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**SUSTAINED DELIVERY SYSTEM OF CURCUMINOIDS RICH PLANT
CURCUMA LONGA, L FOR TOPICAL APPLICATION**

DISSERTATION

Submitted in partial fulfilment of the requirement of

MASTERS

In

APPLIED CHEMISTRY

In the

FACULTY OF CHEMICAL SCIENCE

Of the

UNIVERSITY OF JOHANNESBURG

By

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Signature:

September 2019

DEDICATION

This dissertation is dedicated to my late grandmother Kongkong Elizabeth Magaoganye who died of cancer, my mother Ramatladi Meriam Mphahlele, my father Dr Lethamaga Moses Mphahlele and my grandparents, Moraka and Nelson Sekokotla and Marumo Mphahlele for their support to continue with my studies and guidance. My siblings Tumelo Faith Mphahlele, Katlego Excellent Mphahlele and Fortunate Relebogile Moraka Mphahlele who gave me the motivation to carry on, I love you.



DECLARATION

I, Mokgadi Precious Mphahlele declare that this dissertation is the result of a two years program undertaken at the University of Johannesburg under the supervision of Associate Professor Derek Tantoh Ndinteh and the co-supervision of Dr Lerato Hlekelele.



Signature:

Date:

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ABSTRACT

The research conducted in this study was aimed at extracting and studying the most bioactive elements found in the Southern Asian plant known as *Curcuma Longa*, commercially is known as Turmeric. Curcumin is the most bioactive component of turmeric, it and other phytochemicals including essential oils, particularly the ones relevant for its topical application for skin care were studied. This plant was chosen because of its documented history as an effective active in skin care. This is because some of the plant's phytochemicals have high antioxidant and anti-inflammatory activities, providing skin with nutrients that can shield or protect it from environmental harm. The plant's antioxidant activity makes it useful as a free-radical scavenger. Free radical have oxidation properties that cause skin cancer and aging. During injury (inflammation) of skin, the anti-inflammation of the phytochemicals helps in repairing and healing the wounds. This has led to the wide use of *Curcuma longa* in cosmetics for wound healing, sun protection, and skin lightening.

The essential oils components of turmeric were extracted by the solvent extraction technique and they were studied by 2D GCxGC-TOF/MS. This was done in order to qualitatively study the various components of the essential oils and to quantify them. Various classes of compounds were identified, where it was observed that the essential oils component of turmeric consisted of mainly terpenoids, terpenes, and alkaloids. It was also found that most of these compounds had a chain length varied between 11 and 15 carbon atoms. Most of these 11-15 carbon atoms were identified as sesquiterpenoids. These results were consistent with that turmeric is used as a beauty product because these classes of compounds have been used in cosmetics because of their anti-microbial, antioxidant and therapeutic UV-induced skin care.

In another study, *Curcuma longa*, *L* was subjected to extraction with the aim of isolating curcuminoids. Curcuminoids is a term that encompasses 3 compounds, curcumin, demethoxycurcumin and *bis*-methoxycurcumin. The extraction was achieved by solvent extraction using various organic solvents and isolated by column chromatography. The characterization of the extracts was carried out using FTIR, UV-VIS, NMR. The fraction of interest was characterized by 3 spots observed on the TLC of the fraction. These spots were assigned to curcuminoids. On

the FTIR spectrum of the extract, the major peaks corresponding to the benzene ring, ketone, alcohol functional groups typical of curcuminoids were observed. On UV-Vis analysis of the fraction yielded a spectrum that showed a strong absorption at 410-421 nm which is due to its wide electron delocalization, also typical of curcuminoids. ¹H NMR was used to confirm these results. On NMR the major peaks assigned to methoxy (-OCH₃), phenol of curcumin were observed.

Curcumin which was isolated along with its relatives is the most bioactive component of turmeric but its application is limited by its poor solubility, low bioavailability and it degrades when exposed to sunlight. In order to overcome these disadvantages, inclusion complexes of this compound and β-Cyclodextrin were synthesized using various methods. The inclusion of curcumin inside the cavity of β-Cyclodextrin was studied and characterized UV-vis, FTIR, NMR (¹H NMR and NOESY), PXRD and TGA-DSC. The inclusion complexes were successfully synthesized, with the entrapment of curcumin benzyl rings inside the cavity through the β-Cyclodextrin internal cavity protons H3 and H5. This complex makes it useful in sustained release of the active ingredient in a controlled manner in topical applications



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CHAPTER 1. INTRODUCTION

1.1. Introduction

The defensive and impermeable characteristics of the skin shield human body from dehydration, broke down proteins and minerals as this will happen quicker when the human body is not protected from our surroundings (Souto and Müller, 2008). This requires that the skin is nourished as it is a vital organ. The nourishment of the skin is provided by some bodily mechanisms. However, the human skin is susceptible or is at risk of its functions being aggravated by some nutrient deficiencies, unsettling influences of endocrine organs and environmental factors (Souto and Müller, 2008). In circumstances such as this, the skin's natural defenses may not be adequate necessitating that foreign products be used to protect the skin. In cases such as these, products with relevant pharmacological activities are vital hence the popularity of the cosmetic industry. Cosmetic products are very essential to the skin's protective function, for example, protection against UV radiation using sunscreen, which will prevent as well premature skin aging and skin cancer (Michalun and Dinardo, 2014). Lotions and creams that contain antibacterial properties control or ease the excessive proliferation of bacteria on the skin, which is a problem associated with oily skin and a leading cause of development of acne (Michalun and Dinardo, 2014). Furthermore, the formation of a barrier on the skin's surface using cosmetics products with some moisturizing ingredients assists the skin with retaining moisture thus lessening dehydration (Michalun and Dinardo, 2014).

Many of the actives used in cosmetics are synthetic, these are often synthesized in ways that are not environmentally friendly and many are not biodegradable. Scientists have for this reason looked to natural products to find actives that are environmentally friendly and sustainable. *Curcuma longa*, L. is a plant commonly found in Southern Asian countries. This plant is commercially known as turmeric and it is commonly used as a spice and for medicinal purposes. Furthermore, turmeric is renowned in many cultures for its beautifying properties. This plant contains a variety of essential oils and polyphenols which have been shown to have a variety of pharmacological and beautifying properties. The essential oils extracted from *Curcuma longa*

consist mainly of terpenes (sesquiterpenes), terpenoids (sesquiterpenoids) and alkaloids. These 3 classes of compounds have therapeutic properties on skin. Of the major terpenes found in this plant are turmerone, curcumene, cymene, cineole and etc. Curcuma longa's essential oil are also have potential in food industry as dye for ice cream, mustard, and so on. Their high efficiency at very low concentrations, make them a preservative for storage of food.

A popular example of a group of bioactive components of turmeric polyphenols is known as curcuminoids. This is the case because these compounds are highly antioxidant in nature. This is particularly true for one kind of curcuminoids called curcumin which has been shown to be an even stronger antioxidant than vitamin E. Curcumin is known to be beneficial in cosmetics and skin care product for skin protection and as a natural skin lightener (Prakash and Majeed, 2009, Kyrou et al., 2003, Handog and Macarayo, 2011). Moreover, the skeleton structure of curcumin has a diene ketone that makes it lipophilicity thus it can penetrate the skin easily (Jayaprakasha et al., 2006). The addition of actives such as curcumin in cosmetics is popular and has fuelled the expansion of the cosmeceutical industry.

Unfortunately, many of the actives used for protecting the skin's integrity are unstable and sensitive to environmental factors. Furthermore, the actives of cosmetics aim to have a predominantly local effect and therefore, it's undesirable for the actives to be absorbed into the bloodstream (Souto and Müller, 2008). This means that careful thought has to be put into how to preserve actives and how they should be administered in a healthy way. Encapsulation of the actives is an effective way to achieve this. Encapsulation protects against unwanted degradation and also targets a specific region for the release of active substances at a regulated rate (Ammala, 2013).

Cyclodextrin inclusion complex is used to encapsulate lipophilic water-insoluble drugs in order to form water-soluble inclusion complexes. Cyclodextrin is a non-toxic cyclic polysaccharides and forms inclusion complex with a number of organic molecules (Buschmann and Schollmeyer, 2002). The different Cyclodextrin molecules are made of cyclic oligosaccharides with 6 (α), 7(β), 8(γ) and 9(δ) glucopyranose units (de Paula et al., 2011). Of the four Cyclodextrin, β -Cyclodextrin is mostly used (Mangolim et al., 2014) because of its low cost, availability and that its cavity fits common guests with molecular weights between 200 and 800 g/mol. Cyclodextrin has gained popularity in drug delivery as a complexing agent because it is able to interact with water-insoluble

drugs resulting in an increase in water solubility (Brewster and Loftsson, 2007). Complexing actives with Cyclodextrin also increases their stability and bioavailability. The major benefits of this are i) the reduction of the absorption of the drug into the bloodstream, ii) the release of the active can be controlled and made gradual, and iii) increase in the bioavailability of the active (Loftsson and Masson, 2001). This research makes use of β -Cyclodextrin as a delivery system for the encapsulation of the active drug, curcumin.

1.2. Problem Statement

Overexposure to sunlight accelerates premature aging and wrinkling of skin which may result in skin cancer. This along with other issues which affect the human skin necessitates that cosmetic products be used to help the skin fulfill its purpose of protecting the human body. Some of the products in the market used for assisting the skin in accomplishing its duties are made of products that are environmentally unfriendly, that are expensive, sensitive and may have side effects.

Curcumin, on the other hand, is an active drug offering a wide spectrum of pharmacological activities but its clinical applications are limited by several factors, these include poor solubility, poor bioactivity, low absorption, low bioavailability and instability in neutral and alkaline aqueous solutions and high metabolism rate. These disadvantages limit the use of an otherwise effective active, curcumin and means to address these disadvantages are highly sought out.

1.3. Justification of Study

Turmeric has historical use in the Indian culture, where most Indian women used it for their facial skin (applied topically) for beautifying purposes and for the prevention of sunburn and hyperpigmentation (Remadevi, 2007). Curcumin which is one of the most biologically active components of turmeric is non-toxic with fewer side effects when administered orally or topically. Curcumin is also a natural polyphenol making it a strong antioxidant and a good drug for the treatment of cancer, inflammation and so forth. Curcumin strong antioxidant properties are comparable to those of vitamin C and E (Maheshwari et al., 2006). It is also suggested that curcumin acts at different levels to enhance wound repair (Maheshwari et al., 2006).

Unfortunately, as it was mentioned earlier that the major problems of curcumin are its low bioavailability and this necessitates that its administration is altered so it can be used effectively. One of the most effective ways of increasing bioavailability of lipophilic drugs is by altering their solubility. This strategy suffers from a serious flaw as the process may alter the properties of the drug that makes the drug potent. Therefore, changing the bioavailability of curcumin without compromising their efficacy is what this research aims to address through the use of cyclodextrin as a complexing agent for the actives.

This special structural characteristics of Cyclodextrin of hydrophilic outer surface and a hydrophobic central cavity is the reason why it is commonly utilized to improve the solubility and bioavailability of hydrophobic guest molecule (Saikia et al.).

The hydrophobic cavity shield the hydrophobic guest molecule from aqueous environments, while the polar outer surface of Cyclodextrin provides the solubilizing effect (Saikia et al.). Cyclodextrin and its derivatives have been utilized for a wide range of uses in beauty care products from masking of odours, release profiles of fragrances, stabilizing drugs and etc (Ammala, 2013).

Curcumin phenyl rings were found to be entrapped inside the β -CD cavity meaning that there was formation of inclusion complex between the guest and host (Mangolim et al., 2014). The complex protects the encapsulated material and releases the encapsulated material more effectively in a controlled manner. The complex is biocompatible, biodegradable and non-toxic, permitting its administration to be repeated as a therapeutic agent (Gazori et al., 2009). The entrapped particle will adhere to the skin surface and transport the drug in a more controlled fashion. Controlled drug release and subsequent biodegradation are central for developing successful formulations.

The image below illustrates the comparison of the delivery of an oily active in a conventional manner and an encapsulated product onto the human skin (**Figure 1.1**). The delivery of the conventional product is not as prolonged and it only reaches the epidermis and does not penetrate to the dermis. The delivery of the encapsulated product is protected and prolonged inside a sphere which is made up of the core (containing an active ingredient inside) and shell. The hydrophobic quality of the sphere sustains the rate of diffusion of the active ingredient, which allows their release over an extended period of time. In addition, the substance to be delivered does not have to be soluble in the vehicle since it can be dispersed in the solid. The encapsulated product is

delivered to the epidermis where it ruptures and delivers the encapsulated product to the target side which is the dermis where it is released slowly.

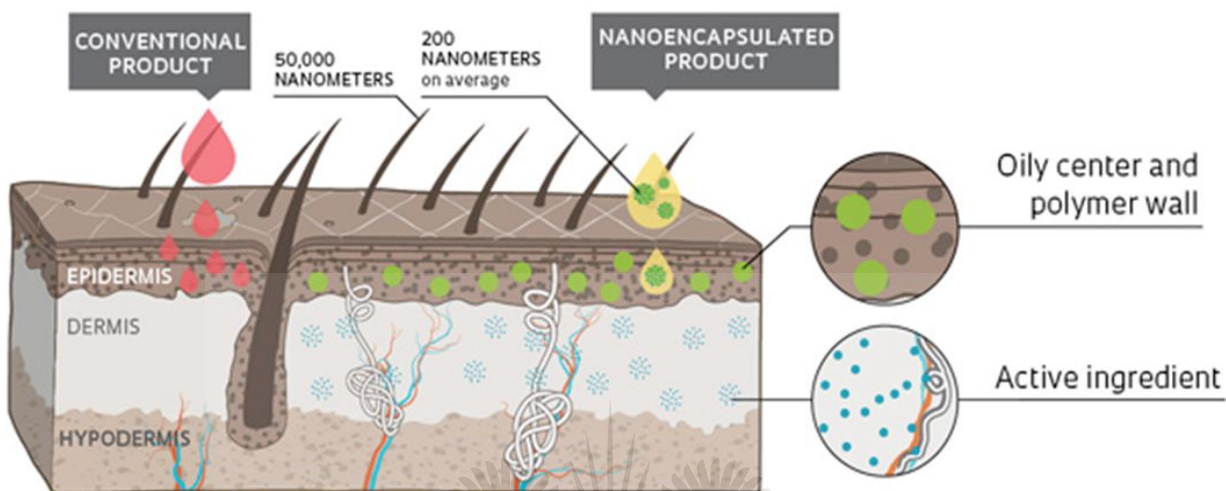


Figure 1.1 Delivery of drugs or active ingredients on the skin (Gupta et al., 2013)

The aim of this research was to use the β -Cyclodextrin to form inclusion complex that will sustain curcumin so as to deliver it at the desired rate. The point of interest of using polymers that are biodegradable in cosmetics applications over synthetic ones is that they are non-responsive and non-toxic when in contact with the body. In contrast, synthetic polymers have a potential of accumulating in different body tissues and cause disturbance.

1.4. Aims and Objectives

1.4.1. Aim:

The main purpose of the study was to develop a sustained release system for topical applications of curcumin using a biodegradable polymer β -Cyclodextrin.

1.4.2. Objectives:

In order to achieve the aim of this study, the following objectives were considered:

1. To extract phytochemicals curcuminoids from *Curcuma longa*, L.
2. To isolate and analyze the extracted curcuminoids using chromatographic analysis.
3. To characterize the isolated curcuminoids using FTIR, UV-VIS, NMR (¹H NMR).
4. To study the secondary metabolites using of the plant essential oils collected from the column using Comprehensive 2D GCxGC-TOF/MS.
5. To prepare and form inclusion complex of the isolated curcumin with β-Cyclodextrin.
6. To characterize the encapsulated drug using FTIR, UV-Vis, SEM, TEM, PXRD, NMR (¹H NMR and NOESY), TGA-DSC.



Dissertation Outline

Chapter 1

This chapter introduces the research undertaken, giving background information on the field of study while covering the problem statement associated with skin and the use of the active drug, curcumin, isolated from *Curcuma longa* and their solutions. The chapter is finalized by presenting the aims and objectives of the study.

Chapter 2

Chapter two covers a literature review on cosmetic industry and their interest in the use of natural products, a representation of human skin, use of botanicals in skin care, background on the plant curcuma longa used in this research and its phytochemical constituents (essential oils, curcuminoids, curcumin) and their pharmacological activities, and lastly the use of delivery systems using Cyclodextrin inclusion complexes.

Chapter 3

This chapter reports on the extraction, isolation, and characterization of the plant constituents (essential oils, curcuminoids, and curcumin). The plant was extracted using solvent extraction and chromatographic techniques followed by characterization.

Chapter 4

In this chapter the essential oils thus the secondary metabolites extracted in chapter 3 were further investigated and studied using Comprehensive 2D GCxGC/TOF-MS instrument.

Chapter 5

Chapter 5 discusses the inclusion complex of the extracted curcumin with β -Cyclodextrin and also comparing the different methods used to form the inclusion complexes by characterization.

Chapter 6

This chapter concludes on the findings obtained in the study, recommendations and their references. Then appendix

CHAPTER 2. LITERATURE REVIEW

Curcuma longa plant extracts, their activities and Curcumin as an antioxidant, anti-inflammation, anti-cancer and anti-microbial on skin

2.1. Introduction

The cosmetic industry is now incorporating natural product extracts into their materials, thus they are branching into cosmeceuticals. The core of the cosmeceuticals industry is to make beauty products that will provide the skin with essential natural products like vitamins, oils, and therapeutic extracts with the purpose of healing, restoring and protecting the human skin.

Coincidentally or by design, beauty products consumers have shown interest that is beyond elegance by seeking cosmetic products that are able to relax, detoxify, moisturize, stimulate, balance and strengthen hair and skin.

Consumers are also interested in skin care products that nourish the skin with necessary natural nutrients. Consumers are in particular looking for nutrients such as antioxidants which protect the skin from environmental factors such as sunlight, smoke, and other pollutants, that may result in the depletion of vitamin C on the skin (Souto and Müller, 2008). These needs of the consumers have necessitated that there be investigations on how natural products could be used in cosmetics. Indeed, this high demand of natural or herbal medicines is also because of that they are made from herbs and shrubs which are reported to have small negative impacts on the human body and improves the body with nutritious supplements (Gediya et al., 2011).

The skin is a vital organ and as such, it should be well taken care of by ways of nourishment as any organ in the body. Such nourishment is usually provided by the body and also by the use of cosmetic formulations that contains natural nutrients (Souto and Müller, 2008). Some cosmetic products have been formulated with antioxidants which protect, rejuvenate and moisturize the skin. Skin make use of these nutritional antioxidants as a protection against free radical damage (BURKE, 2006). Antioxidants are particularly vital in skin care because they minimize cell damage triggered by free radicals, and therefore aid in preventing aging of skin. This has led to

antioxidants being encapsulated in a spectrum of cosmetics from sunscreens, creams, gels and moisturizers products. Therefore, antioxidants are intensely used as a means of preventing skin from aging and damage. Antioxidants which are mostly sourced from plant materials don't just advance and re-establish a typical physical boundary, but additionally help the skin to battle and set itself up against animosity and wounds (Khaiat and Saliou, 2015).

Turmeric is a prompt source of biological active compounds like antioxidants and polyphenols especially flavonoids. Polyphenols have strong antioxidant properties that derives from their high reactivity as electron donors or hydrogens (Dreher, 2015). Moreover, polyphenolic compounds possess anti-inflammatory activities and also beneficial properties for damaged and aged skin (Dreher, 2015). The high activity of antioxidant in turmeric justified its usage in a wide spectrum of applications in plant-medicine, nutraceuticals, and cosmetics; with skin care being the major domain of this aromatic plant (Paulucci et al., 2013).

Additionally to polyphenols, the essential oils of natural products are of great interest in cosmetics as well. Plant's secondary metabolites produces essential oils which are utilized by humans as functions of food in biopolymers, nutraceuticals, nutritional supplements (dietary supplements, culinary), medicines (pharmaceuticals, therapeutic products), manufactured in cosmetics (skin care, aromatherapy, perfumes and etc) and as food additives used in flavourings as antimicrobial and antioxidant (Zengin and Baysal, 2014).

Because of essential oils high efficiency at very low concentrations, they have potential to be added to food as a preservative for storage of food (Mehdizadeh and Moghaddam, 2018). This is vital because essential oils have anti-microbial, anti-mutagenic, antioxidant, insecticidal activities. Therefore this dissertation aims to investigate the polyphenols and essential oils in turmeric and also reports on the encapsulation of one the most bioactive compound isolated from this plant using Cyclodextrin-based delivery systems.

There are limitations with the way that biologically active products are administered and this has necessitated the use of novel delivery systems to encapsulate the active ingredients. The growth interest of plant actives and extracts to be used in delivery systems is derived from their low efficacy in physiological conditions. The low efficacy of these materials is because of their low bioavailability and absorption, elimination and rapid metabolism (Saraf, 2010).

Encapsulating actives in delivery systems helps in to minimize the degradation and loss of the actives. It also prevents harmful side-effects, increases the bioavailability of the actives and also enables the targeting of a specific area and sustain the release of the active substance in a controlled manner.

