible risk of irreversible effects.

APPENDIX E

EC Safety Phrases

- S1 Keep locked up.
- S2 Keep out of the reach of children.
- S3 Keep in a cool place.
- S4 Keep away from living quarters.
- S5 Keep contents under ... (there follows the name of a liquid).
- S6 Keep under ... (there follows the name of an inert gas).
- S7 Keep container tightly closed.
- S8 Keep container dry.
- S9 Keep container in a well-ventilated place.
- S12 Do not keep the container sealed.
- S13 Keep away from food, drink and animal foodstuffs.
- S14 Keep away from ... (a list of incompatible materials will follow).
- S15 Keep away from heat.
- **S16 Keep away from sources of ignition.**
- S17 Keep away from combustible material.
- S18 Handle and open container with care.
- S20 When using, do not eat or drink.
- S21 When using do not smoke.
- S22 Do not breathe dust.
- S23 Do not breathe vapor.
- S24 Avoid contact with skin.
- S25 Avoid contact with eyes.
- **S26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.**
- S27 Take off immediately all contaminated clothing.
- S28 After contact with skin, wash immediately with plenty of soap-suds.
- S29 Do not empty into drains.
- S30 Never add water to this product.
- **S33 Take precautionary measures against static discharges.**
- S35 This material and its container must be disposed of in a safe way.
- **S36 Wear suitable protective clothing.**
- **S37 Wear suitable gloves.**
- S38 In case of insufficient ventilation, wear suitable respiratory equipment.
- **S39 Wear eye / face protection.**
- S40 To clean the floor and all objects contaminated by this material, use (there follows suitable cleaning material).

APPENDIX F

UN Hazard Codes

- Class 1 Explosive
 - 1.1 Substances with a mass explosion hazard
 - 1.2 Substances which present a projection hazard but no mass explosion hazard
 - 1.3 Substances which present both a fire hazard and a minor blast or projection hazard (or both) but not a mass explosion hazard
 - 1.4 No significant hazard
 - 1.5 Very insensitive substances with a mass explosion hazard
 - 1.6 Very insensitive articles with no mass explosion hazard
- Class 2 Gases
 - 2.1 Flammable gases
 - 2.2 Non-flammable, non-toxic gases
 - 2.3 Toxic gases
- **Class 3 Flammable liquids**
- Class 4 Flammable solids
 - 4.1 Flammable solids, self-reactive substances and solid desensitized explosives
 - 4.2 Materials liable to spontaneous combustion
 - 4.3 Substances which, in contact with water, release flammable gases
- Class 5. Oxidizing substances and organic peroxides
 - 5.1 Oxidizing agents
 - 5.2 Organic peroxides
- Class 6 Toxic and infectious substances
 - 6.1 Toxic substances
 - 6.2 Infectious substances
- Class 7 Radioactive substances and articles
- Class 8 Corrosive substances
- Class 9 Miscellaneous dangerous substances