Polymers that are biodegradable are valuable for delivering drugs, hence they have been utilized in delivery systems in light of their versatility, better efficacy and bioavailability (Ammala, 2013) (Hans and Lowman, 2002). In cosmetic applications, biopolymers specifically polysaccharides have advantages over synthetic polymers (which could gather in different body tissues and cause disturbance) because they are non-responsive when in contact with the body via normal metabolic pathways, they are also biodegradable, biocompatible, non-toxic, hydrophilic and have protective properties (Ammala, 2013).

Cyclodextrin was used in this research to encapsulate and improve curcumin's stability and bioavailability. Cyclodextrin is non-toxic naturally occurring polysaccharide produced from starch (Buschmann and Schollmeyer, 2002). Cyclodextrin forms complexes with a variety of materials or actives in their interior cavity. Cyclodextrin-based complexes also protect actives against oxidation and degradation from light or heat and they also increase the shelf life of actives. Furthermore, these kinds of complexes can be designed in a way that they can be used for the controlled release of the actives to the targeted environment (Amiri and Amiri, 2017). The benefits of complexing actives with Cyclodextrin are a lot as it also increases the solubility of lipophilic actives (Hougeir and Kircik, 2012).

In cosmetics, Cyclodextrin functions as odour absorbent by masking the smell of an ingredient, a stabilizer for fragrances, dyes and reduces the foam in cosmetics, toiletries, and food (Szejtli, 1982). Moreover, Cyclodextrin limits the use of preservatives in formulations given its characteristics to enhance, protect and improve the physical and chemical characteristics of the guest compound.

2.2. Skin brief overview

The skin is the largest organ of the body (represented in **Figure 2.1**), carrying a sequence of important functions resulting from numerous physical and chemical reactions which happens inside it. As an excretory function, skin eliminate harmful or toxic substances by secretion of sebum and sweat (Michalun and Dinardo, 2014). As a protective barrier, skin protects the body from foreign elements, injury, and oxidation. It also important for regulating the human body temperature as it aids the body to adjust to ambient temperatures changes and atmospheric conditions through regulation of loss of moisture.

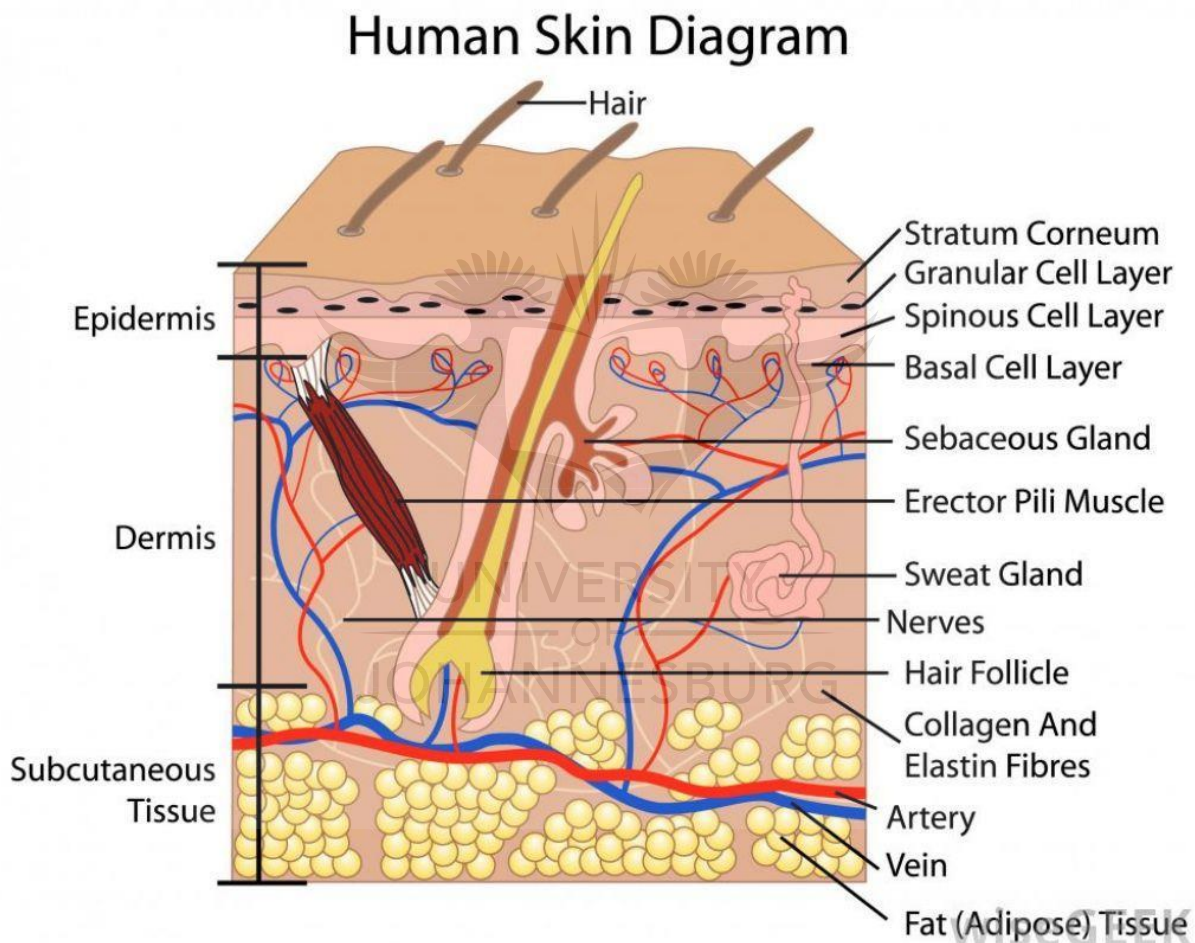


Figure 2.1 Structure of human skin

Furthermore, the skin assumes an immunological job, principally through the Langerhans cells, which deliver antigens from the skin to the lymphatic system (Michalun and Dinardo, 2014). Extreme ultraviolet rays have potential to either inhibits or destroy the performance of Langerhans

cells, increasing skin cancer risk (Michalun and Dinardo, 2014). This occurs because UV rays when in contact with the skin depletes vitamin C in the skin thereby triggering an increase in melanocyte-stimulating hormone (MSH) (Burke, 2006). The MSH ties to a receptor on melanocyte skin cells called the melanocortin 1 receptor (MC1R) and darkens the skin through the production of melanin (Burke, 2006). As a protective layer and a vital organ of the body, skin has its limitations and can still be damaged by UV light-induced reactive oxygen species (ROS).

The harm occurs when skin is overly exposed to UV rays resulting in ROS and reactive nitrogen species (RNS) formation. These radicals make contact by reacting with biomolecules of skin (Dreher, 2015). Radicals that are induced by UV radiation encourages not only skin harm such as sunburn, photo-toxicity, and photo-allergy but also dermatitis (Arakane and Naru, 2015, Briganti and Picardo, 2003, Matsuo et al., 1983, Hayaishi and Imamura, 1988). These radicals disrupt the regulatory mechanisms of common inflammatory genes, including nuclear factor-Kb (NF-kB) and activator protein-1 (AP-1) which are main transcription elements in the oxidative stress reaction (Arakane and Naru, 2015). These shortfalls of the skin have necessitated that means to address them be sought out, thus the popularity of the cosmetic industry.

2.3. Cosmetics, Cosmeceuticals and their Natural and Synthetic ones

Cosmetic is defined according to the European Union as any substance or preparation anticipated for use on the external part of the human body and oral cavity, to deliver a purpose of protection, beautifying, cleaning, skin lightening, perfuming and while also providing health benefits (Nohynek et al., 2010). Cosmeceuticals are described as cosmetics containing biologically active products and ingredients that have medicinal properties (Thaman, 2006). Cosmeceuticals are making waves in the industry as they involve the incorporation of botanicals into them and this provides the skin with proteins, essential oils, terpenoids, hydrocolloids, vitamins, antioxidants and other bioactive molecules (Kapoor, 2005).

Natural cosmetics contain pure raw materials; they are environmentally friendly, biodegradable, low toxicity and cause fewer side effects. For these reasons, they are employed in cosmeceuticals for beautifying and maintaining the physiological balance of human skin. However, they have

short shelf-life and require preservatives. Synthetic ones, on the other hand, have longer shelf-life but improper use of them may cause serious problems and the resulting chemical waste puts the environmental at risk. There are more preservatives in synthetic cosmetics which may cause allergic and irritant reactions (Chen, 2009). Topical application of both natural or synthetic cosmetics involves some degree of risk such as irritation, sensitization or photoreactions (Nohynek et al., 2010). However, sustainability issues, regulatory pressures and consumer desires have led to the need for development of cosmetics using primarily plant-based, renewable resourced raw materials.

2.4. Botanicals in Cosmetics

Natural products from animals, plants, microbes, or of mineral origins have documented history in traditional medicines and as a new drugs (Amalraj, 2016). The most important aspect of the biological activity is the plant source material because each plant part may contain hundreds of different chemicals, ions, and molecules (Thornfeldt, 2006). Therefore, there has been a growing attention in using botanical extract from different parts of plants (i.e. bark, fruit, leaf, seeds *etc*) as cosmeceutical, preventing and minimizing aging and diseases and as well as in nutraceuticals (Ebeler and Mitchell, 2015). A number of compounds extracted from different parts of plant materials have beneficial medicinal effects on humans.

Botanicals are mainly used for the treatment of signs and symptoms of diseases rather than for reversing the disease dissection. Botanical extract according to the cosmetic industry, is the active ingredient that improves skin moisturization, brightens and soothes the skin, reduces aging or cellulite signs and make scars less noticeable (Khaiat and Saliou, 2015). The extract is also used in the cosmetic industry to thicken, stabilize or preserve and emulsify products. For example, coconut oil from the seed or fruit of *Cocos nucifera*, family *Arecaceae*, is used to soften and moisturizes dry skin. The root of *Rhodiola* from *Rhodiola rosea* is used in anti-aging treatment. The roots, stems, and leaves of *Echinacea purpurea* are used for skin regeneration and turmeric, *Curcuma longa*, *L* is used on the skin to produce golden glow (Gediya et al., 2011). In dermal application, *Mahonia*, *Hypericum*, tea tree oil, *Glycyrrhiza*, and *Saccharomyces* are used to treat atopic dermatitis and acne (Reuter et al., 2010).

Botanicals provide biologically active molecules necessary to keep the skin healthy (Kapoor, 2005). Botanical extracts from herbs, fruits, vegetables, are used in oral administration and topical application to provide skin with protection against effects caused by UV radiations, thus early aging, cancer and induced erythema (Reuter et al., 2010). Black and green tea leaves from *Camellia sinensis* are known for their health-protecting antioxidants effects (Gediya et al., 2011). In this work, we investigate the polyphenols and essential oils in *Curcuma longa*.

2.5. Historical Background and uses of Aromatic Plant, *Curcuma longa*, L (Turmeric)

Curcuma longa L., commercially known as turmeric, belonging to ginger (*Zingiberaceae* family) (Chattopadhyay, 2004), is a perennial plant having a short stem with big elliptical leaves and ovate rhizomes, which are often branched (Nisar, 2015). The plant is yellow-orange in color (Premavalli, 2007) (**Figure 2.2**). *Zingiberaceae* accounts for more than 70 *Curcuma* varieties originating from Southeast Asian countries (Afzal, 2013). This plant is mostly cultivated in India, followed by other countries in the Southeast Asia (Shrishail et al., 2013, Amalraj, 2016). India is the one that largely produces, consumes and export this plant. It is grown on a small scale in America, Pacific Ocean Islands and Africa, America and Pacific Ocean Islands (Shrishail et al., 2013). Plants belonging to the *Zingiberaceae* family have known history to have strong anti-inflammatory, antioxidant and many biological properties and therefore many of these plants are used for medicinal purposes (Afzal, 2013, Ammon, 1991).



Figure 2.2 *Curcuma longa* (a) leaves and (b) rhizome(El-Sayed and Safar, 2014)

The name *Curcuma* is derived from either or both its Arabic term (Kurkum) or the Hebrew term (Karkom) meaning yellow (Meng et al., 2018). Whereas the name *longa* comes from the rhizome's elongated shape (Meng et al., 2018). The genus *Curcuma longa* have many taxa which are of economical importance as food, condiment, coloring agents, medicinal and ornamental materials (Skornickova, 2004, Shrishail et al., 2013). The plant have yellowish-orange color rhizome, which can be attributed to its commercial uses in spice that is called turmeric (Damalas, 2011). Turmeric is the commercial name for *Curcuma Longa*. Turmeric is related to many other *Curcuma* species with the main ones being *Curcuma amada* Roxb., *Curcuma angustifolia* Roxb., *Curcuma aromatica* salisb., *Curcuma caesia* Roxb, *Curcuma zedoaria* (christm.) Rosc., that are used as herbal or tribal medicine (Ravindran et al., 2007). The Linnaeus describe turmeric as *Curcuma longa* by the following taxonomic positions below:

Table 2.1 *Curcuma longa* taxonomic position

Class	<i>Liliopsida</i>
Subclass	<i>Commelinids</i>
Order	<i>Zingiberales</i>

Family	<i>Zingiberaceae</i>
Genus	<i>Curcuma</i>
Species	<i>Curcuma longa</i>

The root powdered form of turmeric is utilized in the food industry as a coloring ingredient, to preserve food and in spices (Damalas, 2011). The name turmeric originates from The Medieval Latin originated the term turmeric naming it *terramerita*, which then in French became *terre merite*, meaning meritorious earth or earth deserving (Ravindran et al., 2007). The Indian tribe refer to turmeric as a medicinal plant used in socio-religious practices having documented history of 6000 years in that area (Nisar, 2015) (Shrishail et al., 2013). Turmeric with a colorful yellow, has a characteristic fragrance and a bitter and slightly acrid taste (Sarker and Nahar, 2007), and these characteristics are the reason why it is used as a spice (Premavalli, 2007). In the Sanskrit language, turmeric has about 55 synonyms associated with its medicinal or religious uses (Ravindran et al., 2007). To name a few Sanskrit synonyms of turmeric that indicate its color enlightening ability, *varna-datri*: which means giving color, indicating its application as body complexion enhancer, *hemaragi* and *hemaragini*: both indicating a golden color, used by women folks for its golden complexion, *yoshti priya*: indicates its use for enhancing beauty, meaning favorite of young women and *hridayavilasini*: meaning giving delight to heart, charming (Shrishail et al., 2013, Ravindran et al., 2007). In English, turmeric was identified as an Indian saffron and a roof of yellow color (Ravindran et al., 2007).

Turmeric uses differs from a country or culture. In all South Asian countries, it has historical uses in traditional medicine and in food (Chattopadhyay, 2004). It is also used for ritual purposes. It was extensively used in old Hindu for medicinal purposes to treat injuries (Ammon, 1991). In the past, turmeric and its wild relatives, *C. aromatic*, were used as a dye (Ravindran et al., 2007). In recent years, turmeric coloring properties coming from its bioactive ingredient, curcumin, made entry in the food industry as safe for ice creams, mustards, cereals, cheese, yogurt, spices, pickles and so forth (Ravindran et al., 2007).

Medical application of turmeric range from its use in cosmetic creams for sun protection to the prevention of Alzheimer's disease (Ravindran et al., 2007). Research findings have shown that turmeric is not toxic to humans even when taken continuously at a dose of 8000 mg/d (HSIEH,

2001, Ravindran et al., 2007). Traditionally, the Indians used turmeric as medication to treat diabetic wounds, anorexia, cough, sinusitis, coryza amongst other medical conditions (Chattopadhyay, 2004). In Nepal the powdered rhizomes are used for treatment of wounds, bruises, inflamed joints and sprain (Surh, 2002). Chinese people use turmeric for diseases associated with abdominal pains (Chattopadhyay, 2004, Araujo, 2009). Reports on a mixture of turmeric with other plants are known to purify blood and heal pain associated with menstrual-abdominal (Eigner, 1990). There are also reports showing turmeric to be anti-diabetic, anti-inflammatory and effective against blood-related diseases (Remadevi, 2007).

Data also suggests that when turmeric powder is administered as capsules to patients with respiratory disease, it relieves the patients from symptoms like dyspnoea, cough, and sputum (Chattopadhyay, 2004). Some of the traditional medicinal uses of turmeric are shown below in

Figure 2.3.

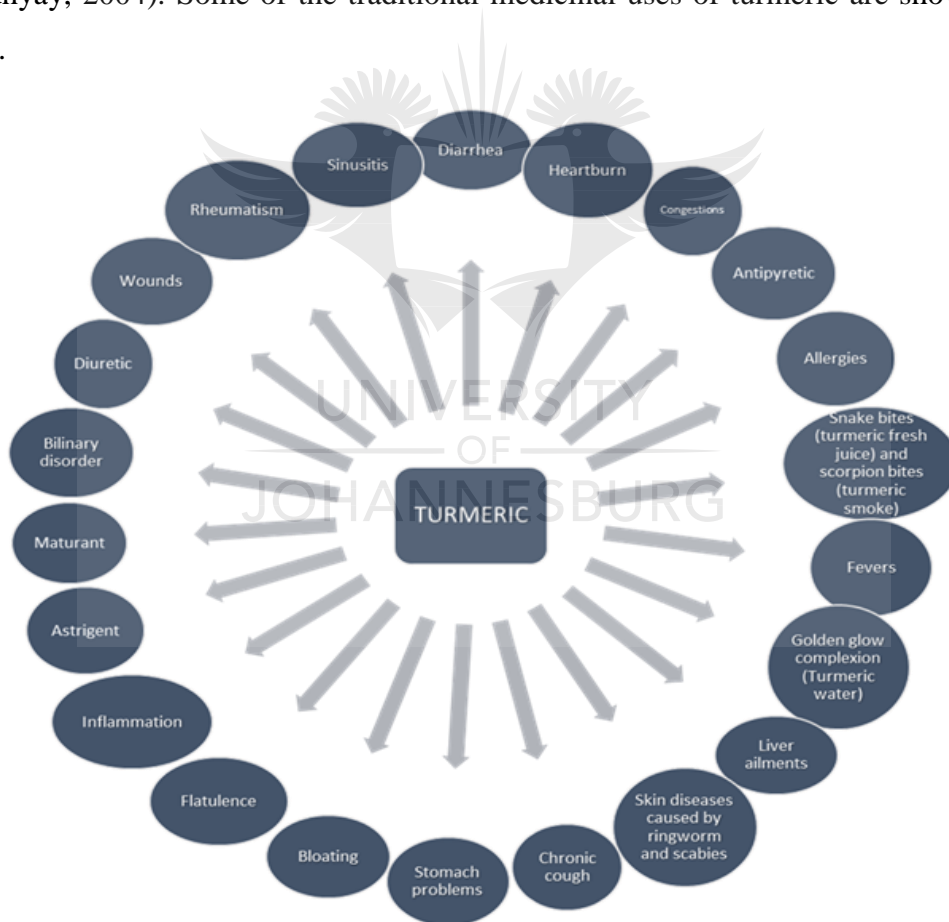


Figure 2.3 Traditional medicinal uses of turmeric

2.5.1. Phytochemistry/Major Chemical Constituents of Turmeric

Plants have active/bio-active components which give them recognition in traditional and modern medicine, cosmeceuticals and nutraceuticals. Turmeric as well has active compounds that are responsible for its popularity and widespread usage. The most biological active groups of compounds in Turmeric are curcuminoids, monoterpenoids, and sesquiterpenoids (Amalraj, 2016, Meng et al., 2018, Nisar, 2015). Turmeric has other constituents which are carbohydrates (69.4%), moisture (13.1%), proteins (6.3%), fats (5.1%), minerals (3.5%) and essential oils (Amalraj, 2016) (Nisar, 2015). The volatile component of turmeric which includes essential oils consists of mainly turmerone, zingiberene, curone (β -turmerones), α -turmerone and various monoterpenes and sesquiterpenes (Premavalli, 2007).

2.5.2. Turmeric essential oil constituents

The essential oils component of *Curcuma* species mainly consists of sesquiterpenes and monoterpenes. Many of the specific kinds of the individual sesquiterpenes and monoterpenes are particular to the *Curcuma* genus. The essential oil component of this plant contains most of the major terpenes including α -turmerone, *p*-cymene, α -turmerone, α -curcumene, β -turmerone and β -curcumene (Premavalli, 2007). Furthermore, within *Curcuma longa* species different volatile oils are extracted in various parts of the plant, for example the rhizome oil of turmeric has 84 constituents, some of the main constituents include turmerone, cineole, caryophyllene, sesquiphellandrene and α -turmerone (Premavalli, 2007). Sabinene, borneol, α -phellandrene, cineol, sesquiterpenes, and zingiberene are some of the other rhizome oil constituents (Nisar, 2015). On the other hand, oil from *Curcuma* leaf contains 83 components with the major ones being terpinolene, 1,8-cineole, phellandrene, and terpinen-4-ol, respectively (Raina, 2002).

2.5.3. Polyphenolic Constituents of turmeric

Plant constituents (carotenoids, phenolic compounds and terpenoids), are of importance in inflammation, itchiness and reducing redness of skin (Khaiat and Saliou, 2015). Phytochemicals such as phenols are amongst diverse and rich in strong natural anti-inflammatory constituents (Khaiat and Saliou, 2015). Phenolic compounds are strong antioxidant, providing protective barrier against oxidation (Khaiat and Saliou, 2015) to defend the human body against free radicals and also for their photo-protective activities. Medicinal and dietary plants constituents are gaining interest in topical application for skin protection against photo-damage (Dreher, 2015). Turmeric extracts have been extensively studied because it contains polyphenols known as curcuminoids which have high antioxidant properties and are of beneficial to human health, for example in aged and damaged skin. Polyphenols are generally multifunctional, having strong antioxidant activity derived from their highly reactive hydrogen or as electron donors, stabilizing the unpaired electron thus disturbing the production of hydroxyl radicals (Dreher, 2015).

2.5.4. The biological activities of turmeric constituents

Plants survive environmental stresses (climate change, pest, bacteria's, UV) by inducing their phytochemical responses to pressure (Khaiat and Saliou, 2015). These phytochemicals are comprised of a mass of compounds that have antimicrobial activities (Khaiat and Saliou, 2015, Suffredini et al., 2004, Cowan, 1999). Plants have numerous essential oils providing antibacterial, antifungal, antiviral properties. Amongst those essential oils, terpenoids (linalool, citral) or phenylpropanoids (eugenol) are responsible for their defense (Hammer and Carson, 2011, Khaiat and Saliou, 2015, Carson and Hammer, 2011). Turmeric oil contains turmerene and curlone, which are the major compounds responsible for the plant's antibacterial activity (Premavalli, 2007). The growth of bacterias like *Streptococcus*, *Staphylococcus*, *Lactobacilus*, etc. are suppressed by turmeric oil and curcumin (Chattopadhyay, 2004). In-vitro studies curcumin inhibited the progression of *H. pylori* CagA⁺ strains (Sarker and Nahar, 2007). This finding suggest that

curcumin could be therapeutic that is active against pathogenic processes initiated by *H. pylori* infections (Sarker and Nahar, 2007). The essential oils of turmeric as well were reported to be active pathogenic strains of Gram-positive (*Staphylococcus aureus*, *Staphylococcus epidermidis*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*, *Salmonella typhimurium*) bacteria (Sarker and Nahar, 2007, Singh et al., 2002). The antifungal activity of turmeric essential oils has also been reported, where it was demonstrated to be effective against *Aspergillus flavus*, *A. parasiticus* and *Fusarium moniliforme* (Saju et al., 1998, Jayaprakasha et al., 2001). In another study, it was observed that clinical isolates of *Staphylococcus aureus* were more sensitivity towards turmeric essential oils than the positive controls (Khaiat and Saliou, 2015).

Turmeric oil has also been shown to be therapeutic against other ailments that are non-infectious as the aforementioned examples. In one report, for instance, it was reported that powdered rhizomes of turmeric are effective in the treatment of sprain inflammation (Khare and Chopra, 2000). In another report, it was shown that turmeric is a useful treatment for painful traumatic conditions and deep-rooted pains showing analgesic action (Sharma, 2009). A decoction of turmeric in purulent conjunctivitis is very effective in relieving pain (Remadevi, 2007).

This potency is not only exclusive to turmeric essential oils, it was also demonstrated that even the aqueous extracts of turmeric rhizome have antibacterial effects (Chattopadhyay, 2004). Curcuminoids, isolated from the rhizome turmeric are known to possess a variety of health benefits like the prevention of cancer, inflammation, etc (Sarker and Nahar, 2007). This group of compounds possess antimicrobial, anticancer and antitumor, anti-inflammatory, antioxidant/radical scavenging properties, digestive disorders, wound healing, lowers blood glucose levels and *etc*. Furthermore, turmeric powder has been found to have a healing properties on wounded rabbits and rats (Gujral et al., 1953). Curcumin increased mucin secretion in rabbits (Chattopadhyay, 2004). In an experiment conducted on cancer models, it was observed that turmeric powder had adjuvant chemo-protection (Azuine and Bhide, 1994).

2.5.5. Pharmacological activities of turmeric

Turmeric is medicinal plant, with a vast spectrum of pharmacological properties, for example, as an antioxidant (Chattopadhyay, 2004, Khor, 2016, Araujo and Leon, 2001, Wojdyło et al., 2007), anti-protozoal (Amalraj, 2016), anti-septic (Damalas, 2011), anti-venom (Chattopadhyay, 2004,

Araujo and Leon, 2001), antimalarial (Amalraj, 2016), anti-inflammatory (Shrishaail et al., 2013, Heng, 2015, Araujo and Leon, 2001, Jurenka, 2009), anti-proliferative (Amalraj, 2016), anticancer (Sarker and Nahar, 2007, Maheshwari et al., 2006, Wilken et al., 2011), anti-angiogenic (Maheshwari et al., 2006, Yue et al., 2015), antitumor (Sarker and Nahar, 2007, Araujo and Leon, 2001), anti-depressant (Kulkarni et al., 2009), anti-diabetic (Shrishaail et al., 2013), anti-aging (Haque et al., 2017, Amalraj et al., 2017), antifungal (Chattopadhyay, 2004), antibacterial (Sarker and Nahar, 2007), anti-ulcer (Maheshwari et al., 2006, Shrishaail et al., 2013), anti-fibrotic (Shrishaail et al., 2013), anti-rheumatic (Shrishaail et al., 2013), antiviral (Shrishaail et al., 2013), anti-hepatotoxic (Shrishaail et al., 2013), analgesic (Damalas, 2011, Remadevi, 2007), digestive (Sarker and Nahar, 2007), disinfectant (Damalas, 2011), choleric (Shrishaail et al., 2013), insect repellent (Shrishaail et al., 2013), immunomodulatory (Paulucci et al., 2013), gastroprotective (Paulucci et al., 2013) and hypocholesteremic (Shrishaail et al., 2013) activities. Addition to this, turmeric has been successfully used in cardiac disorders. Different parts of the plant have different medicinal uses. For instance the rhizomes are used as a carminative, stomachic and emmenagogue (Shrishaail et al., 2013). And the fresh juice from turmeric possess anti-parasitic property in many skin afflictions (Shrishaail et al., 2013, Remadevi, 2007). India people used turmeric for face protection during sun worship, which it was believed that the golden yellow color of turmeric possessed sun protective properties (Nisar, 2015). Women were more dependent on turmeric using a mixture of turmeric to smear their bodies in order to gain a golden glow on their skin (Remadevi, 2007, Remadevi, 2005). Turmeric is used in cosmetics to help remove hairs and impart color by improving skin complexion (Remadevi, 2007). The Himalayans use it mostly to tone their skin, to treat wounded areas, pimples (Nisar, 2015). Its volatile oil is known to be a curative drug on skin diseases (Remadevi, 2007), greying of hair and for charming away jaundice (Shrishaail et al., 2013). Turmeric also aid in digestion problems and irritation of skin (Damalas, 2011). It is antiseptic (Damalas, 2011, Remadevi, 2007) and can acts as a cholagogue (Akram et al., 2010). In the digestive system, it acts as a carminative and protect against intestinal gas formation (Shrishaail et al., 2013). The digestive and stimulant properties of turmeric comes from its hot potency (Shrishaail et al., 2013). Health benefits of turmeric on the digestive system, also enhances the mucin secretion in the digestive tract (Nisar, 2015). This pharmacological activities of turmeric comes its biologically active compounds curcuminoids consisting of the main component curcumin (CUR) and demethoxycurcumin (DMC) and *bis*-methoxycurcumin (BDMC) (**Figure 2.4**)

2.5.6. Antioxidant activity of turmeric

Human skin consists of antioxidant network made up of vitamins, carotenoids and enzymes that act as a protection, protecting the skin from free radicals (Dreher, 2015). These antioxidants protect the human body cells against free radical damage which are caused by ROS (Nisar, 2015). The free radicals offend lipid peroxidation, therefore compounds that can scavenge this free radicals are able to treat many diseases and pathological cells (Nisar, 2015). Plants containing bioactive molecules have been shown to possess powerful antioxidant properties (Nisar, 2015).

Natural antioxidants are not only important to skin as free radical scavenger but also to plants, protecting them from free radical damage. Turmeric's curcuminoids prevent the development of free radicals, i.e. scavenge radicals (Maizura et al., 2011), and have been shown to have greater activity of antioxidant compared to those of vitamin C and E (Akram et al., 2010). Due to its free radicals scavenging ability, it has been accepted or labelled as a specie with the utmost antioxidant activity (Wojdyło et al., 2007), justifying its wide spectrum in applications, with skin care being the major domain of this aromatic plant (Shrishail et al., 2013). These attribute of turmeric can be due to its curcuminoids rich content, especially the bioactive one, curcumin, giving this plant recognition as a medicinal specie. Turmeric is a wellspring of naturally active ingredients like polyphenols, cancer preventing agents (antioxidants) (Nisar, 2015), which might be the substitute of the anti-infection agents utilized in food products (Nisar, 2015).

Phenolic compounds extracted from natural products are gaining considerable attention as good natural antioxidants. This growing attention of phenolic compounds comes from their powerful antioxidant activity. Turmeric having abundance of phenolic compounds such as curcuminoids (Maizura et al., 2011), makes it useful to the human body as a defender or protector against free radicals. These turmeric phenolic compounds prevent the development of free radicals (Nisar, 2015, Maizura et al., 2011). High levels of antioxidant in human skin act as an efficient antiaging strategy. Among curcuminoids, curcumin has shown great antioxidant and immune-suppressive activity in animals. Curcumin is a powerful antioxidant having therapeutic properties like free radical scavenging properties. Curcumin has been reported to be pro-oxidant (Araújo et al., 2001). The pro-oxidant behaviour of curcumin is associated with the conjugated β -diketone configuration

of it (Yoshino et al., 2004). These pro-oxidants are ROS categorized as non-radicals and radicals. Curcumin encases a blend of strong enemy of oxidant phytonutrients, for example, curcuminoids and inhibits cancer at initiation, progression, and promotion stages (Nisar, 2015).

2.5.7. Curcuminoids

Deep yellow characteristic color of turmeric derive from a group of fat-soluble, polyphenols pigments which are said to be curcuminoids (Akram et al., 2010). Curcuminoids are lipophilic poly-phenols found in the rhizome of turmeric and are used in spices, as a pigment, and as an additive in food (Kocher et al., 2015) (Amalraj, 2016). The chemical features of curcuminoids make them significantly less dissolvable in water and yet dissolvable in methanol, ethanol, acetone and dimethyl sulfoxide (Amalraj, 2016). Curcuminoids have been recognized as the most bioactive compounds of turmeric. This group of compounds is represented by a *bis*- α , β -unsaturated β -diketone polyphenol skeleton.

Every one of these mixtures show fluorescence under ultraviolet light, and this component can be utilized for identifying turmeric within the sight of other yellow colors (Premavalli, 2007). These three compounds can be separated by TLC and column chromatography along with their geometrical isomers, which are also expected to form in traces (Premavalli, 2007). Curcuminoids yellowish to orange color comes from its high electron delocalization within the molecules exhibiting strong UV absorption between 420-430 nm (Amalraj et al., 2017). The content estimation of curcuminoids in a turmeric plant is achieved by extracting it with different organic solvents including alcohol, dichloromethane, ethyl acetate and followed by collecting an absorption profile of the samples. This is followed by measuring at 429, 424, and 419 nm for curcumin, demethoxycurcumin and *bis*-demethoxycurcumin, respectively (Premavalli, 2007). Demethoxycurcumin and *bis*-methoxycurcumin stabilize curcumin in a portion subordinate way and are the natural stabilizers of curcumin.

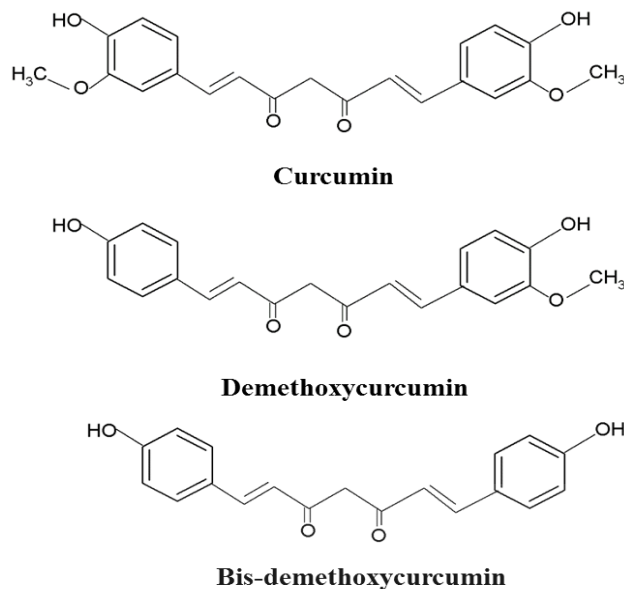


Figure 2.4 Structures of different types of curcuminoids

Curcuminoids possess powerful antioxidant activity (Amalraj, 2016) which is basically because of the phenol group on their structures. They also appeared to be strong antibacterial, anti-carcinogenic among other activities (Amalraj et al., 2017). Therefore they can be valuable in the treatment and inhibition of various diseases. These compounds are able to prevent the activation of NF- κ -B in human monocytic derived cells (Sarker and Nahar, 2007). Hydrogenation of curcumin produces a color-free mixture of tetrahydrocurcumin, which is esteemed as a topical antioxidant and anti-inflammatory agent having super free radical scavenging and lipid peroxidation inhibition efficacy contrasted with vitamin E (Prakash and Majeed, 2009). In vivo investigations of this topical antioxidant revealed it as a viable skin lightening agent with multifunctional topical advantages and no irritant or sensitization side effects (Pari and Amali, 2005, Majeed and Prakash, 2008).

Despite the fact that curcuminoids are the promising natural compound with a broad diversity of remedial properties, particularly organic targets and interactions linked to different ailments (Amalraj, 2016), their clinical uses are limited by their poor dissolvability (Amalraj, 2016, Kocher et al., 2015), bioavailability and low assimilation (Amalraj, 2016), instability in neutral and alkaline aqueous solution (Zamarioli et al., 2015) and hydrophilic topical formulations (Zamarioli

et al., 2015), high metabolism rate (Amalraj et al., 2017), and that only little portion of ingested curcuminoids is absorbed (Kocher et al., 2015). To enhance this is by encapsulation of curcuminoids in delivery systems, such as liposomes, nanoparticles or Cyclodextrin. This approach of administering curcuminoids (curcumin in particular) will be discussed later on in **section 2.6**.

2.5.8. Chemistry of curcumin

Curcumin (C₂₁H₂₀O₆), is the active ingredient of turmeric responsible for many of the plant's biological activities (Amalraj, 2016). The chemical skeleton of curcumin is a *bis-α, β*-unsaturated β-diketone and its IUPAC name is diferuloylmethane or 1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione (Paramasivam et al., 2009) with a molecular weight of 368.37 g/mol (Nisar, 2015). Curcumin was first discovered by Vogel and Pelletier in 1815 when they isolated a yellow coloring compound from rhizomes of *C. longa* and named it curcumin (Amalraj, 2016). In 1973 Roughley and Whiting determined the chemical structure of curcumin (Araujo, 2009).

The melting point of curcumin is between 176-177⁰C and forms red-brown salts with alkalis (Shrishaile et al., 2013). Curcumin has a bright yellow color at pH 2.5 to 7 and takes on a red color at pH levels higher than 7. It is hydrophobic therefore it does not dissolve in water but is dissolvable in alkalis, ketone, ethanol, acetic acid and chloroform, and insoluble in water (Shrishaile et al., 2013).

2.5.8.1. Properties of curcumin

Curcumin has been labelled as a natural medicine because of its documented studies in-vivo and -vitro, shown to have chemo-preventive properties, therapeutic potency and potent pharmacological activities (Khor, 2016, Shrishaile et al., 2013). This active ingredient exist in two tautomeric forms, thus the keto, and enol form (Akram et al., 2010). The enol part of it stabilizes in the solid phase and in solution (Akram et al., 2010). Literature on toxicity of curcumin proved that is harmful to

humans in clinical trials, even dozed at large quantity (Chattopadhyay, 2004, Sarker and Nahar, 2007, Akram et al., 2010). Curcumin possess free radical scavenging properties (Lee et al., 2013). The pro-oxidant activity of curcumin might be coming from conjugated β -diketone configuration it possesses (Nisar, 2015). The diketone moiety of it is essential for cancer and tumor activities (Sarker and Nahar, 2007).

As an antioxidant, this active constituent is said to be as a powerful antioxidant as vitamins E, C and Beta-Carotene (Akram et al., 2010, Aggarwal et al., 2006). It was reported that curcumin is 8x more powerful as vitamin E in inhibiting lipid peroxidation (Nisar, 2015). In the same study, the authors found that it inhibits cancer at different stages like initiation, progression, and promotion (Nisar, 2015). In another study that complements the results obtained by Nasir *et.al.*, curcumin was found to apply the high inhibitory impacts for different cancers by preventing the initiation and proliferation of carcinogen and inducing apoptosis of the tumor cells (Sarker and Nahar, 2007). It can, therefore, be utilized to improve the impacts of existing chemotherapeutic drugs. The antioxidant behaviour of curcumin, discloses its defensive activity on the brain (Aggarwal et al., 2006).

Furthermore, curcumin can tamper with the replication of human immunodeficiency virus (HIV) (Chattopadhyay, 2004), which makes it a promising anti-HIV agent being an HIV integrase inhibitor (Araujo and Leon, 2001).

2.5.8.2. Structural antioxidant activity of curcumin

In 1975 a report was given on the antioxidant activity of curcumin (Chattopadhyay, 2004). The natural antioxidant activity of curcumin, give a wide range of biological functions. The antioxidant mechanism of curcumin is ascribed to its special conjugated structural make, that incorporates two methoxylated phenols and an enol form of β -diketone; showing radical trapping ability as a chain-breaking antioxidant (Chattopadhyay, 2004). When comparing the activity of curcumin structural analogs, phenolic analog was more active than non-phenolic group (Aggarwal et al., 2006, Venkatesan and Rao, 2000). This high antioxidant activity of the phenol group was obtained by steric hindrance of two methyl groups introduced at the ortho position, implying that the

antioxidant activity increases when the phenolic group with a methoxy at the ortho position (Araujo and Leon, 2001, Aggarwal et al., 2006). The phenolic group is important as a scavenger for the free-radicals and the methoxy group increases the scavenging activities. In another study, the hydrogens attached to the phenol and the $-CH_2$ hydrogens on the heptanoid chain evaluated on their antioxidant activity (Aggarwal et al., 2006). The authors concluded that the phenolic hydrogens plays an essential in the antioxidant activity and it was also found to be liable for abstraction compared to $-CH_2$ hydrogens in curcumin (Aggarwal et al., 2006).

2.5.8.3. Antioxidant Properties of curcumin

Skin is equipped with nitrous antioxidant network that are able to reverse oxidation-induced damage to proteins (Taungjaruwinai et al., 2009) by scavenging free radicals so as to oppose ROS and RNS induced oxidative stress (Thiele et al., 2000, Thiele and Elsner, 2001). However, continuous exposure to these sources overwhelms the antioxidant defense in cutaneous tissues leading to damage of skin (Dreher, 2015).

In a case of skin stratum corneum being excessively exposed to oxidative events like UV rays, the skin homeostasis malfunction as a result of insufficient endogenous antioxidant, which will alter the performance of skin and its functions resulting in damage to the skin barrier (unsaturated fatty acids), proteins (collagen, elastin), and DNA (Khaiat and Saliou, 2015). If the skin continues to be overly exposed to these oxidative insults, they will trigger skin pigmentation (hyperpigmentation), aging, as well as inflammatory reactions (Khaiat and Saliou, 2015, Bickers and Athar, 2006). Exposing the skin to the sun as well, stresses the stratum corneum in activating an inflammatory cascade that invokes the wound repairing mechanism (Heng, 2015). These repair processes, result in the formation of new blood vessels and fibroblastic proliferation, which often lead to dermal scarring.

In *in-vitro* studies, curcumin was reported to inhibit the generation of ROS' like superoxide radicals (O_2^-), hydrogen peroxide (H_2O_2) and the nitrite radical (NO_2^-) by activated macrophages. This process plays an essential role in inflammation (Chattopadhyay, 2004). In the inhibition of ROS generation, curcumin exert strong inhibitory effect against H_2O_2 -induced damage in human

keratinocytes and fibroblasts (Chattopadhyay, 2004). So essentially, given this curcumin have the ability to control diseases associated with ROS through its antioxidant activity (Lee et al., 2013).

Curcumin is an inhibitor of phosphorylase kinase (PhK), which make it particularly useful to help skin in repairing itself after injury because of its special biochemical property (Heng, 2015). Curcumin inhibits PhK, by blocking PhK-dependent signals, which may lead to mitigation of skin tissue injury (Heng, 2015). Applying curcumin topically enhances the antioxidant tissue levels on the skin. Therefore, the stratum corneum being the outermost part of the skin exposed to environmental factors (UV, air pollution) which may depletes skin antioxidants, will benefit from the increased antioxidant supplied topically (Sivamani et al., 2015). This accounts for topical curcumin wide spectrum and longstanding popularity as a therapeutic cosmetic (Heng, 2015).

2.5.8.4. Anti-inflammatory activities of curcumin

Inflammation is known to be the 7th feature of cancer (Mantovani et al., 2009). The anti-inflammatory activity of curcumin was first investigated in 1971 (Srimal et al., 1971). When the skin is injured, it initiate cascade of events in the injury healing process. One of the earliest inflammatory cells the skin respond to when is injured is the initiation of the transcription activator NF- κ B in dendritic cells (Heng, 2015).