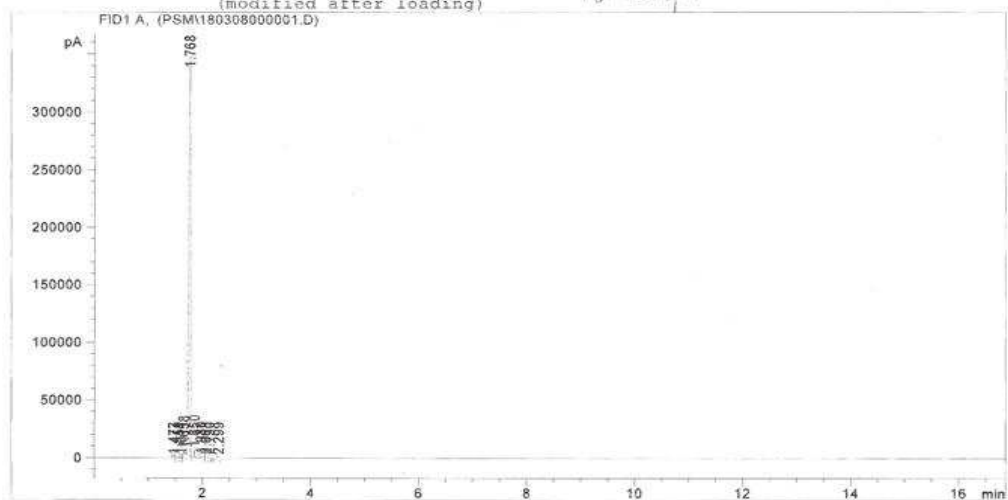
APPENDIX G

Result Chromatogram

Data File C:\CHEM32\1\DATA\PSM\180308000001.D
Sample Name: 98PA

```
=====
Acq. Operator   : NORA                      Seq. Line :    1
Acq. Instrument : Instrument 1              Location  : Vial 1
Injection Date  : 18/03/2008 11:25:06      Inj       :    1
                                           Inj Volume: 1 µl

Acq. Method     : C:\CHEM32\1\METHODS\ISOOCCTANE230108.M
Last changed    : 18/03/2008 11:04:51 by NORA
Analysis Method : C:\CHEM32\1\METHODS\DEF GC.M
Last changed    : 19/03/2008 11:30:05 by NORA
                  (modified after loading)
=====
```



Area Percent Report

```
=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.477	BV	0.0194	3.73417	2.83350	0.00047
2	1.559	VV	0.0295	227.13031	104.11143	0.02868
3	1.611	VV	0.0243	96.27958	55.42627	0.01216
4	1.658	VV S	0.0340	1.50068e4	5656.37842	1.89475
5	1.768	VV S	0.0370	7.69967e5	3.46753e5	97.21544
6	1.850	VB S	0.0143	6012.63037	6228.57861	0.75915
7	1.980	BV X	0.0144	32.08628	36.07384	0.00405
8	2.068	VV X	0.0244	17.38913	9.94302	0.00220
9	2.130	VB X	0.0176	657.23083	561.84955	0.08298
10	2.299	BB	0.0157	1.03004	1.02412	0.00013

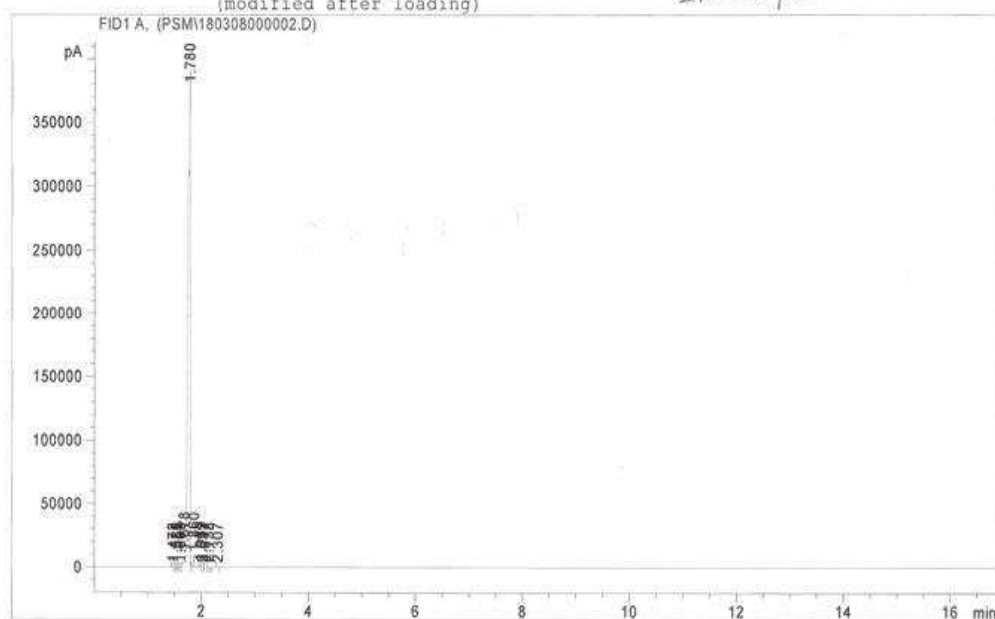
Totals : 7.92021e5 3.59409e5

Data File C:\CHEM32\1\DATA\PSM\180308000002.D
Sample Name: 200PA