NF- κ B is a transcription factor activated by UVB irradiation. It plays a fundamental role in the expression of genes involved in inflammatory and immune responses (Khor, 2016, Arakane and Naru, 2015). Curcumin blocks NF- κ B-induced signals by inhibiting PhK, which is initiated minutes following injury upstream of NF-KB. This reduces fibroblast proliferation and myofibroblast change (Heng, 2015). Curcumin inhibits various molecules that play role in inflammation, which might be reason why it has anti-inflammatory activities (Sarker and Nahar, 2007). Anti-inflammatory properties of curcumin might be a promising approach to suppression of inflammatory reactions for UV-caused damage and ROS scavenging (Heng, 2015).

2.6. The novel delivery systems of curcumin

The curcumin applications is limited by its low dissolvability in water, poor absorption, bio-availability and sensitivity to physical (thermal, light) and chemical (acid, metallic ions) conditions. These components confine the application of curcumin, thus improvements are necessary for the stability and solubility of curcumin. Encapsulation techniques have been used to overcome these advantages. These include encapsulation of curcumin with polymeric nanoparticles, liposomes, biodegradable microspheres, yeast cells, cationic micelles, gelatin, modified starch, and Cyclodextrin, which have been investigated to enhance the dissolvability of curcumin and reduce the side effects of actives as well as to avoid the use of toxic substances (Shrishail et al., 2013). In this study, curcumin will be incorporated in β -CD to form inclusion complexes so as to improve its application. When encapsulating drugs, the aim is to increase the solubility and pharmacokinetics, and sometimes enables further clinical improvement of new chemical entities that have stalled in light of poor pharmacokinetic properties (Saraf, 2010). The importance of using biodegradable polymers is the vanishing of embedded foreign materials from the body because of their biodegradation.

2.6.1. Cyclodextrin-curcumin inclusion complex

Cyclodextrin (CD) are cyclic oligosaccharides consisting of α , seven β , eight γ or more glucopyranose units, linked by α -(1, 4) bonds (de Paula et al., 2011). They have a hydrophilic outer surface, making it soluble in water, apolar cavity and a hydrophobic central cavity. Because of Cyclodextrin special molecular structure with a hydrophilic outer surface (provide the guest molecule with solubilizing effects) and a hydrophobic central cavity (protects the hydrophobic guest from aqueous environment), they have become useful as an enhancer for the solubility and bioavailability of hydrophobic drugs (Saikia et al.). The commonly used cyclodextrins in pharmaceutical applications are α , β , and γ -CD, and their derivatives such as hydroxypropyl- β -CD (HP β CD) and methyl β -CD (M β CD)(Saikia et al.). The preparation of β -CD–curcumin inclusion complexes was reported(Mangolim et al., 2014) were the complex enhanced the stability and solubility of curcumin, followed by its application in food (ice-cream colorant). In the inclusion

complex of curcumin with β -Cyclodextrin, Cyclodextrin incorporates one of the phenyl rings of curcumin inside its cavity and enhances curcumin's chemical and physical characteristics.



CHAPTER 3. Chromatographic and Spectroscopic Study of *Curcuma longa* L. Extracts and Compounds

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Abstract:

The active product in this plant is believed to be curcumin belonging to a class of compounds known as curcuminoids extracted from *Curcuma longa*, therefore this study was undertaken to isolate and characterize curcumin. The rhizomes of *Curcuma longa* were dried, ground and extracted using various organic solvents. The objective of this study was to extract, isolate and characterize curcuminoids and curcumin. It was observed from TLC analysis that the extracts contained curcuminoids including curcumin, given by the 3 spots on TLC plate. The curcuminoids collected from different solvents were characterized with respect to UV-Vis and FTIR. The extracts gave similar results, therefore they were then combined and fractionated by column chromatography guided by TLC to isolate curcuminoids. The fractions gave 3 spots on TLC plates and when viewed under UV at wavelength 252 nm. Column chromatography led to the isolation of a pure compound, curcumin which was confirmed by characterization techniques. Curcumin absorption on UV-Vis yielded peaks at 420 nm and a shoulder at 442 nm indicating the presence of more than one isomer. FTIR showed a sharp phenolic OH peak at 3494 cm⁻¹, the spectrum also confirmed that curcumin exists in keto-enol tautomeric form with no peaks at the carbonyl region (1800-1650 cm⁻¹). The aromatic C-C vibrations at 1588 and 1492 cm⁻¹ were also observed. ¹H NMR results showed a singlet peaks at δ 3.8ppm assigned to proton attached to O-CH₃, proton at δ 6.0ppm attached to -CH₂ and a proton at δ 9.7 ppm attached to OH, confirming the structure of curcumin.

Keywords: *Curcuma longa* rhizomes, curcuminoids, solvent extraction, column chromatography (CC), thin-layer chromatography (TLC), UV-VIS and FTIR

3.1.Introduction

Natural plant extracts and/or isolated compounds are used in the skin care industry to improve skin moisturization, lessen the indication of aging or cellulite, brighten and soothing the skin (Khaiat and Saliou, 2015). Plants constituents can be isolated, purified and identified by using various methods of extraction and chromatographic techniques. Chromatographic, including thin-layer chromatography and column chromatography, and spectroscopic (UV-Vis) techniques have been employed for the separation, investigation and quantification of curcuminoids. Spectrophotometric methods are used to give the total color content of the sample (Péret-Almeida et al., 2005). *Curcuma longa* has long been used for various purposes including for health and cosmetics for skin protection e.g. protection against UV damage of skin cells (Korać and Khambholja, 2011) and coloring agent (Sharma et al., 2012). This chapter aims at extracting, isolating and characterizing different compounds found in the plant but mainly curcumin.

3.2.Materials and Methods

3.2.1. Materials

Curcuma longa (Turmeric) rhizomes were purchased from Gravel Sparg industries in Cape Town, South Africa. All solvents/chemicals were of analytical grade and obtained from E-Merck.

3.2.2. Method

3.2.2.1. Plant Sample Collection and Extraction

The stems of *Curcuma longa*, L known commercially as Turmeric were water washed, cut into pieces and dried for 3-5 days, then ground into fine powder.

3.2.2.2.Solvent extraction

The fine plant material was weighed into sealable 500 mL glass bottles (100 g), to which 300 mL of different organic solvents (methanol (MeOH), ethyl acetate (EA), dichloromethane (DCM),

hexane (Hex) and acetone) were added separately. The extraction process was carried out for 7 days with mild daily shaking on a shaker. The extract which was contained in the liquid phase was collected by decanting into a round bottom flask then dried under vacuum in a rotary evaporator (rotavapor R210, BUCHI).

3.2.2.3.TLC analysis using different solvent systems

Upon TLC analysis of the extracts, curcuminoids were separated by column chromatography using hexane with increasing gradient of polar solvents (ethyl acetate and methanol) as the mobile phase. Different compositions of mobile phase used for the separation of curcuminoids include. This was conducted for both the crude extract and the various fractions (MP1, MP2 etc). In the case of the fractions, the developed plates were dried and viewed under a UV light at 252 nm. TLC was carried out using aluminium plates pre-coated with silica 60-F₂₅₄.

3.2.2.4.UV-Vis analysis

The absorbance of curcuminoids and curcumin were analyzed using Shimadzu UV-2450 UV-Vis spectrophotometry in the UV range of 200 nm to 700 nm. In order to carry analysis, 0.01g of curcumin was diluted in 50ml of ethanol and filtered through 0.45 µm filter. A volume of 2 mL was pipetted into 3 mL quartz cuvette.

3.2.2.5.FTIR analysis

Fourier Transform Infrared spectra of the crude extract and curcumin were studied using PerkinElmer100 spectrometer. The spectra were recorded from 4000 cm⁻¹ to 650 cm⁻¹ in attenuated total reflectance (ATR) mode fitted with a germanium crystal.

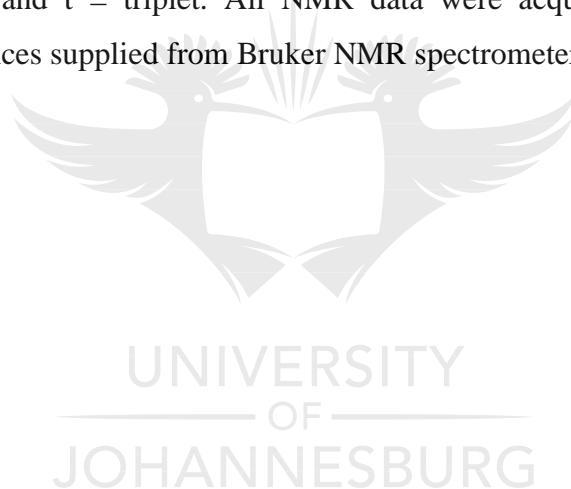
3.2.2.6.Column chromatography (CC)

The crude extract was subjected to column chromatography using a glass column packed with 60 – 120 mesh silica gel. The crude of 100g was impregnated with 100g of silica gel, loaded on the

column and eluted with 100% hexane followed by hexane: ethyl acetate with increasing polarity to 100% ethyl acetate and ethyl acetate: methanol with increasing polarity to 100% methanol for isolation of different compounds. The fractions were collected and grouped according to their TLC profiles, concentrated under a vacuum at 50°C and characterized by UV-Vis and FTIR. The fractions were collected as MP 1, MP 2 (Mokgadi Precious) and etc.

3.2.2.7. Nuclear Magnetic Resonance (NMR) spectroscopy

¹H NMR spectra were recorded at room temperature (298 K) at 400 MHz and 100 MHz respectively, using Bruker Avance III 400 MHz FTNMR spectrometers. All chemical shifts, δ , were reported in parts per million (ppm) relative to tetramethylsilane. Multiplicity is as follows: s = singlet, d = doublet, and t = triplet. All NMR data were acquired and processed using TopSpin™ pulse sequences supplied from Bruker NMR spectrometer manufacturer.



3.3. Results and Discussion

3.3.1. Solvent extraction and TLC analysis for crude extract

Curcuminoids have low polarity making them immiscible with water; therefore the five organic solvents chosen are good solvents for extraction of organic compounds that are insoluble in water. The hexane extract was a yellow volatile oil, the DCM extract was an orange powder whereas the ethyl acetate extract was a sticky dark orange solid with deep brown oil. The methanol extract was characterized as a slurry consisting of a thick deep brown solid and oil. In addition, the acetone extract was a little bit of solid and thick oil. TLC analysis of these solvents were similar except for hexane, in which the color was faint on a TLC plate, possibly consisting of mostly hydrocarbon given the solvents low polarity. A similar observation was seen with ethyl acetate **Image 3.1**

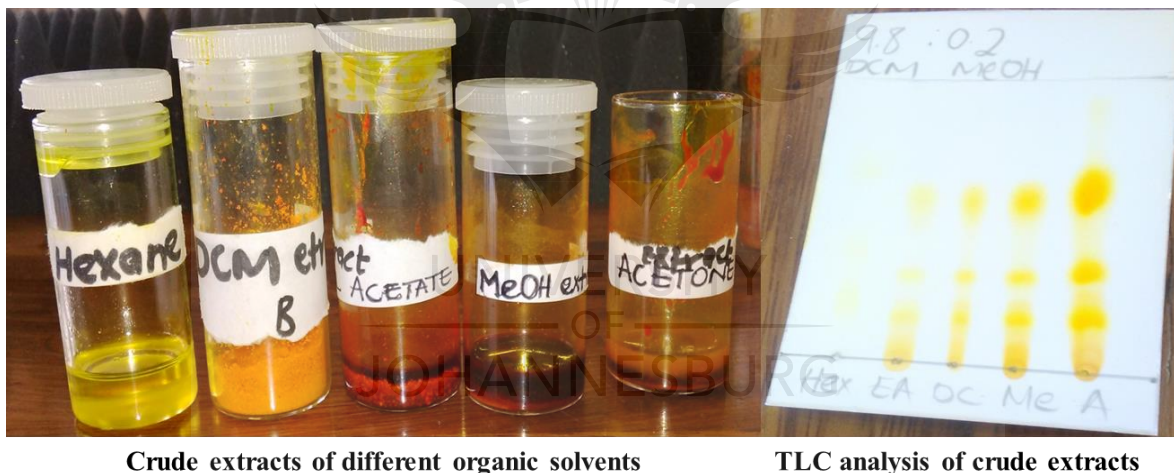


Image 3.1 Different solvent systems on separation of curcuminoids and their TLC results

The mobile phases used for TLC analyses were in ratios EA: MeOH (95:5; 7:3), Hex: EA (5:5; 7:3), DCM: MeOH (9.9:0.1; 9.8:0.2), 100% DCM, CF: MeOH (5:5, 8:2), CF: CHCl₃ (9:1), 100% CHCl₃ and PE: EA (7:3; 9:1). The desired TLC separation of compounds was achieved by using 2 % methanol in dichloromethane as the mobile phase. The reason for this is that curcuminoids are diarylheptanoids having a negative and positive charge making them polar compounds suitable for this dichloromethane/methanol composition which favors the polar compounds dissolving

them better. On this system, the separation between curcuminoids was larger and the spots were well defined.

3.3.2. FTIR analysis of different solvents extract

All 4 extracts showed similar results with the peaks of different solvents vibrating a broad peak around 3352-3342 cm^{-1} assigned to asymmetric and symmetric stretching of OH. The vibration band of $-\text{CH}$ at 2921 cm^{-1} and aromatic C-C stretching appear at 1620-1575 and 1525-1475 cm^{-1} . These peaks identified or confirmed the presence of the functional group in curcuminoids.

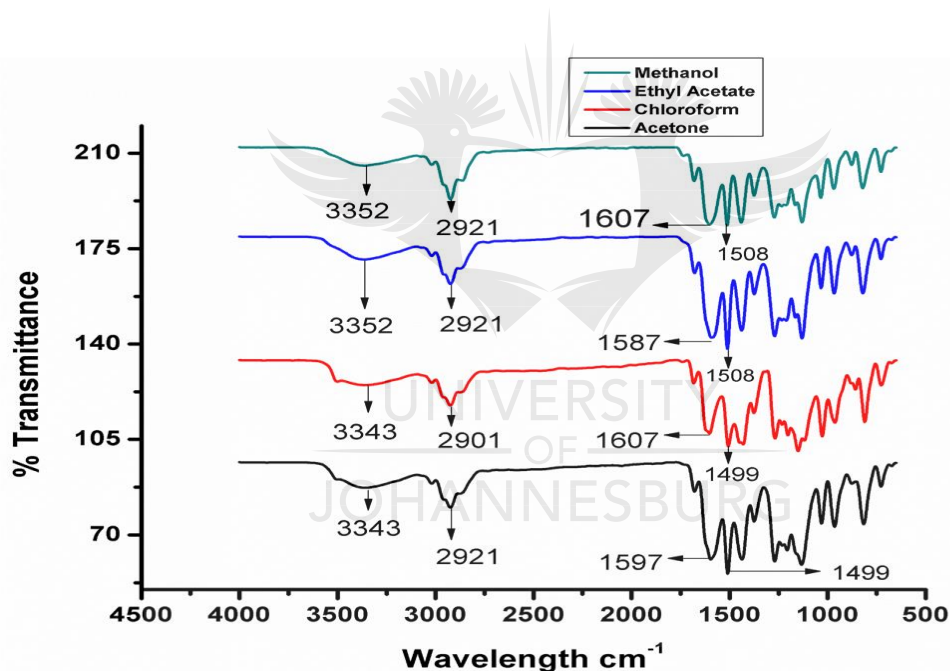


Figure 3.1 FTIR spectrum of crude extracts

3.3.3. UV-Vis analysis of different analysis extract

The 1, 3-diketone group of curcuminoids tautomerizes to keto or enol form (Meng et al., 2018). This change is caused by the transfer of intramolecular hydrogen atoms at the diketone chain. The enol form of this chain has a large conjugating system which absorbs strongly at 410-430 nm in the UV-Vis region (Meng et al., 2018), giving it its yellowish color due to the wide electronic

delocalization inside the molecule (Amalraj et al., 2017). The results on UV-Vis analysis gave similar results with literature where the absorption of curcuminoids for organic solvents ethyl acetate, chloroform, methanol, and acetone were measured at 411, 418, 421 and 421 nm, respectively. The absorption bands at 258, 245, 251 and 253 for EA, CF, MeOH and acetone, respectively, corresponds to the transfer of pi bonds in the benzene ring (Masek et al., 2013).

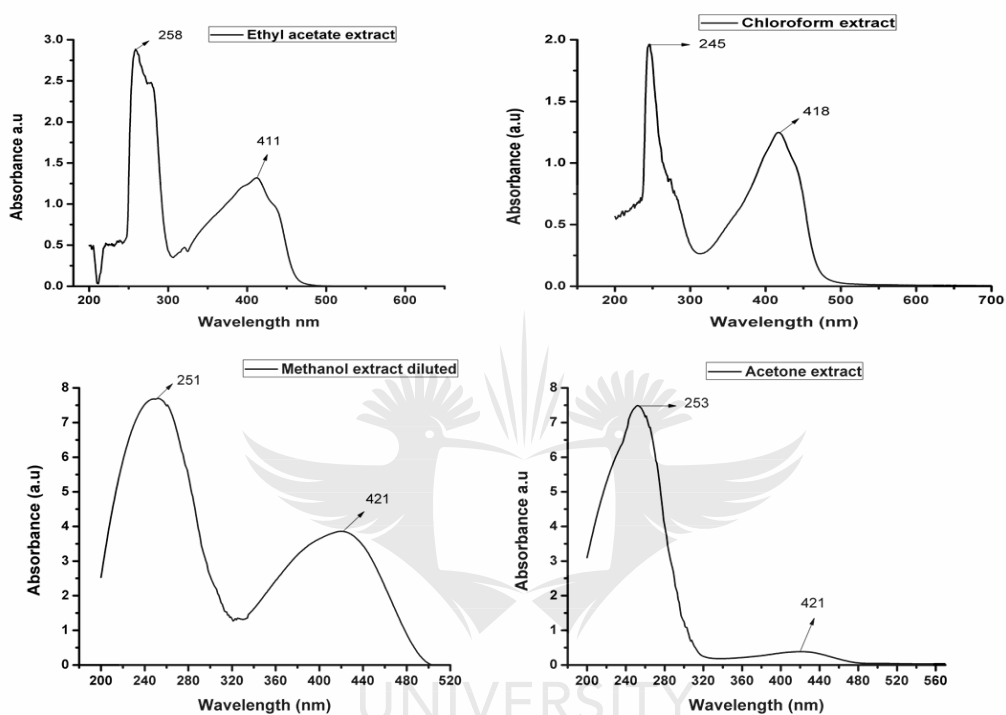


Figure 3.2 UV-Vis spectrum of crude extracts

3.3.4. Column Chromatography and TLC analysis

The crude extracts from all four solvents were combined because they were similar to each other based on TLC, UV-Vis and FTIR data (Figure 3.1 & Figure 3.2). The combined extracts were then separated by column chromatography. Hexane is non-polar, therefore it eluted non-polar compounds that is the hydrocarbons. The combination of hexane and ethyl acetate is non-polar, favoring non-polar compound as well. Combination of ethyl acetate and methanol is very polar, eluting very polar compound on the column. Methanol is polar protic, favoring the polar compound as well.

Some compounds collected from the column remained at the baseline of the TLC plates and others were not visible at all, hence the use of polar mobile phases at different fractions to check for other possible compounds in the plant extract. The other compounds extracted could be those of phenolics, sugars, carbohydrates, volatiles and antioxidants as they have been conducted and identified in another study (Santana and Meireles, 2016). The authors identified these compounds by developing mobile phases for TLC analysis that favored them. Mobile phases used for phenolics, antioxidants and volatile compounds were chloroform, ethyl acetate and glacial acetic acid. And for sugars and carbohydrates were ethyl acetate, acetic acid, methanol and water. Mobile phases that favored curcuminoids were dichloromethane: methanol, chloroform: methanol and chloroform: methanol and glacial acetic acid (Li et al., 2014, Revathy et al., 2011). This concludes that successive chromatographic (CC and TLC) analysis of *Curcuma longa*, L crude extracts led not only to the isolation of curcuminoids but other compounds as well, including essential oils, sugars, phenolics, carbohydrates, antioxidants. The results are reported in **appendix 1**. The crude extracts results were then compared to the curcumin.

3.3.5. UV-Vis analysis of curcumin

UV-Vis analysis of curcumin on this part was dissolved in ethanol. Curcumin exerted a strong and intense peak at 321 nm and a broad band at 420 nm with a shoulder at 442 nm in **Figure 3.3**. The presence of a shoulder indicates the possibility of more isomeric forms in the ground state (Masek et al., 2013). The absorption band at 420 nm corresponds to the enol group whereas the band at 442 nm is for the keto group in the molecule (Mondal et al., 2016).

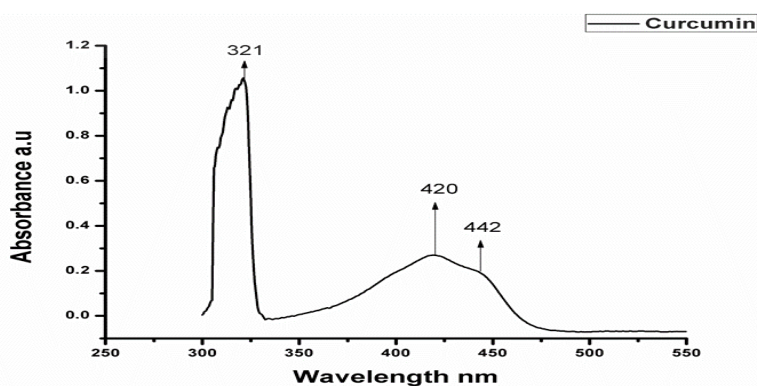


Figure 3.3 UV-Vis spectrum for curcumin

3.3.6. FTIR analysis of curcumin

Curcumin has characteristics of two benzyl rings joined by a 1,3-diketone group on a heptanoid chain. Therefore FTIR was used to identify/confirm these functional groups in curcumin. According to literature, (Akram et al., 2010, Mangolim et al., 2014, Meng et al., 2018) curcumin exists in tautomeric form. This was evident in our finding, as there were no visible peaks at 1800-1650 cm^{-1} region belonging to carbonyl. Another observation in the FTIR spectrum of curcumin shown in **Figure 3.5**, was a sharp peak for phenolic O-H in region 3494 cm^{-1} and the aromatic C-C vibrations appearing at 1588 cm^{-1} and 1492 cm^{-1} regions.

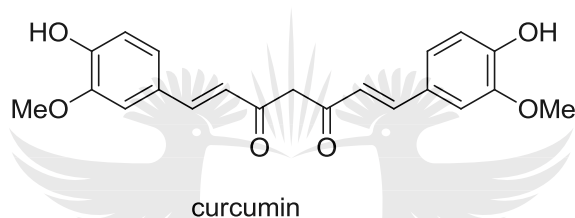


Figure 3.4 Structure of curcumin

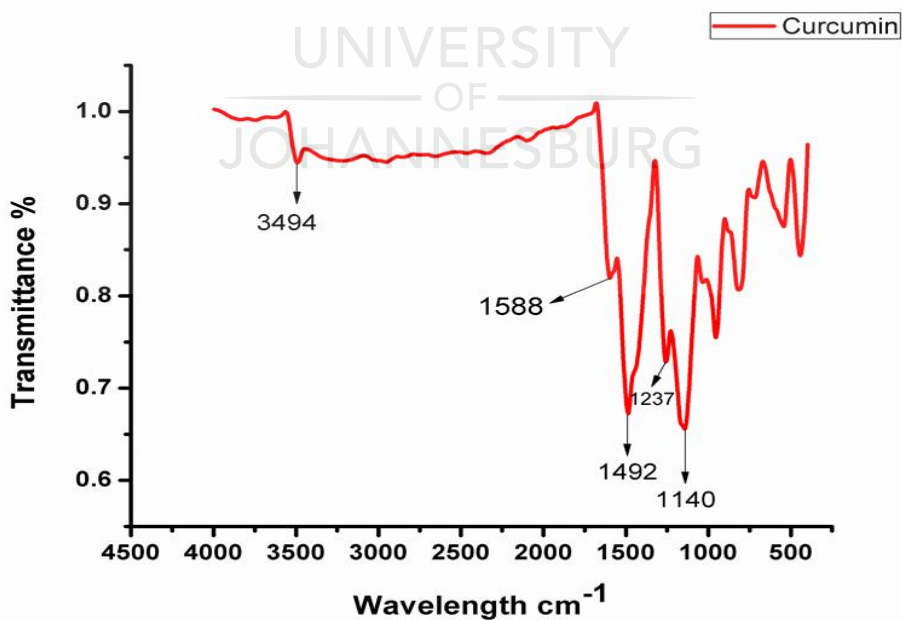


Figure 3.5 FTIR spectrum for curcumin

3.3.7. ^1H NMR Spectroscopy of curcumin

Curcumin is a diphenylheptanoid with a symmetry at methylene region. This compound was subjected to proton NMR to assign the protons in the structure. A prominent singlet peak of a methoxy ($\text{O}-\text{CH}_3$) group was observed at region $\delta 3.8$ ppm (6H, s) and another signal at region $\delta 6.04$ ppm (1H, s) assigned to protons on $-\text{CH}_2$. A sharp singlet peak at $\delta 9.64$ ppm indicate the hydroxyl groups of curcumin. Protons (H_2) were observed as a doublet in region $\delta 7.30$ ppm (d, 2H, H_2 and H_2').

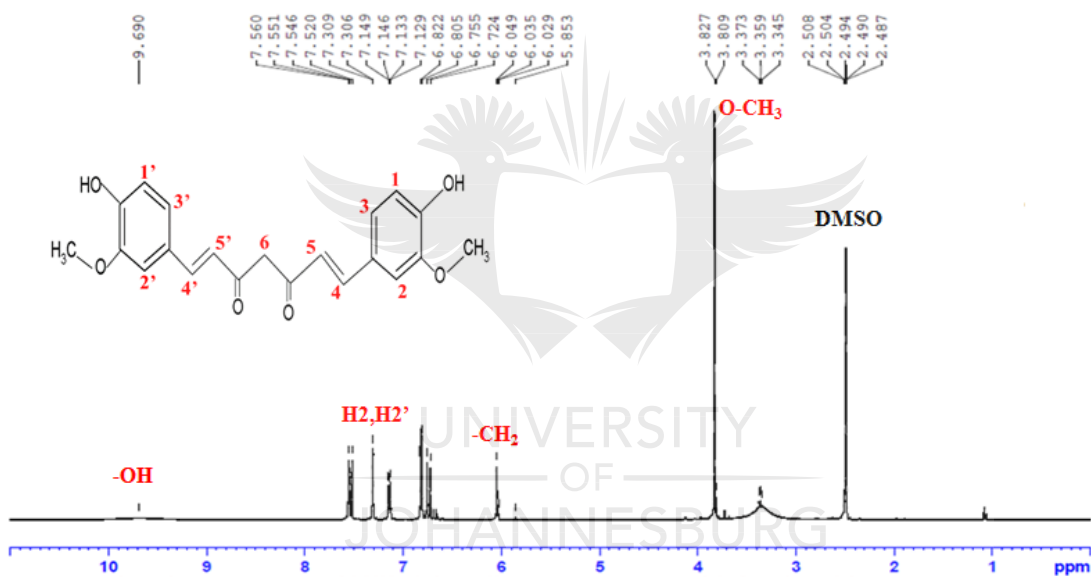


Figure 3.6 Curcumin H NMR

3.4. Conclusion

Solvent extraction method was efficient in extracting the curcuminoids. The crude extracts were then characterized on UV-Vis and FTIR. Both techniques showed similar spectrum for all chosen solvents. For this reason the extracts were then combined and fractionated by column chromatography guided by TLC to isolate curcuminoids. The fractions had three spots on TLC plates when viewed under UV at wavelength 252 nm. In the fractionation, the pure curcumin was isolated and analyzed by UV-vis, FTIR and NMR techniques. On UV-Vis the significant peaks corresponding to the isomeric forms of curcumin were observed. FTIR showed major peaks assigned to functional groups on curcumin structure, it also revealed that curcumin exist in tautomeric form because the peaks belonging to carbonyl in the 1800-1650 cm^{-1} region were not visible. ^1H NMR results showed a prominent singlet peak at $\delta 3.82$ ppm assigned to proton attached to O-CH_3 , and two more singlets assigned to protons attached to $-\text{CH}_2$ ($\delta 6.04$ ppm) and OH ($\delta 9.69$ ppm), confirming the structure of curcumin.

CHAPTER 4. COMPREHENSIVE GCxGC-TOFMS ANALYSIS OF *CURCUMA LONGA, L.*

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Abstract:

The medicinal and aromatic plant *Curcuma longa*, L. which belongs to the *Zingiberaceae* family, was chosen for analysis because of its multiple uses in cosmetics, nutraceuticals and phytomedicines. In this chapter, the focus is mainly on the volatile compounds which were extracted and fractionated as described in Chapter 4. The classes of compounds of interest are terpenes, terpenoids and alkaloids because of their usefulness in skin care. Some of the fractions were analysed for chain length, amount of terpenes and terpenoids, heteroatom content and chemical class identification by gas chromatography coupled to time of Flight mass spectrometry (GCxGC-TOFMS). It was found that the majority of the volatile compounds in the extracts had a chain length range between C11 and C15. This also reflected in the terpenes-terpenoids content as it was found that the majority of them had 15 carbon atoms, defined as sesquiterpenoids. It was also found that most of the compounds in the analyzed extracts had 1-2 heteroatoms.

Keywords: *Curcuma longa* L., rhizomes, GCxG-TOFMS, alkaloids, terpenes and terpenoids

4.1.Introduction

Phytochemical investigation on *Curcuma longa* lead to the isolation and identification of numerous types of secondary metabolites (Meng et al., 2018), with its main bioactive components being curcuminoids (diarylheptanoids) and essential oils (monoterpenoids and sesquiterpenoids) (Nisar, 2015) which are present in essential oil extract from *Curcuma longa* root (Amalraj, 2016). This bioactive compounds show various bioactivities in in-vivo and in-vitro studies (Li et al., 2011). The oil extracts from *Curcuma* rhizome consist mostly of monoterpenoids, monoterpenes, sesquiterpenes, and sesquiterpenoids (Premavalli, 2007, Li et al., 2011), except that in this chapter the rhizomes were rich in alkaloids, sesquiterpenoids, monoterpenoids and diterpenoids, respectively. The interest in using *Curcuma longa*/ Turmeric for the analysis is derived from its wide cosmeceutical uses as a natural topical medicine in skin care, since it has documented uses for the skin disorders treatment such as acne and skin discoloration (1999), wounds, burns, including sun burns, and psoriasis, as well as in antiseptic agents, allergic reaction formulation, anti-inflammatory products, anti-aging and anti-oxidants products (Bommarito, 2010). Of the plant extracts, terpenoids and alkaloids are of interest as components for human skin protection (Lee et al., 2012). Alkaloids and terpenoids having physicochemical and biological effect on control and/or treatment of various diseases (Mehdizadeh and Moghaddam, 2018) and their anti-bacterial, anti-fungal effects on skin (Modak et al., 2011) makes them of interest to this chapter. To quantify this phytochemicals, comprehensive 2D GCxGC-TOFMS analysis was conducted.

4.2.Materials and Methods:

4.2.1. Materials

GC grade dichloromethane sourced from Merck (South Africa) was used to prepare GC samples. The organic solvents used here are same as those used in chapter 3

4.2.2. Method

4.2.2.1.GCxGC-TOFMS

Fraction 1 to 62 collected from column chromatography in chapter 4 were essential oils. This essential oils samples were injected in 1µl splitless on a GCxGC-TOFMS (LECO Pegasus 4D, Agilent 7890A, Agilent Technologies, USA). The analyte was fractionated in a 5 MS fused silica capillary column (30 m x 0.25 mm x 0.25 mm). Helium was used as a carrier gas at a constant flow rate of 1mL/min and an oven temperature of 60 °C/5min, which was increased to 300 °C at a rate of 10 °C/min. The mass spectrometry conditions were optimized where the electron ionization potential was set to 200 eV (optimized voltage offset 200 eV and acquisition voltage 1526 eV) and the acquisition rate was set to 60 spectra/s. Peaks obtained after solvent delays (from 260 s onwards) were considered as significant peaks and the S/N ratio was 400. The subsequent GCxGX-TOF/MS raw files obtained were converted to netCDF format via Chemstation (Agilent Technologies), while retention time alignment, matched filtration, peak detection and peak matching were done on ChromaTOF software (LECO, USA). Subsequent identification of the volatile compounds was done by matching their spectral databases (NIST, Adams and EO libraries). Peak tables obtained from ChromaTOF were further analyzed in Microsoft Excel. Compound classes were identified based on heteroatoms and chain length using filtering procedures.

4.3.Results and Discussion

The secondary metabolites found in the plant's essential oil, from fractions MP 1-60, were analyzed to study and identify the distribution of the various compounds. The chain length of compounds was used in order to investigate different compound classes in the plant extracts. The graphs and tables were plotted and tabulated using peak area percentages (Area %), except for graph in **Figure 4.5**, which was calculated manually. The results that were found are represented in **Table 4.1** and **Figure 4.2**. The green colour on **Table 4.1** represents high abundance (carbon chain > 44 carbon atoms) whereas the fading green colour represents moderately high abundant molecules with carbon chain length that is between 20 and 44 carbon atoms. The deep red colour represents molecules with the least amount of carbon atoms, ranging between 0 and 2 carbon atoms and the slightly faint red colour represent molecules with carbon atoms ranging between 2 and 10 carbon atoms (**Table 4.1**).

Table 4.1 Representation of the various molecules chain lengths from different fractions.

	MP 1-6	MP 7-13	MP 15-16	MP 17-21	MP 22-33	MP 33-37	MP 38	MP 39	MP 40-45	MP 46-49	MP 50	MP 52-62
C1-C5	1.91	0.05	11.57	2.98	0.41	0.26	1.11	0.45	0.07	2.31	0.38	3.60
C6-C10	14.17	7.02	16.71	31.63	25.18	11.17	13.87	17.08	20.95	20.15	24.57	15.18
C11-C15	52.94	51.50	25.67	33.95	30.84	58.49	53.92	61.94	52.07	44.89	55.18	49.90
C16-C20	16.77	26.01	16.92	14.01	26.02	18.27	14.67	17.26	13.10	29.01	17.36	14.24
C21-C25	8.61	13.25	24.14	6.62	9.49	6.36	7.48	1.38	1.81	1.62	0.90	12.23
C26-C30	0.06	0.66	1.04	0.00	0.01	0.03	0.00	0.00	0.00	0.00	0.00	0.00

Table 4.2 Representation of the various molecules heteroatom content from different fractions.

	MP 1-6	MP 7-13	MP 15-16	MP 17-21	MP 22-33	MP 33-37	MP 38	MP 39	MP 40-45	MP 46-49	MP 50	MP 52-62
O1	37.58	3.79	3.99	37.81	39.16	20.85	31.79	43.66	30.19	37.21	28.25	43.89
O2	15.52	1.08	1.21	11.77	10.38	16.61	11.65	14.18	17.23	22.41	36.32	13.49
O3	7.16	0.03	0.29	6.44	6.82	1.08	0.70	1.05	5.66	1.35	1.73	2.23
O4	1.66	0.38	1.12	5.05	1.40	3.67	3.43	1.89	0.44	1.66	3.02	2.59
O5	0.03	0.003	0.00	2.99	0.18	2.63	0.35	8.92	4.39	4.86	2.29	0.41
O6	0.00	0.00	0.00	0.01	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O7	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N1	0.69	0.33	0.62	0.53	0.40	0.01	1.68	1.36	1.59	1.32	0.44	0.00
NO	9.92	0.84	0.09	3.31	6.41	1.45	0.95	1.09	3.84	2.61	2.79	0.64
N2O	1.57	0.08	0.001	1.15	2.06	1.78	1.03	0.06	4.01	0.69	3.08	0.02
N3O	0.03	0.01	0.12	0.62	0.06	0.01	0.18	0.00	0.06	0.00	0.08	0.45
N4O	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.28	0.84	0.00	0.68	0.13
N5O	0.00	0.00	0.00	1.46	0.00	0.00	2.40	0.10	1.03	0.00	0.00	0.00
N6O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N7O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	62.08	5.27	6.61	64.06	57.63	44.84	49.19	69.30	57.91	66.80	71.61	63.24

Here it was found that the bulk of the compounds had a chain length that ranges between 11 and 15 carbon atoms with fraction MP 39 having the most of these compounds. It was also found that molecules with carbon chains that ranges between 26 and 30 carbon atoms were the least abundant with fractions MP 1-6, MP 7-13, MP 15-16, MP 22-23 and MP 33-37 being the only fractions that contained these compounds. Molecules with small chain length (1-5 carbon atoms) were also not frequently detected, where the highest abundance of 11.57 % was detected for MP 15-16. The rest of the fractions contained less than 3 % of molecules with carbon chain length that ranges between 1-5 carbon atoms.

The results discussed were also represented graphically as shown in **Figure 4.1** where it is evident that peaks with higher areas were for molecules with a carbon chain length that ranges between 11 and 15 carbon atoms (**Figure 4.1**). Fewer bars were observed for molecules with chain lengths of 1-5 and 26-30, with the latter being the fewest of the two, clearly indicating fewer atoms with such carbon chain lengths.

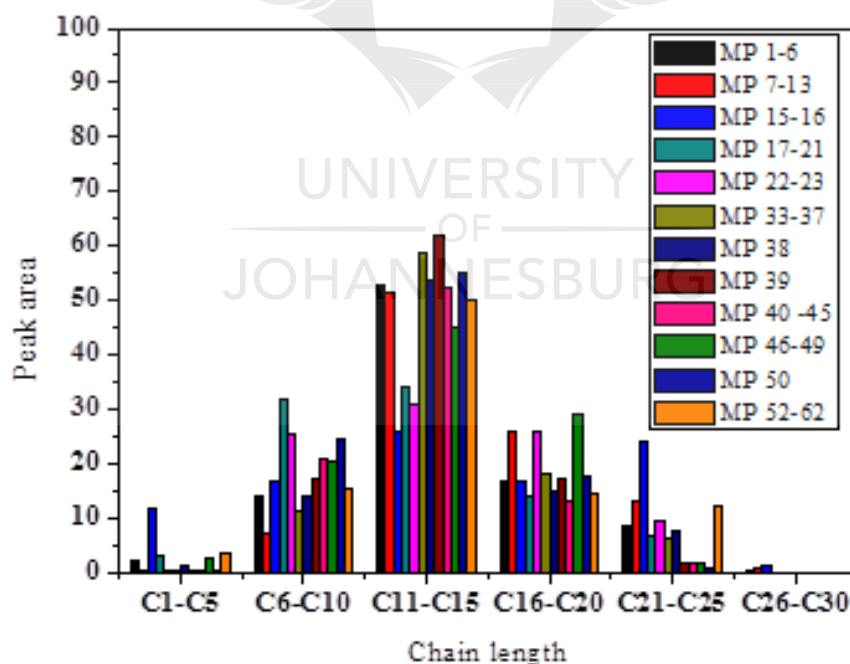


Figure 4.1 Chain length distribution of molecules in different fractions.

The amount of heteroatoms (oxygen and nitrogen atoms) in the molecules (volatile compounds) contained in the different extracts was also measured. The results are tabulated in **Table 4.2** and

plotted in **Figure 4.2**. The colour coding on **Table 4.2** is the same representation as it was on **Table 4.1**, i.e. the green colour represents molecules that are highly abundant whereas the deep red colour represents molecules that are the fewest. It was observed that between 48 and 72 % of the compounds in the fractions analyzed contain heteroatoms, with fractions MP 50 having the most molecules with heteroatom based functional groups (**Table 4.2** and **Figure 4.2**). Fractions MP 7-13 and MP 15-16 showed highly irregular results where the total amounts of heteroatoms were 5.27 and 6.61 %, respectively (**Table 4.2** and **Figure 4.2**). This might have been attributed to the polarity changes in the column. In the first fraction, which was 100% hexane (non-polar), lots of oxygen containing compounds were eluted first, then the polarity increased from 15% Ethyl acetate/Hexane to 30% Ethyl acetate/Hexane which is a non-polar and polar composition. This increase in polarity explains fluctuation of the results.

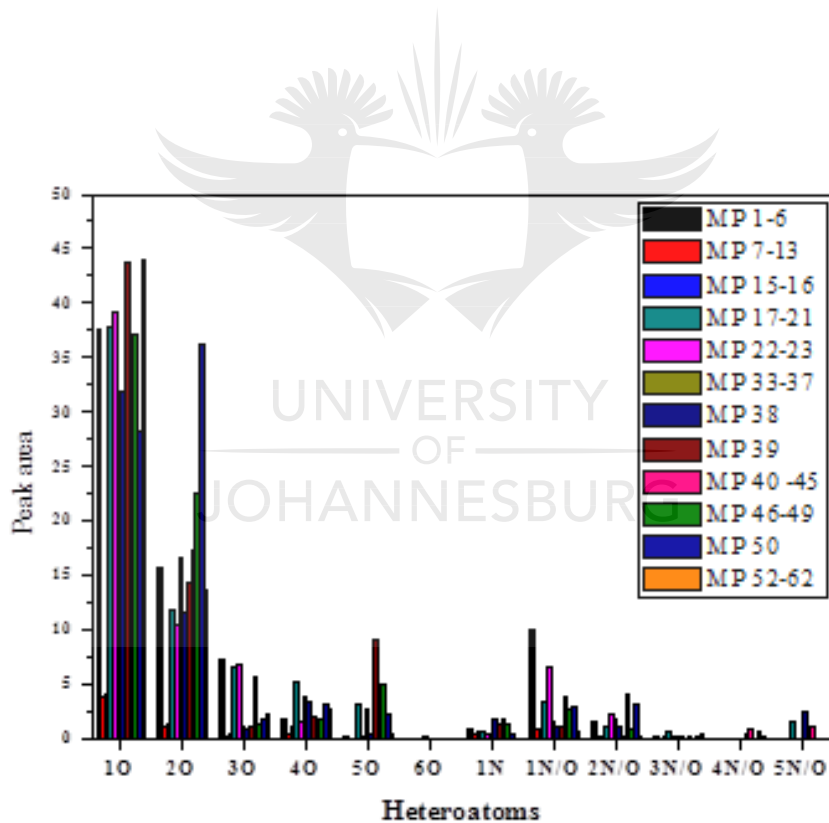


Figure 4.2 Heteroatom in different fractions.