```
=====
Acq. Operator   : NORA                      Seq. Line :    2
Acq. Instrument : Instrument 1              Location  : Vial 2
Injection Date  : 18/03/2008 11:48:42      Inj       :    1
                                           Inj Volume: 1 µl

Acq. Method     : C:\CHEM32\1\METHODS\ISOCTANE230108.M
Last changed    : 18/03/2008 11:04:51 by NORA
Analysis Method : C:\CHEM32\1\METHODS\DEF GC.M
Last changed    : 19/03/2008 11:30:05 by NORA
                (modified after loading)
=====
```

2nd sample



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.472	BV	0.0178	4.46343	3.78646	0.00037
2	1.529	VV	0.0184	99.57352	80.70969	0.00826
3	1.555	VV	0.0190	190.94455	159.47812	0.01583
4	1.608	VV	0.0222	132.09825	89.79237	0.01095
5	1.678	VV S	0.0335	1.92801e4	8820.38965	1.59878
6	1.780	VV S	0.0500	1.17697e6	3.92158e5	97.59833
7	1.860	VB S	0.0194	8131.28711	8329.32129	0.67428
8	1.989	BV X	0.0134	44.45758	49.70765	0.00369
9	2.022	VV X	0.0133	69.13501	78.32195	0.00573
10	2.077	VV X	0.0229	29.82965	18.39495	0.00247
11	2.138	VB X	0.0167	978.80133	898.07068	0.08117
12	2.307	BB	0.0159	1.69924	1.66136	0.00014

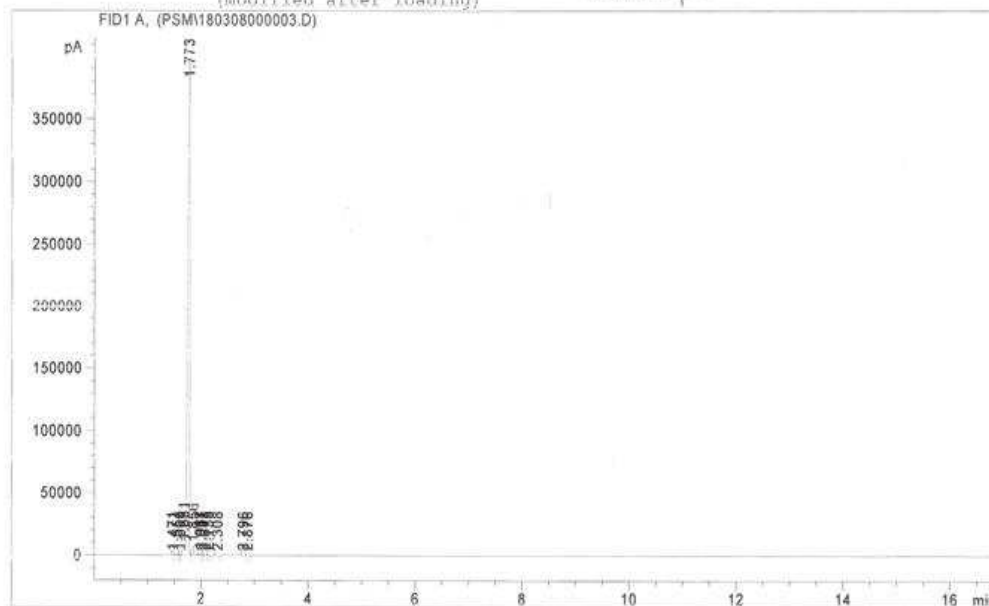
Totals : 1.20593e6 4.10688e5

2.307
- 2.290
0.017

Data File C:\CHEM32\1\DATA\PSM\180308000003.D
Sample Name: 300PA

```
=====
Acq. Operator   : NORA                      Seq. Line :    3
Acq. Instrument : Instrument 1              Location  : Vial 2
Injection Date  : 18/03/2008 12:12:17      Inj       :    1
                                           Inj Volume: 1 µl