The amount of molecules that contain 1 oxygen atom were present at a higher abundance in all the fractions except for irregular MP 7-13 and MP 15-16. MP 39 and MP 52-62, which had the least molecules with a single oxygen atom. Molecules with 2 atoms were also well represented with an

average abundance of 14 % across all fractions. This indicated that many of the molecules either had one oxygen or two oxygen atoms. Compounds with 3 and 4 oxygen atoms accounted for almost 5 % of the fractions. Molecules rich in nitrogen and molecules with both nitrogen and oxygen were not detected in large quantities; most of these compounds are shaded in red in **Table 4.2** showing low abundance.

Having studied the ‘primitive’ structural properties of the various compounds contained in the fractions analyzed, the compound classes of these molecules were also identified.

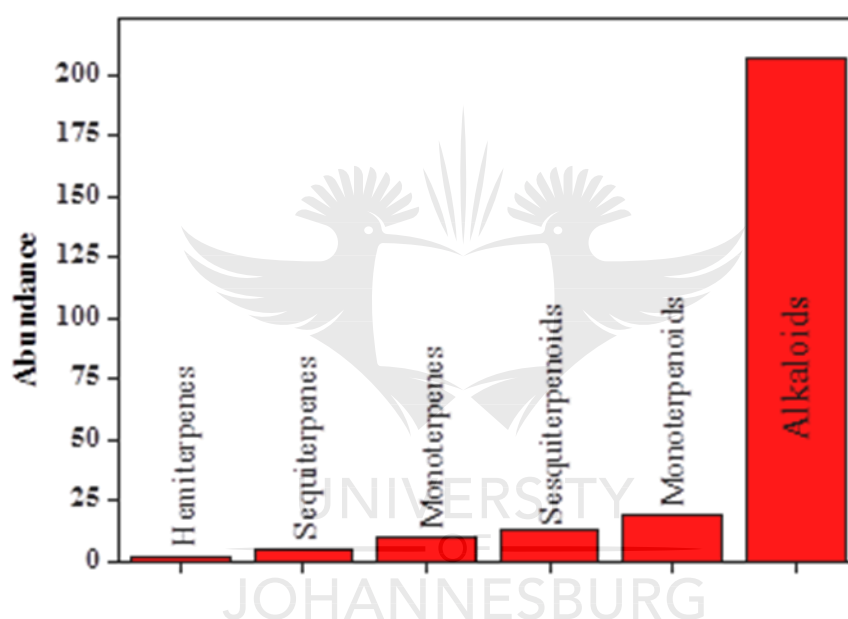


Figure 4.3 Identified classes of compounds identified in the extracts.

It was found that alkaloids formed the overwhelming majority. Terpenes and terpenoids were detected at small amounts, ranging between 2 and 19 molecules (**Figure 4.3**). It is noteworthy that the results represented in **Figure 4.3** excluded the isomers of the counted compounds (**Appendix 2**). This explains why the quantities of terpenes and terpenoids detected were smaller as they had a high number of isomers in the previous figures and tables in every fraction. Here the isomers were excluded.

The identified groups of molecules have been shown of important in the skin treatment industry and this is not only because of their properties (listed below) but also because they are biodegradable. The uses of some classes of compounds extracted in this chapter are discussed below:

Sesquiterpenes are used in skin care because of their properties that soothes the skin and have anti-inflammation properties. They also inhibit melanin formation caused by frequent shaving and antiperspirants thereby promoting skin lightening (Srivilai et al., 2017).

Terpenoids have been shown to have interesting characteristic and distinct activity patterns towards micro-organisms. Different terpenes have been demonstrated to have a synergistic effect on pathogens and bacteria (Zengin and Baysal, 2014, Mehdizadeh and Moghaddam, 2018, Li et al., 2011).

Monoterpenoids have high antioxidant activities, they are chemo-preventive and also have chemo-therapeutic activities (Zengin and Baysal, 2014) (Edris, 2007).

Alkaloids are effective for treating proliferating skin diseases such as psoriasis (Voorhees, 1977). They play an important role in modulating pro-inflammatory signaling pathways in rosacea, a chronic skin condition that affect the central face (Lanier et al., 2013).

Having identified that terpenes and terpenoids formed a significant part of the extracts; the subsequent step was to study the chain lengths of the various terpenes and terpenoids (**Figure 4.4**). It was observed that a large portion of the terpenes and terpenoids in the various extracts had molecules with 15 carbon atoms. This is consistent with what was observed when studying the number of carbon atoms in all the molecules present in the various extracts (refer back to **Figure 4.1** and **Table 4.1**). These were mainly attributed to a large number of sesquiterpenes.

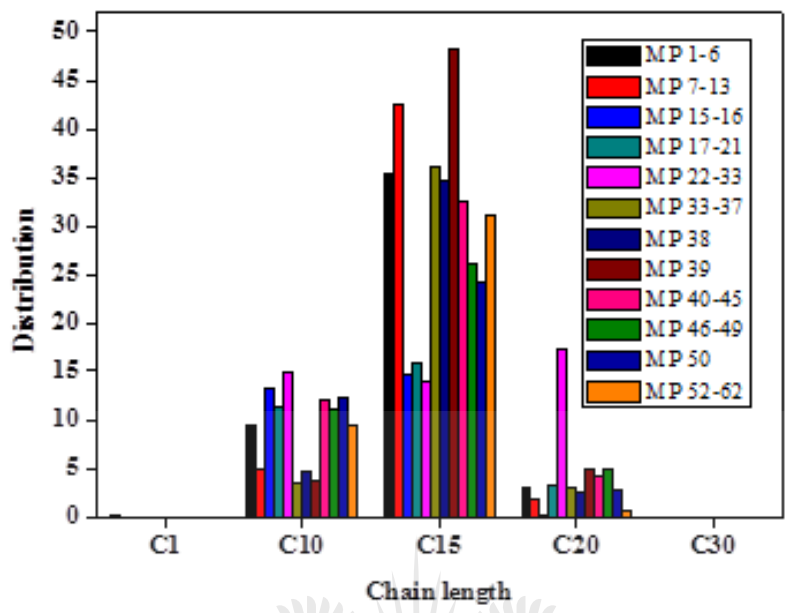


Figure 4.4 Distribution of the various terpenes and terpenoids chain lengths.

Another study was conducted in order to study what the various terpenes and terpenoids were. Here in **Figure 4.5** it was found that sesquiterpenoids and sesquiterpenes dominated in abundance among all the other terpenes and terpenoids in the analyzed fractions.

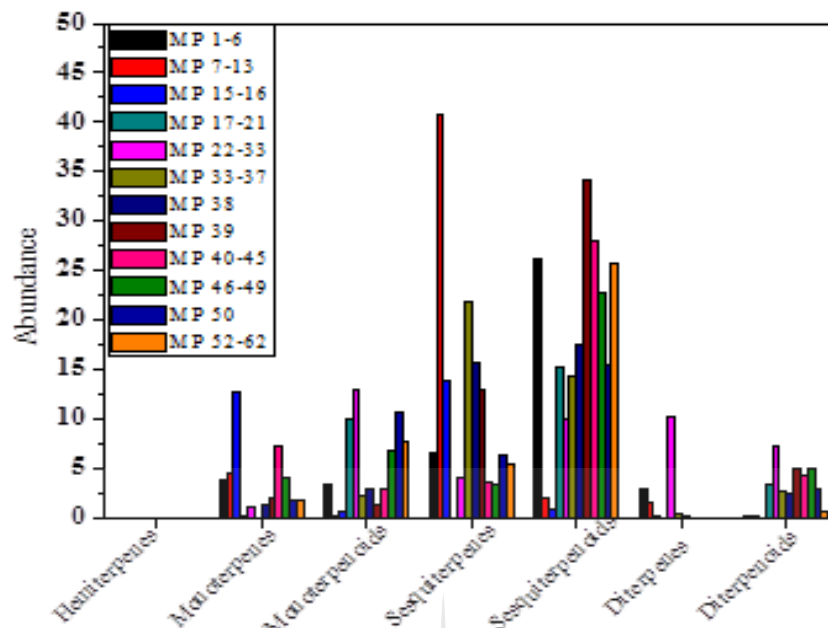


Figure 4.5 Different classes of terpenes and terpenoids found in the fractions

4.4. Conclusion

We set out to characterize volatile oil extracted in chapter 4 and identified them in this chapter using comprehensive 2D GCxGC-TOFMS. We achieved this and found that the extracts contained 207 alkaloids, 26 sesquiterpenoids, 13 sesquiterpenes, 19 monoterpenoids, 10 monoterpenes, 13 diterpenoids and 5 diterpenes and 2 hemiterpenes. This classes of compounds have already been previously demonstrated to have anti-microbial, anti-fungal, anti-oxidants, anti-inflammatory, therapeutic UV-induced skin care and chemo-therapeutic activities, and as components for human skin protection by moisturizing and soothing skin. This explains the wide use and efficacy of *curcuma longa* extracts.

CHAPTER 5. INCLUSION COMPLEX OF CURCUMIN WITH β -CYCLODEXTRIN

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Abstract

Curcumin has beneficial properties that can be used in cosmetics and in pharmaceuticals, but because of its poor physicochemical properties, its potential has not been realized. This then sparked an interest in designing delivery systems that solves the physicochemical properties of curcumin that hinder its use, *i.e.* poor solubility and low dissolution thus very low bioavailability. The β -Cyclodextrin has a hydrophobic interior that can entrap or encapsulate the lipophilic curcumin by forming an inclusion complex. On the other hand, the exterior of β -CD is hydrophilic which and this makes the entire inclusion complex more soluble in an aqueous medium. This Chapter reports the synthesis of various curcumin/ β -CD complexes. These were synthesized by co-precipitation, freeze-drying, and solvent evaporation synthetic procedures. The materials were then characterized using several analytical techniques including UV-Vis, FTIR, NMR (¹H and NOESY), SEM, PXRD, TGA-DSC where the pure β -CD and curcumin were compared with the complex formed to check for inclusion of curcumin's protons (H3, H5 and OH) and any significant changes in their morphology. Solvent evaporation method enabled complex formation as indicated by UV-Vis and IR techniques via peak vibrational changes, inclusion of H3, H5 and OH protons inside β -CD on NMR and peak disappearance on TGA-DSC.

Keywords: Curcumin, β -Cyclodextrin, Inclusion complex

5.1.Introduction

Curcumin ($C_{21}H_{20}O_6$), is a phytochemical, extracted from the dried rhizomes of the plant *Curcuma longa L* (turmeric). This chemical is responsible for most of the pharmacological activities *Curcuma longa L*. Curcumin has a bright yellow color, it is it that responsible for turmeric being used fairly successfully for improving the skin complexion (Remadevi, 2007). The poor solubility of curcumin makes it difficult for it to be able to interact sufficiently at a desired site hence its encapsulation with Cyclodextrin is required to make it more potent. Cyclodextrin form an inclusion complexes with a variety of hydrophobic molecules/drugs/actives wherein the lipophilic molecule moiety binds to the inner cavity, while the hydrophilic outer surface of the cyclodextrin helps in solubilizing the complex and by extension the lipophilic drug (Pushpalatha et al., 2018). These types of inclusion complexes have a characteristic structure of an adduct; one compound (host molecule) spatially encloses another compound (guest molecule) in the cavity of the host without affecting the host (Szejtli, 1988). Studies on complexes between Cyclodextrin (host) and guest molecules are investigated using various analytical and characterization techniques such as NMR, FTIR, DSC, XRD, X-ray crystallography, UV-Vis, mass spectroscopy, calorimetry, electrochemistry, fluorescence measurements, and chromatographic techniques. However, in this chapter, the inclusion complex was studied using FTIR, DSC, NMR (1H and NOESY), PXRD, UV-Vis, and SEM.

5.2.Materials and Method

5.2.1. Materials

Cyclodextrin and curcumin were purchased from Sigma-Aldrich (South Africa), and both were used as received. All reagents and solvents used in this Chapter were of analytical grade.

5.2.2. Method

5.2.2.1.Preparation of inclusion complexes

The general synthetic procedure for the inclusion complex of β -Cyclodextrin with curcumin was adapted from previous studies on Cyclodextrin inclusion complexes with minor changes

(Mangolim et al., 2014, Zhao et al., 2016, Lakkakula et al., 2012). The inclusion complexes were prepared by dissolving 0.6 g β -Cyclodextrin in 30 ml of deionized water for 3-5 minutes under intensive magnetic stirring (600 rpm at 60 °C) in a beaker. In another beaker, 0.1 g of curcumin was also dissolved in 5 ml acetone by swirling gently which was then added to the β -cyclodextrin solution and stirred for 8 hours at 600 rpm at room temperature. The co-precipitation, freeze-drying, and solvent evaporation synthetic procedures were also used to synthesize other β -cyclodextrin and curcumin inclusion complexes, and the details are discussed below.

5.2.2.2.Co-precipitation

An aqueous solution β -CD was prepared by dissolving 1.0 g of β -CD in 40 ml deionized water by stirring at 600 rpm kept at 60°C. In another beaker, 0.34 g of curcumin was dissolved by stirring at 600 rpm in 6 ml of ethanol at 60°C. This ethanoic solution was then added to the β -CD aqueous solution with continuous stirring. The curcumin and β -CD mixture was then refluxed with vigorous agitation at 100-140 °C for 5 minutes to remove the ethanol. The now aqueous mixture of curcumin and β -CD was then cooled to room temperature while stirring magnetically at 600 rpm for 8 h. The mixture was then stored overnight at 4 °C. The mixture was then filtered by vacuum and the collected solid was dried at 50-55 °C for 10 minutes. The obtained crystalline product was stored for further analysis

5.2.2.3.Freeze-drying

An aqueous solution of β -CD was made by dissolving 1.0 g in in 30 ml of deionized water in a 250 ml stoppered conical flask. The mixture was then magnetically stirred at 600 rpm until a clear solution was obtained. In another beaker, an ethanoic solution of curcumin was created by the dissolution of 0.5 g of curcumin in 6 ml ethanol. Another solution was prepared in a similar manner excluding ethanol. The reaction mixture was then stirred in an incubator shaker at 180 rpm for 7 days at 37 °C. Afterward, the mixture was then filtered through a 0.45 μ m filter paper and the solution was freeze-dried to obtain a solid complex which was kept for analysis.

5.2.2.4.Solvent evaporation

An aqueous solution of β -CD was made by dissolving 0.61 g in 12 ml of deionized water in a glass vial with a magnetic stirrer bar. While the solution was being stirred, 0.06 g of curcumin dissolved in 1 ml of acetone in a separate glass vial was added to the aqueous solution of β -CD. The mixture was then magnetically stirred overnight and centrifuged at 134xg for 5 min. The supernatant, which contained the complex, was collected and the complex was recovered by freeze-drying. The product was stored for analysis. This inclusion complex was the last one synthesized so therefore 4 different complex mixtures were synthesized, namely: Cur- β -CD prepared by co-precipitation method, Cur- β -CD acetone 1 and 2 prepared by solvent extraction and Cur- β -CD incubator and incubator (-ethanol) prepared by freeze-drying. The following sections describe how these inclusion complexes were characterized.

5.2.3. Characterization of solid state inclusion complex:

5.2.3.1.FTIR

Fourier transmission infrared spectroscopy (FTIR) characteristics of curcumin, β -Cyclodextrin and the various inclusion complexes were studied using a PerkinElmer Spectrum 100 spectrometer. The spectra were recorded from 4000 to 650 cm^{-1} in attenuated total reflectance (ATR) mode fitted with a germanium crystal. The samples were analyzed in solid form without further modifications.

5.2.3.2.UV-Vis

The absorption characteristics in the ultraviolet-visible light part of the spectrum of curcumin, β -cyclodextrin and the various inclusion complexes were analyzed using Shimadzu UV-2450 UV-Vis spectrophotometry. The absorption spectra were collected at wavelengths between 200 to 700 nm. In order to carry out these analyses, 0.01 g of each of the samples was diluted separately in 50 ml of ethanol and filtered through a 0.45 μm filter.

5.2.3.3.NMR

The ^1H NMR spectra of curcumin, β -cyclodextrin and the different inclusion complexes were recorded using a BRUKER Avance 500 MHz spectrometer. The samples were prepared by weighing 10 mg of the different samples and separately dissolved in 0.4 ml of DMSO and referenced to residual solvent. 2D-NOESY experiments were carried out in phase sensitive mode, set up applying a continuous wave with spinlock for mixing.

5.2.3.4.SEM

The specimens of the various inclusion complexes, curcumin and β -cyclodextrin were prepared by individually placing small amounts of the powder onto a 2-sided carbon tape immobilized on a stub. The individual specimens were gold coated using scope SC 500 and then examined on a VEGA3 TESCAN scanning electron microscope (SEM) at an accelerating voltage 20kV.

5.2.3.5.PXRD

The powder X-ray diffraction patterns of the various samples, which were analyzed as they were, (curcumin, β -cyclodextrin and the different inclusion complexes) were recorded using X-Pert PRO, PANalytical diffractometer system, operated at a voltage of 40kV and a current of 40mA. The diffraction patterns were collected at a 2θ angle range of 4-90 ° at a step size of 0.0170 seconds.

5.2.3.6.TGA-DSC

The thermal gravimetric analysis coupled with Differential scanning calorimetry analyses of the various samples (curcumin, β -cyclodextrin and the different inclusion complexes) were carried out at a temperature range of 25-350°C ramped at 10 °C/min. The analyses were conducted in a nitrogen environment maintained at 40 ml/min. The individual sample specimens were prepared by weighing 7.5 mg onto an aluminum pan whereas an empty aluminum pan was used as a reference.

5.3. Results and Discussion

5.3.1. Fourier transmission infrared spectroscopy (FTIR)

FTIR spectroscopy is an important tool giving information about vibrations inside the molecule confirming the formation of an inclusion complex. Thus any changes in the signal intensity or frequency of the inclusion complex give information about the complex formation (Lakkakula et al., 2012). FTIR spectra of pure curcumin and β -CD were discussed in the tables below (**Table 5.1** and **Table 5.2**).

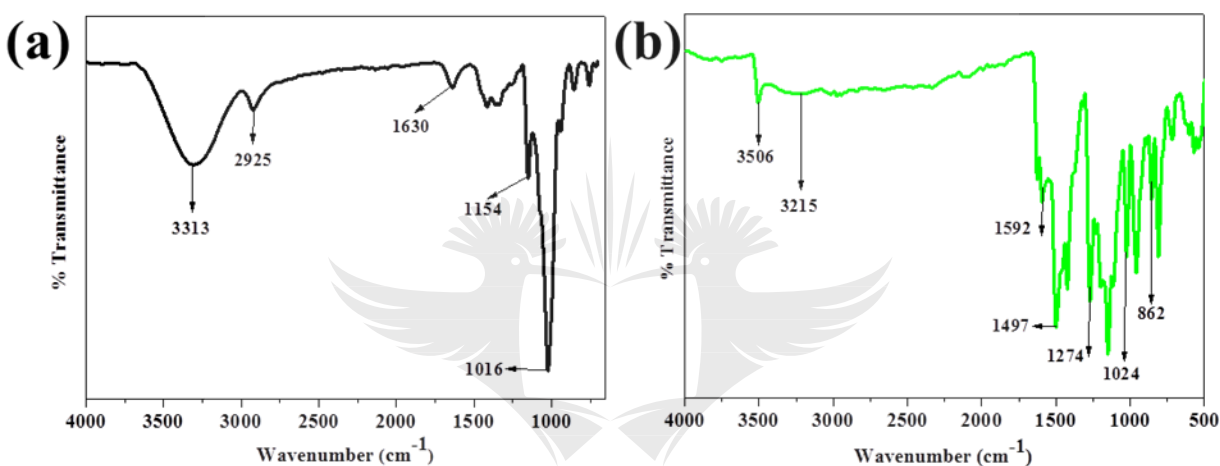


Figure 5.1 FTIR spectrum of (a) β -Cyclodextrin and (b) Curcumin

Table 5.1 FTIR results of pure β -CD

Wavenumber (cm-1)	Functional Groups
3303	Broad band of OH stretching
2919	C-H asymmetric and symmetric stretching
1619	H-O-H water bands in CD
1151 and 1013	C-H and C-O stretching

Table 5.2 FTIR results of pure curcumin

Wavenumber (cm-1)	Functional Groups
3494	Phenolic OH stretching
1588	Benzene ring stretching
1502	C=O vibration
1237	The enol C-O peak
810	C-O-C stretching

The FTIR spectra of all the inclusion complexes synthesized were similar to the FTIR spectrum of β -Cyclodextrin (**Figure 5.2**). The most important vibrational change was observed for the peaks belonging to curcumin. Benzene ring peak of 1588 cm⁻¹ disappear in solvent extraction method for acetone 1. This change is brought about the entrapment of the ring inside β -CD cavity by van der Waal forces, hydrophobic interactions and formation of curcumin hydrogen bond inside the cavity as a result of its electron donor group (Rachmawati et al., 2013). However, the inclusion complex of curcumin in β -CD, shifted peaks of β -CD to either high or low wavenumber, i.e., 3303-3292, 2919-2897, 1013-1023 cm⁻¹ and curcumin peaks 1588-1589, 1237-1290, 810-788 cm⁻¹. All

this changes were observed for co-precipitation, solvent extraction and freeze-drying methods. Therefore this data suggest the inclusion complex formation of curcumin/ β -CD.