Acq. Method     : C:\CHEM32\1\METHODS\ISOCTANE230108.M
Last changed    : 18/03/2008 11:04:51 by NORA
Analysis Method : C:\CHEM32\1\METHODS\DEF_GC.M
Last changed    : 19/03/2008 11:30:05 by NORA
                  (modified after loading)
3rd sample.
```



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.471	BV	0.0192	4.23257	3.46966	0.00039
2	1.554	VV	0.0292	261.21362	126.08791	0.02405
3	1.608	VV	0.0258	117.98956	69.42856	0.01086
4	1.681	VV S	0.0310	1.79983e4	7787.11084	1.65734
5	1.773	VV S	0.0449	1.05901e6	3.93241e5	97.51717
6	1.856	VB S	0.0202	7529.75830	6636.45215	0.69336
7	1.987	BV X	0.0207	52.57343	44.88389	0.00484
8	2.021	VV X	0.0170	60.76396	59.56838	0.00560
9	2.078	VV X	0.0264	30.01020	15.61306	0.00276
10	2.138	VB X	0.0208	894.45276	704.42517	0.08236
11	2.308	BB	0.0218	1.55715	1.22846	0.00014
12	2.796	BB	0.0273	5.69365	3.27900	0.00052
13	2.876	BB	0.0246	6.35030	3.98460	0.00058

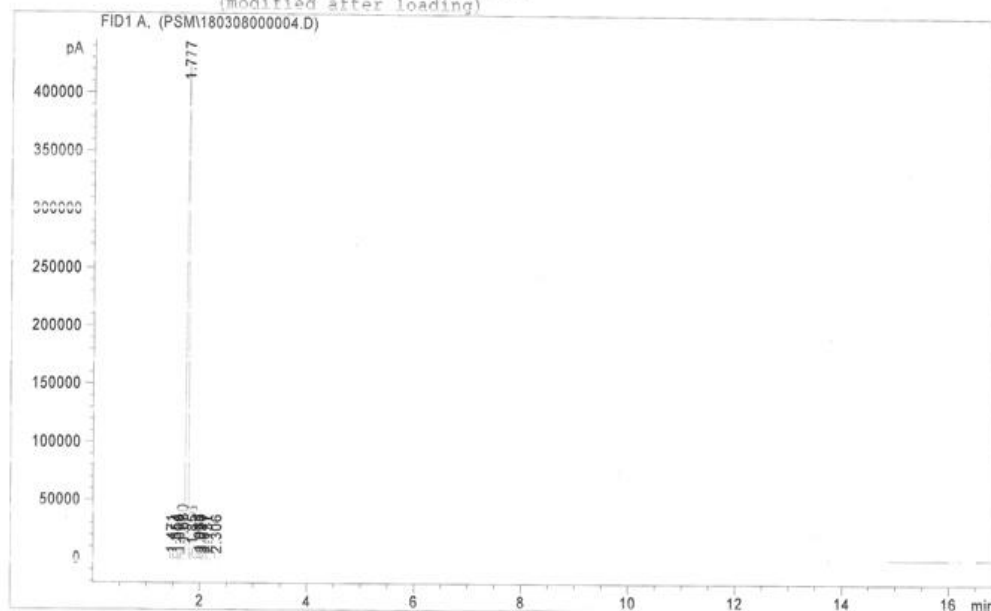
Totals : 1.08597e6 4.08696e5

Instrument 1 19/03/2008 11:43:39 NORA

Page 1 of 2

FILE C:\CHEM32\1\DATA\PSM\180308000004.D
 Sample Name: 330PA