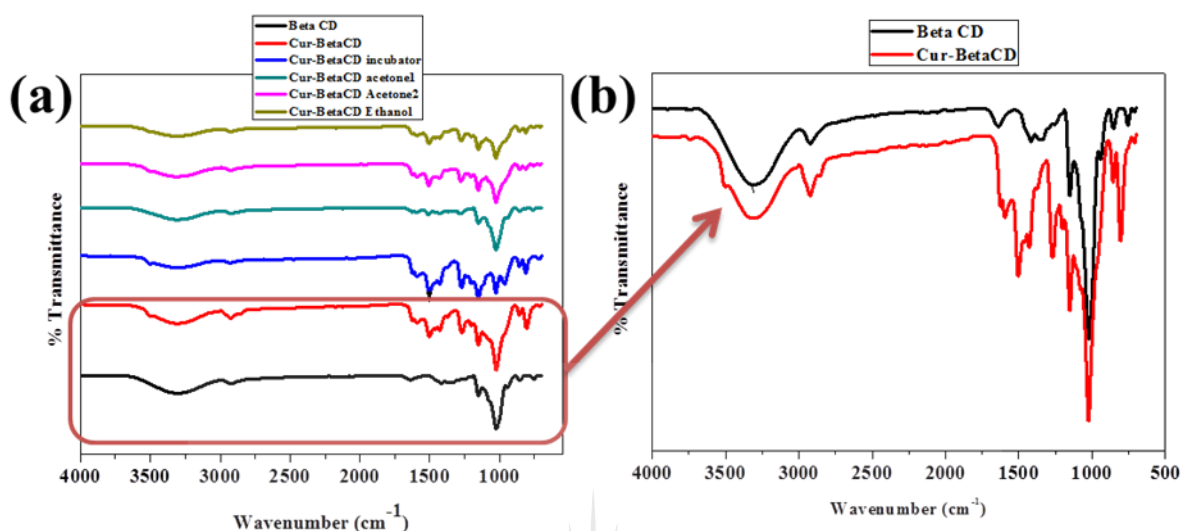


Figure 5.2 FTIR spectra of (a) β -Cyclodextrin and the inclusion complexes (b) enlargement of the FTIR spectra of β -Cyclodextrin and the inclusion complex labelled Cur-BetaCD.

5.3.2. Ultraviolet spectroscopy (UV-Vis)

Ultraviolet spectroscopy measurements were conducted in order to further investigate if inclusion complexes between β -Cyclodextrin and curcumin were synthesized using different methods. This is possible because both β -Cyclodextrin and curcumin have different chromophores therefore will absorb UV light at different wavelengths, and the difference observed on the UV spectra of the inclusion complexes may show evidence of complexation. First, the UV absorption signature of β -Cyclodextrin and curcumin were studied (**Figure 5.3**). Here, it was observed that β -Cyclodextrin absorbed UV light at 290 and 313 nm whereas the UV spectrum of curcumin absorbed at 420 nm with a shoulder at 442 nm, assuming existence of more than one isomeric form.

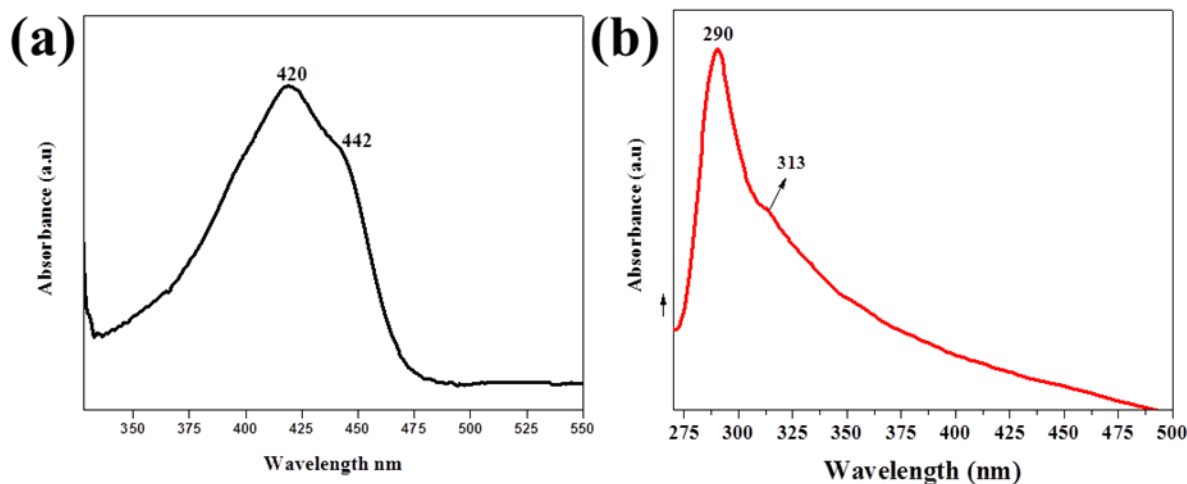


Figure 5.3 UV-Vis spectrum of (a) Curcumin and (b) β -Cyclodextrin

On the other hand, when investigating the UV-Vis spectra of the various inclusion complexes, it was observed that they were similar to that of curcumin (**Figure 5.4**). Indeed, the peak observed at 420 for curcumin was observed at 419 for the inclusion complexes and there were no absorption of β -Cyclodextrin peaks. This could mean that the benzene ring of curcumin possessing methoxy phenolic group was successfully entrapped within the cavity of β -Cyclodextrin. It was also expected that the absorption peaks of curcumin when complexed with β -Cyclodextrin would be enhanced to the shielding of excited species and increased molar absorption coefficient of curcumin/ β -CD (JA et al., 2018). Solvent extraction method for both Acetone 1 and 2 showed better results on UV-Vis and FTIR, as compared to the other methods of synthesis, therefore the inclusion complex of solvent extraction was further investigated on NMR.

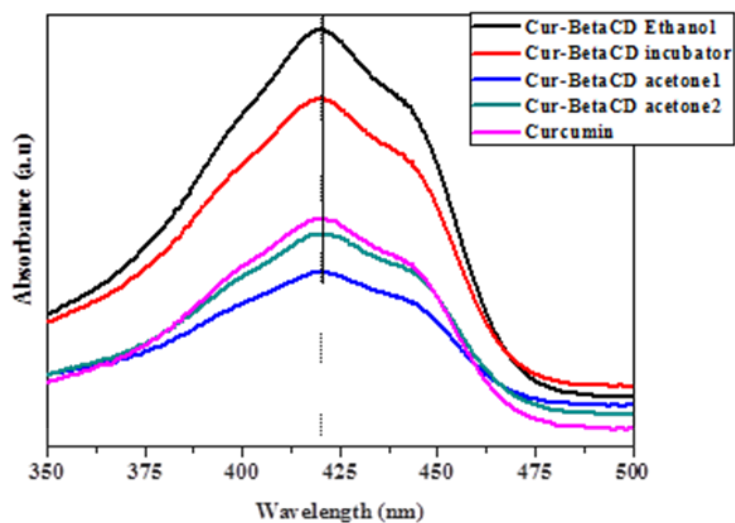


Figure 5.4 UV-Vis spectrum of Curcumin and the various inclusion complexes

5.3.3. Nuclear Magnetic Resonance (NMR) study

5.3.3.1. Proton NMR (^1H NMR)

In order to further investigate if inclusion complexes were formed, ^1H NMR experiments were conducted on curcumin, β -cyclodextrin and the various inclusion complexes. The aim here was to investigate if there would be changes to the chemical shifts of the protons of β -cyclodextrin when complexed with curcumin. This would be an indication if complexation has occurred or not (de Paula et al., 2011). The ^1H NMR spectra for β -CD (**Figure 5.5a**), curcumin (**Figure 5.5b**) and inclusion complexes (**Figure 5.5c** & **Figure 5.5d**) were studied and compared. In the inclusion complex, the protons (H-5, H-3) inside β -CD internal cavity shift when the guest molecule is placed inside the β -CD cavity (Jahed et al., 2014). The chemical shift changes ($\Delta\delta$) was used to identify the difference in chemical shift in the presence and absence of other molecules. The negative sign is given to downfield shift and a positive sign means an up-field shift. Comparing the chemical shift changes of free β -CD and presence of curcumin in the complex, the internal cavity protons (H-3, H-5) are shielded. This is attributed to the up-field shift ($\Delta\delta = \text{positive}$). The external protons (H-4, H-1) as well, showed a chemical change by shifting towards a negative atom in the downfield region ($\Delta\delta = \text{negative}$). Graph (d), showed the opposite with internal proton

(H-5) in a down-shield region. The narrow rim protons (H-6), showed an up-field shift, shifting the protons in a shielding environment. The chemical shift changes results are tabulated in **Table 5.3, Table 5.4, Table 5.5** and **Table 5.6**. In the ¹H NMR spectra of inclusion complex in **Figure 5.5** we see the peaks attributed to the methoxy protons (-OCH₃) attached to the aromatic ring appearing at position δ (ppm) = 3.813 (**Figure 5.5c**) and 3.818 ppm (**Figure 5.5d**). The peaks attributed to protons H2 and H2', appeared at position = 7.286 ppm (**Figure 5.5c**) and 7.296 ppm (**Figure 5.5d**). Comparing this results with that of free curcumin, we observed that the signals for -OCH₃ protons undergo a shift suggesting that aromatic rings of curcumin are complexed inside the β -CD cavity (Jahed et al., 2014). Same thing with -CH₂ protons.

5.3.3.2. Nuclear Overhauser Effect Spectroscopy (NOESY)

The formation of inclusion complex was further studied using 2D NOESY NMR. NOESY investigate intermolecular interactions and provide information about conformation of inclusion complex (Raovv et al., 2013), as well as the distances and relative orientation of the host and guest molecules in a complex (de Paula et al., 2011). On NOESY spectrum in **Figure 5.6**, the cross peak aligning to the diagonal peak, is NOE peak. Both curcumin/ β -CD Acetone 1 and Acetone 2 spectra gave similar results. It is observed that H2, H3 and H5 from β -CD internal and external cavity correlates with aromatic (H2, H2') and OH protons of curcumin. It can be concluded that the aromatic ring of curcumin has been sheltered/ accommodated inside the β -CD cavity.

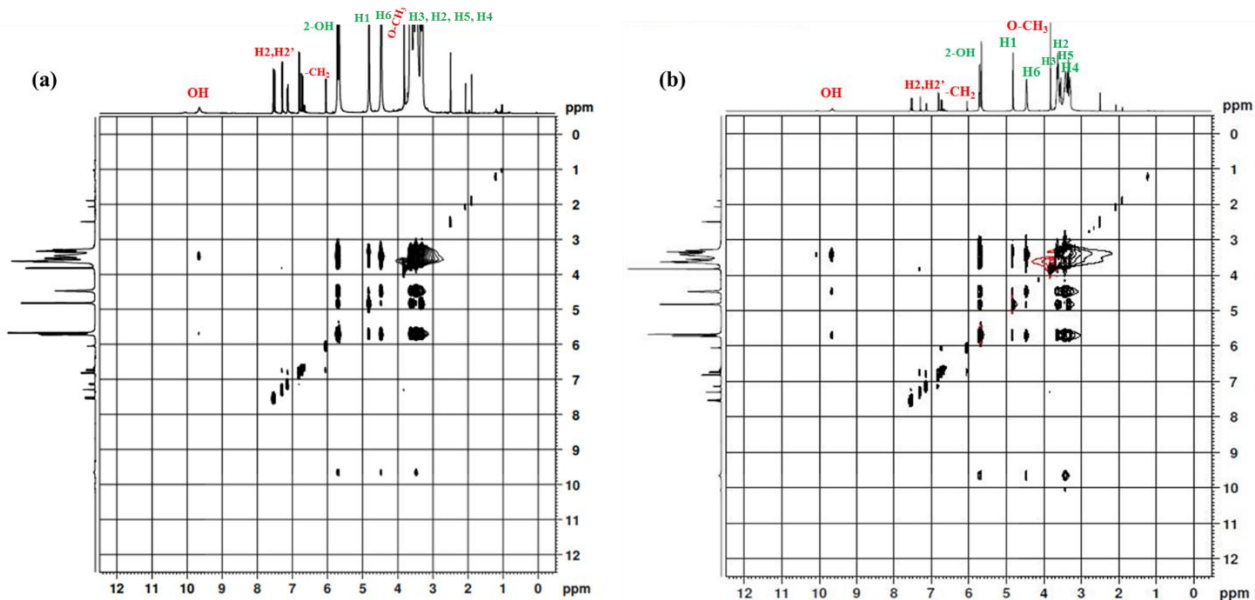


Figure 5.6 NOESY NMR of (a) Cur/B-CD Acetone 1 and (b) Cur/B-CD Acetone 2

Table 5.3 ^1H NMR chemical shift of protons of β -CD free and complexed (prepared in acetone 1) with curcumin in DMSO

^1H assignment	δ β -CD _{free} (ppm)	δ β -CD _{complexed} Acetone 1 (ppm)	Δ (β -CD _{complexed} - β -CD _{free}) (ppm)
H4	3.539	3.535	-0.004
H5	3.562	3.615	0.053
H2	3.591	3.634	0.043
6-OH	4.446	4.446	0
H3	3.641	3.710	0.069
H1	4.818	4.816	-0.002
2-OH	5.712	5.716	0.004

Table 5.4 ^1H NMR chemical shift of protons of β -CD free and complexed (prepared in acetone 2) with curcumin in DMSO

^1H assignment	δ β -CD _{free} (ppm)	δ β -CD _{complexed} Acetone 2 (ppm)	Δ (β -CD _{complexed} – β -CD _{free}) (ppm)
H4	3.539	3.540	0.001
H5	3.562	3.559	-0.003
H2	3.591	3.606	0.009
6-OH	4.446	4.455	0.015
H3	3.641	3.715	0.074
H1	4.818	4.813	-0.005
2-OH	5.712	5.717	0.005

Table 5.5 ^1H NMR chemical shift of protons of curcumin free and complexed (in acetone 1) with β -CD in DMSO

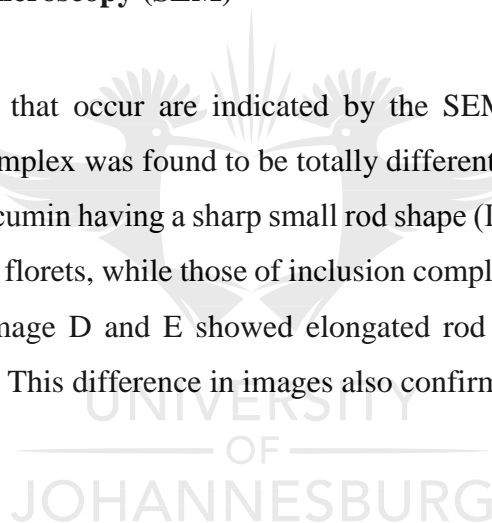
^1H assignment	δ Curcumin _{free} Acetone 1 (ppm)	δ Curcumin _{complexed} (ppm)	Δ (Curcumin _{complexed} – Curcumin _{free}) (ppm)
H2,H2'	7.312	7.286	0.026
-OCH ₃	3.829	3.813	0.016

Table 5.6 ^1H NMR chemical shifts of protons of curcumin free and complexed (in acetone 2) with β -CD in DMSO

^1H assignment	δ Curcumin _{free} Acetone 2 (ppm)	δ Curcumin _{complexed} (ppm)	Δ (Curcumin _{complexed} – Curcumin _{free}) (ppm)
H ₂ ,H ₂ '	7.312	7.296	0.016
-OCH ₃	3.829	3.818	0.011

5.3.4. Scanning electron microscopy (SEM)

The morphological changes that occur are indicated by the SEM study. The morphology of curcumin- β -CD inclusion complex was found to be totally different from that of curcumin and β -CD in **Image 5.1** below. Curcumin having a sharp small rod shape (Image B) and the β -CD (Image A) showed presence of small florets, while those of inclusion complex were different images from free β -CD and curcumin. Image D and E showed elongated rod like shape whereas Image C showed a folded feather like. This difference in images also confirms complexation.



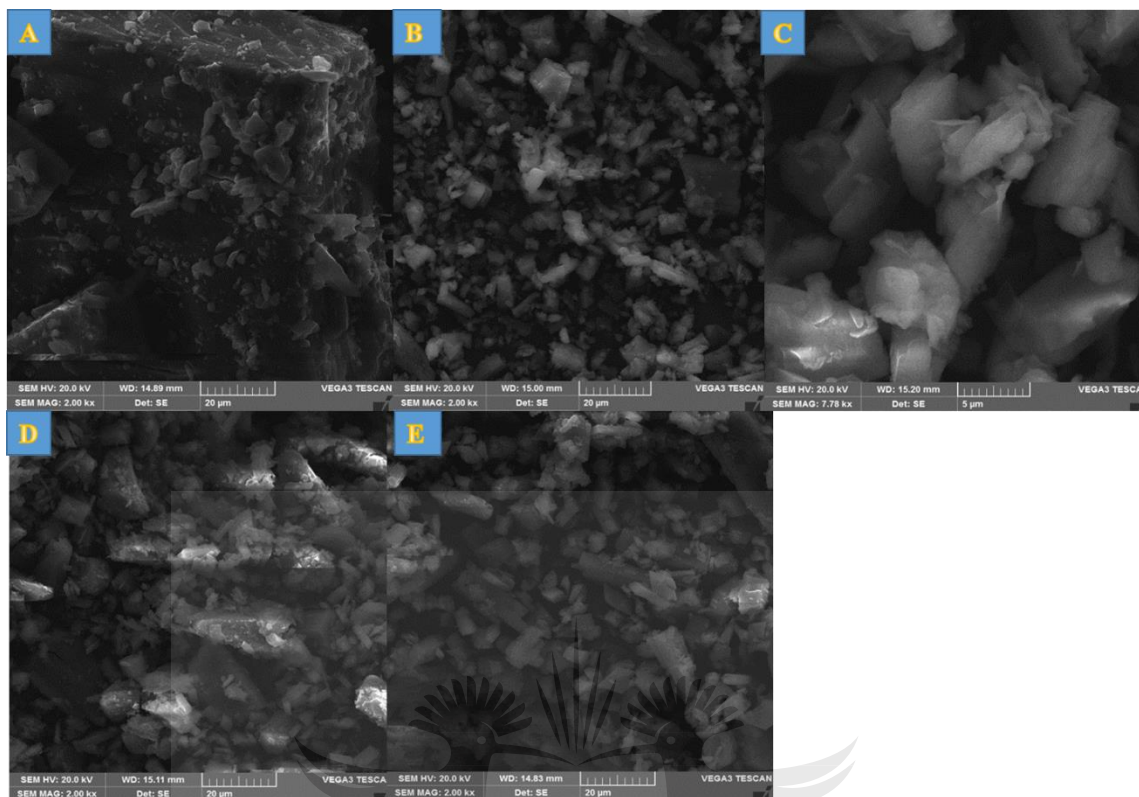


Image 5.1 SEM images of (a) β -CD (b) Curcumin (c) Curcumin/ β -CD complex (d) Curcumin/ β -CD Acetone 1 (e) Curcumin/ β -CD Acetone 2

5.3.5. Powder X-ray diffraction (XRD) study

When a molecule forms an inclusion complex, the diffraction pattern of the inclusion complex formed will be different from that of the pure host and guest molecules. The diffractograms of curcumin and β -CD obtained here in **Figure 5.7**, exhibited a series of sharp intensive lines indicating their crystallinity. The most thin intense peaks of curcumin were observed at $2\theta = 8.98^\circ$ and 17.95° , which disappear in graph c, f and g. Similar to curcumin, the most intense peaks of β -CD that appeared at $2\theta = 4.35^\circ$, 8.86° and 10.04° disappeared in the complex. This changes confirms formation of inclusion complex. Additionally, there's appearance of intense peaks at $2\theta = 10.01^\circ$, 11.99° , 14.87° , 18.20° and 19.01° , indicating the presence of new solid crystalline phases that corresponds to an inclusion complex of the same nature (Mangolim et al., 2014).