```
=====
Acq. Operator   : NORA                      Seq. Line :    4
Acq. Instrument : Instrument 1              Location  : Vial 4
Injection Date  : 18/03/2008 12:35:56      Inj       :    1
                                           Inj Volume: 1 µl
Acq. Method     : C:\CHEM32\1\METHODS\ISOCTANE230108.M
Last changed    : 18/03/2008 11:04:51 by NORA
Analysis Method : C:\CHEM32\1\METHODS\DEF_GC.M
Last changed    : 19/03/2008 11:30:05 by NORA
                (modified after loading)
=====
```



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

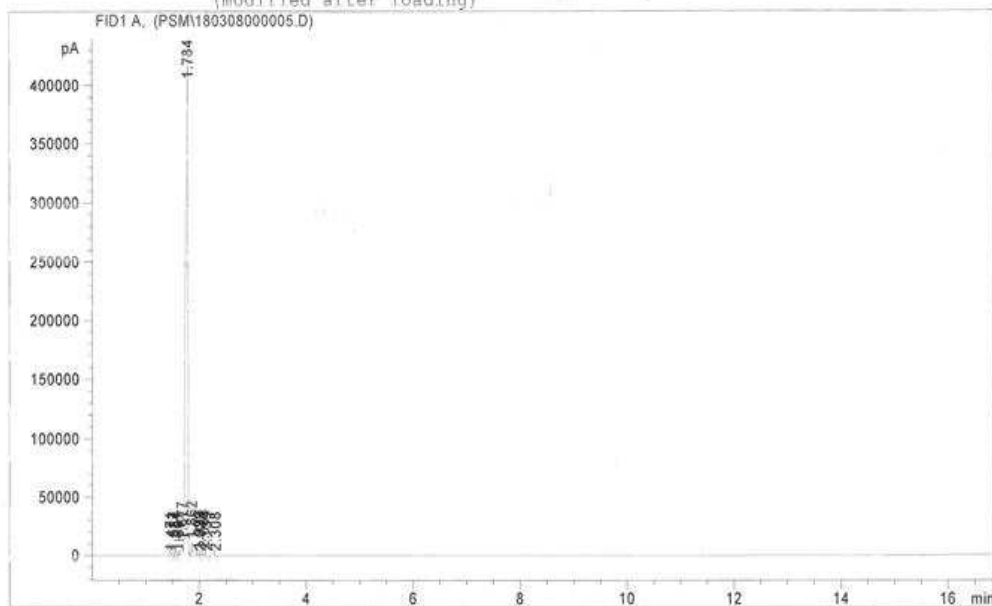
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.471	BV	0.0180	4.10852	3.42344	0.00035
2	1.554	VV	0.0286	277.70157	137.34618	0.02374
3	1.608	VV	0.0252	127.43944	77.30470	0.01089
4	1.680	VV S	0.0312	1.92941e4	8593.01270	1.64921
5	1.777	VV S	0.0443	1.14090e6	4.28794e5	97.52126
6	1.856	VB S	0.0180	8182.32813	7326.43115	0.69940
7	1.987	BV X	0.0173	44.14463	41.93139	0.00377
8	2.020	VV X	0.0168	68.24841	67.88493	0.00583
9	2.077	VV X	0.0245	33.27420	18.93506	0.00284
10	2.137	VB X	0.0201	965.77350	796.72125	0.08255
11	2.306	BB	0.0207	1.73327	1.37500	0.00015

Totals : 1.16990e6 4.45858e5

Data File C:\CHEM32\1\DATA\PSM\180308000005.D
 Sample Name: 350PA

```
=====
Acq. Operator   : NORA                      Seq. Line :    5
Acq. Instrument : Instrument 1              Location  : Vial 5
Injection Date  : 18/03/2008 12:59:29      Inj       :    1
                                           Inj Volume: 1 µl

Acq. Method     : C:\CHEM32\1\METHODS\ISOCTANE230108.M
Last changed    : 18/03/2008 11:04:51 by NORA
Analysis Method : C:\CHEM32\1\METHODS\DEF GC.M
Last changed    : 19/03/2008 11:30:05 by NORA
                  (modified after loading)
=====
```



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.471	BV	0.0159	5.24573	4.73137	0.00040
2	1.527	VV	0.0171	106.81397	94.81392	0.00806
3	1.554	VV	0.0187	220.89143	188.34250	0.01667
4	1.607	VV	0.0227	145.34619	101.50749	0.01097
5	1.677	VV S	0.0354	2.11993e4	9365.96875	1.59988
6	1.784	VV S	0.0520	1.29134e6	4.13578e5	97.45585
7	1.862	VV S	0.0135	8969.66309	9964.27832	0.67693
8	1.990	BV X	0.0127	52.67149	63.10130	0.00398
9	2.023	VV X	0.0143	76.27290	88.74428	0.00576
10	2.088	VB S	0.0131	1860.12720	2153.94019	0.14038
11	2.139	BB X	0.0158	1073.29834	1062.85510	0.08100
12	2.308	BB	0.0135	1.70571	1.89481	0.00013

Totals : 1.32505e6 4.36668e5

2.308
 - 2.290

 0.018