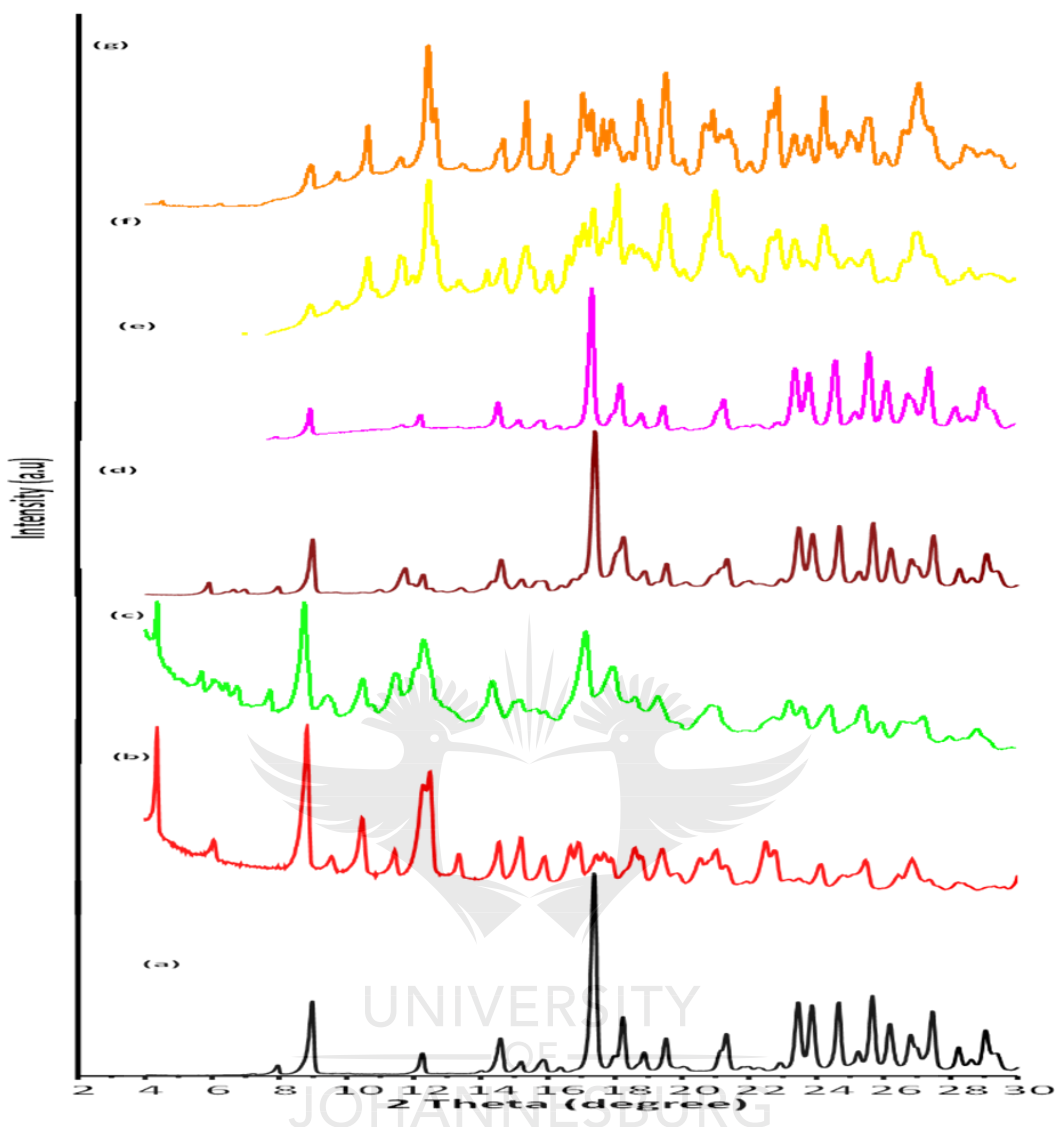


Figure 5.7 PXRD results of (a) Curcumin (b) β -CD (c) Curcumin/ β -CD complex (d) Incubator Curcumin/ β -CD complex (e) Incubator Curcumin/ β -CD complex excluding ethanol (f) Acetone 1 Curcumin/ β -CD complex (g) Acetone 2 Curcumin/ β -CD complex

5.3.6. Differential thermal analysis (DTA)

Thermal techniques are widely employed for analysis and stability evaluation of Cyclodextrin complexes, where the formation of Cyclodextrin inclusion complexes is evidenced by disappearance of the thermal characteristics (melting or boiling points) of the guest molecule after encapsulation (Hădărugă et al., 2018). In this study, the thermal stability of Curcumin/ β -CD was

evaluated using DTA and the results were compared with that of free β -CD and curcumin in **Figure 5.8**. Free β -CD in both graph **A** and **B**, show a broad endothermic peak at 100 °C, corresponding to water loss in β -CD cavity, while degradation appears from 310 to 330 °C. No effect is observed between 125 and 290 °C. In the inclusion complex graph, the endothermic peak belonging to curcumin at 168 °C disappears due to the encapsulation of curcumin in the cavity of β -CD.

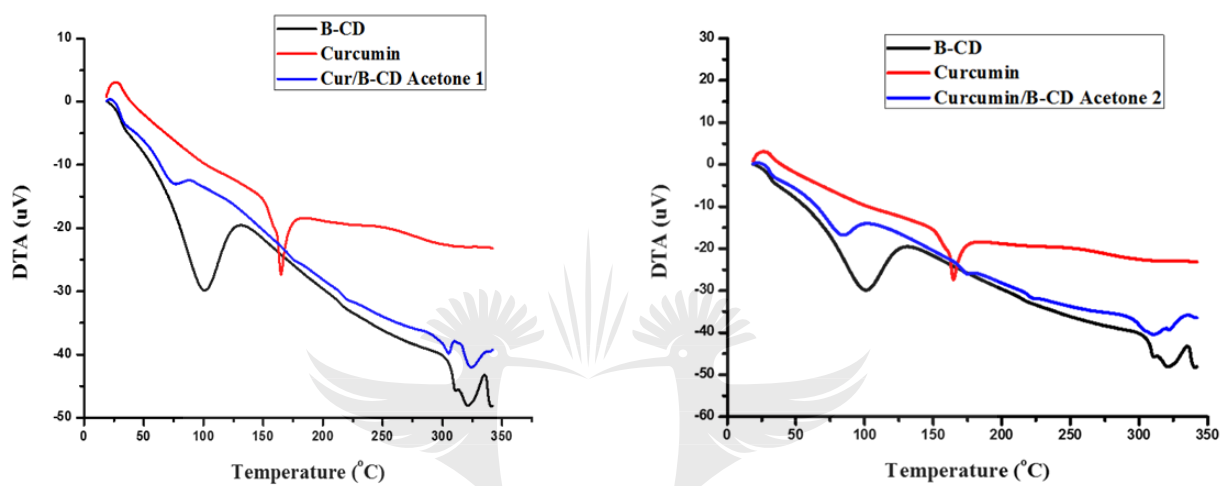


Figure 5.8 Differential thermal studies of β -CD, curcumin and Cur/ β -CD prepared in **A**) Acetone 1 and **B**) Acetone 2

5.4. Conclusion

Curcumin physicochemical characteristics of poor solubility and dissolution, limit its application hence the use of delivery systems to improve this physicochemical properties. Therefore the objective of this chapter was to improve curcumin disadvantages by forming inclusion complex with β -CD. The inclusion complex was prepared by co-precipitation, freeze-drying and solvent evaporation methods. Solvent showed good results in all characterization techniques, hence this method was further used for all characteristics. This was achieved as the pure β -CD and curcumin results obtained in all characterization were different from those of the inclusion complex which confirms that there was inclusion of guest curcumin in the β -CD cavity.

CHAPTER 6. CONCLUSION AND RECOMMENDATIONS

6.1. Conclusions

This research was conducted to study and analyze the extracts from *Curcuma longa*, *L.* plant in order to find safer actives that can be incorporated in skin care cosmetics. The extract of this plant contained curcuminoids, phenolics, carbohydrates, antioxidants and sugars and further phytochemical studies of the plant secondary metabolites on GCxGC/TOF-MS showed that the plant is rich with alkaloids, terpenoids and terpenes which have been used in skin care as good classes of compounds for skin treatment and protection.

Most plant extracts contain actives that have low efficacy in physiological conditions, *Curcuma longa* is also one of the plant that contains actives (curcuminoids) with low efficacy. Curcuminoids gave this plant recognition as a medicinal plant because of their studied pharmacological activities on cancer, diabetes, inflammation, aging and etc. Curcuminoids which are made of curcumin, demethoxycurcumin and *bis*-methoxycurcumin, were isolated in this research. Curcumin is the most bioactive compound of this *Curcuma longa*, which was further analyzed in novel delivery system. The low efficacy of curcumin, led to novel delivery system using β -Cyclodextrin to form inclusion complex. This complexation protects curcumin from oxidation and degradation by improving its chemical and physical properties. The inclusion complex was formed by coprecipitation, solvent evaporation and freeze-drying method. Solvent evaporation gave good results in all characterization techniques (UV-Vis, IR, NMR, PXRD, TGA, SEM) of the complex.

6.2. Recommendations

Cyclodextrin inclusion complexes are designed in such a way that the encapsulated drug or actives be delivered to the desired site in a controlled manner. Therefore, it is recommended that release profiles of curcumin/ β -CD complex in topical application be studied to see how long curcumin can be prolonged between 1 to 5 days on skin when applied to area of interest. This will be useful in skin care as it will help in reducing re-application of a lotion while delivering the active to the

targeted site. This complex can be incorporated in sunscreens and gels since curcumin has documented use as a sun protection active and possess wound healing properties.

Both curcumin and β -CD are non-toxic, making it of safe use in skin treatment. Therefore this complex can also be further studied in clinical trials for treatment melasma, skin pigmentation, as a safer method that will phase out the uses of toxic chemicals (hydroquinone) and methods (chemical peel) on skin tanning.



REFERENCES

1999. Turmeric for treating skin disorders. Google Patents.
- AFZAL, A., ORIQAT, G., AKRAM KHAN, M., JOSE, J. & AFZAL, M. 2013. Chemistry and biochemistry of terpenoids from *Curcuma* and related species. *Journal of Biologically Active Products from Nature*, 3, 1-55.
- AGGARWAL, B. B., BHATT, I. D., ICHIKAWA, H., AHN, K. S., SETHI, G., SANDUR, S. K., NATARAJAN, C., SEERAM, N. & SHISHODIA, S. 2006. 10 Curcumin—Biological and Medicinal Properties.
- AKRAM, M., SHAHAB-UDDIN, A. A., USMANGHANI, K., HANNAN, A., MOHIUDDIN, E. & ASIF, M. 2010. *Curcuma longa* and curcumin: a review article. *Romanian Journal of Biology - Plant Biology*, 55, 65-70.
- AMALRAJ, A., PIUS, A., GOPI, S. & GOPI, S. 2017. Biological activities of curcuminoids, other biomolecules from turmeric and their derivatives—A review. *Journal of traditional and complementary medicine*, 7, 205-233.
- AMALRAJ, A., PIUS, A., GOPI, S. & GOPI, S. 2016. Biological activities of curcuminoids, other biomolecules from turmeric and their derivatives—A review. *Journal of traditional and complementary medicine*, 7, 205-233.
- AMIRI, S. & AMIRI, S. 2017. *Cyclodextrins: properties and industrial applications*, John Wiley & Sons.
- AMMALA, A. 2013. Biodegradable polymers as encapsulation materials for cosmetics and personal care markets. *International journal of cosmetic science*, 35, 113-124.
- AMMON, H. P. A. W., M.A. 1991. Pharmacology of *Curcuma longa*. *Planta medica*, 57, 1-7.
- ARAKANE, K. & NARU, E. 2015. UV care. *Cosmeceuticals and Active Cosmetics*, 281.
- ARAUJO, C. & LEON, L. 2001. Biological activities of *Curcuma longa* L. *Memórias do Instituto Oswaldo Cruz*, 96, 723-728.
- ARAUJO, C. A. C. L., L.L. 2009. Biological activities of *Curcuma longa* L. *Memórias do Instituto Oswaldo Cruz*, 96, 723-728.
- ARAÚJO, M. C. P., ANTUNES, L. M. & TAKAHASHI, C. S. 2001. Protective effect of thiourea, a hydroxyl-radical scavenger, on curcumin-induced chromosomal aberrations in an in vitro mammalian cell system. *Teratogenesis, carcinogenesis, and mutagenesis*, 21, 175-180.
- AZUINE, M. & BHIDE, S. 1994. Adjuvant chemoprevention of experimental cancer: catechin and dietary turmeric in forestomach and oral cancer models. *Journal of ethnopharmacology*, 44, 211-217.
- BICKERS, D. R. & ATHAR, M. 2006. Oxidative stress in the pathogenesis of skin disease. *Journal of Investigative Dermatology*, 126, 2565-2575.
- BOMMARITO, A. A. 2010. Topical turmeric skin care products. Google Patents.
- BREWSTER, M. E. & LOFTSSON, T. 2007. Cyclodextrins as pharmaceutical solubilizers. *Advanced drug delivery reviews*, 59, 645-666.
- BRIGANTI, S. & PICARDO, M. 2003. Antioxidant activity, lipid peroxidation and skin diseases. What's new. *Journal of the European Academy of Dermatology and Venereology*, 17, 663-669.
- BURKE, K. E. 2006. Topical nutritional antioxidants. *Cosmetic science and technology series*, 30, 377-402.
- BUSCHMANN, H.-J. & SCHOLLMEYER, E. 2002. Applications of cyclodextrins in cosmetic products: a review. *Journal of cosmetic science*, 53, 185-192.

- CARSON, C. F. & HAMMER, K. A. 2011. Chemistry and bioactivity of essential oils. *Lipids and essential oils as antimicrobial agents*, 203-238.
- CHATTOPADHYAY, I., BISWAS, K., BANDYOPADHYAY, U. & BANERJEE, R.K. 2004. Turmeric and curcumin: Biological actions and medicinal applications. *Current science-Bangalore*, 87, 44-53.
- CHEN, Q. 2009. Evaluate the effectiveness of the natural cosmetic product compared to chemical-based products. *International Journal of Chemistry*, 1, 57.
- COWAN, M. M. 1999. Plant products as antimicrobial agents. *Clinical microbiology reviews*, 12, 564-582.
- DAMALAS, C. A. 2011. Potential Uses of Turmeric ('*Curcuma longa*') Products as Alternative Means of Pest Management in Crop Production. *Plant Omics*, 4, 136.
- DE PAULA, E., RIBEIRO DE ARAUJO, D. & FRACETO, L. F. 2011. Nuclear Magnetic Resonance Spectroscopy tools for the physicochemical characterization of cyclodextrins inclusion complexes. *ChemInform*, 42, no-no.
- DREHER, F., THIELE, J. & LEVIN, J. 2015. Antioxidants. *Cosmeceuticals and Active Cosmetics*, 3, 177-190.
- EBELER, S. E. & MITCHELL, A. E. 2015. Analytical Chemistry of Botanical Extracts. *Cosmeceuticals and Active Cosmetics*, 411.
- EDRIS, A. E. 2007. Pharmaceutical and therapeutic potentials of essential oils and their individual volatile constituents: a review. *Phytotherapy Research: An International Journal Devoted to Pharmacological and Toxicological Evaluation of Natural Product Derivatives*, 21, 308-323.
- EIGNER, D. S., D 1990. Das Zauberbüchlein der Gyani Dolma. *Pharmazie in unserer Zeit*, 19, 141-152.
- EL-SAYED, N. & SAFAR, E. 2014. A brief insight on anti-Toxoplasma gondii activity of some medicinal plants. *Aperito Journal of Bacteriology, Virology Parasitology*, 1, 2.
- GAZORI, T., KHOSHAYAND, M. R., AZIZI, E., YAZDIZADE, P., NOMANI, A. & HARIRIAN, I. 2009. Evaluation of Alginate/Chitosan nanoparticles as antisense delivery vector: formulation, optimization and in vitro characterization. *Carbohydrate Polymers*, 77, 599-606.
- GEDIYA, S. K., MISTRY, R. B., PATEL, U. K., BLESSY, M. & JAIN, H. N. 2011. Herbal plants: used as a cosmetics. *Journal of Natural Products and Plant Resources*, 1, 24-32.
- GUJRAL, M., CHOWDHURY, N. & SAXENA, P. 1953. The effect of certain indigenous remedies on the healing of wounds and ulcers.
- GUPTA, S., BANSAL, R., GUPTA, S., JINDAL, N. & JINDAL, A. 2013. Nanocarriers and nanoparticles for skin care and dermatological treatments. *Indian dermatology online journal*, 4, 267.
- HĂDĂRUGĂ, N. G., BANDUR, G. N. & HĂDĂRUGĂ, D. I. 2018. Thermal Analyses of Cyclodextrin Complexes. In: FOURMENTIN, S., CRINI, G. & LICHTFOUSE, E. (eds.) *Cyclodextrin Fundamentals, Reactivity and Analysis*. Cham: Springer International Publishing.
- HAMMER, K. A. & CARSON, C. F. 2011. Antibacterial and antifungal activities of essential oils. *Lipids and essential oils as antimicrobial agents*. Chichester: John Wiley & Sons, 255-306.
- HANDOG, E. B. & MACARAYO, M. J. E. 2011. Melasma. *Color Atlas of Chemical Peels*. Springer.

- HANS, M. & LOWMAN, A. 2002. Biodegradable nanoparticles for drug delivery and targeting. *Current Opinion in Solid State and Materials Science*, 6, 319-327.
- HAQUE, M. I., UDDIN, M. K. & AKTER, S. 2017. Value Chain Development and Technology Practices of Spice Crop Research and Development in Bangladesh Cardamom (small and large), Ginger, Turmeric, Black Pepper and Cinnamon. *Challenges and Opportunities in Value Chain of Spices in South Asia. SAARC Agriculture Centre*, 12.
- HAYAISHI, O. & IMAMURA, S. 1988. The biological role of reactive oxygen species in skin. *Book reviews*, 18.
- HENG, M. C. 2015. Curcumin in Cosmetics: Biochemical Basis for Skin Repair with Use of Topical Curcumin. *Cosmeceuticals and Active Cosmetics*, 31.
- HOUGEIR, F. G. & KIRCIK, L. 2012. A review of delivery systems in cosmetics. *Dermatologic therapy*, 25, 234-237.
- HSIEH, C. Y. 2001. Phase I clinical trial of curcumin, a chemopreventive agent, in patients with high-risk or pre-malignant lesions. *Anticancer research*, 21, 2895-2900.
- JA, M. H., KAMAL, N., HUI, B. Y. & FAHMI, M. 2018. Inclusion of Curcumin in β -cyclodextrins as Potential Drug Delivery System: Preparation, Characterization and Its Preliminary Cytotoxicity Approaches. *Sains Malaysiana*, 47, 977-989.
- JAHED, V., ZARRABI, A., BORDBAR, A.-K. & HAFEZI, M. S. 2014. NMR (1H, ROESY) spectroscopic and molecular modelling investigations of supramolecular complex of β -cyclodextrin and curcumin. *Food chemistry*, 165, 241-246.
- JAYAPRAKASHA, G., RAO, L. J. & SAKARIAH, K. 2006. Antioxidant activities of curcumin, demethoxycurcumin and bisdemethoxycurcumin. *Food chemistry*, 98, 720-724.
- JAYAPRAKASHA, G. K., NEGI, P. S., ANANDHARAMAKRISHNAN, C. & SAKARIAH, K. K. 2001. Chemical composition of turmeric oil-A byproduct from turmeric oleoresin industry and its inhibitory activity against different fungi. *Zeitschrift für Naturforschung C*, 56, 40-44.
- JURENKA, J. S. 2009. Anti-inflammatory properties of curcumin, a major constituent of *Curcuma longa*: a review of preclinical and clinical research. *Alternative medicine review*, 14.
- KAPOOR, V. 2005. Herbal cosmetics for skin and hair care.
- KHAIAT, A. & SALIOU, C. 2015. Botanical Extracts. *Cosmeceuticals and Active Cosmetics*, 385.
- KHARE, C. & CHOPRA, R. N. 2000. *Indian herbal therapies*, Vishv Books.
- KHOR, T. O. K., A.N.T 2016. Curcumin from Turmeric Spice, Anti-inflammatory and Antioxidant Phytochemical, and Cancer Prevention. *Inflammation, Oxidative Stress and Cancer: Dietary Approaches for cancer*, 343-354.
- KOCHER, A., SCHIBORR, C., BEHNAM, D. & FRANK, J. 2015. The oral bioavailability of curcuminoids in healthy humans is markedly enhanced by micellar solubilisation but not further improved by simultaneous ingestion of sesamin, ferulic acid, naringenin and xanthohumol. *Journal of functional foods*, 14, 183-191.
- KORAĆ, R. R. & KHAMBHOLJA, K. M. 2011. Potential of herbs in skin protection from ultraviolet radiation. *Pharmacognosy reviews*, 5, 164.
- KULKARNI, S., DHIR, A. & AKULA, K. K. 2009. Potentials of curcumin as an antidepressant. *The Scientific World Journal*, 9, 1233-1241.
- KYROU, C. D., SIMPSON, S. E., PTHELINTSEV, D., MARTIN, D. M. & TEAL, J. J. 2003. Skin whitening composition comprising bearberry and tetrahydrocurcumin. Google Patents.

- LAKKAKULA, J., KRAUSE, R. W. M., NDINTEH, D. T., VIJAYLAKSHMI, S. & RAICHUR, A. M. 2012. Detailed investigation of a γ -cyclodextrin inclusion complex with l-thyroxine for improved pharmaceutical formulations. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, 74, 397-405.
- LANIER, R. K., COHEN, A. E. & WEINKLE, S. H. 2013. Effects of a facial cream containing the minor alkaloid anatabine on improving the appearance of the skin in mild to moderate rosacea: an open-label case series study. *Case reports in dermatology*, 5, 347-356.
- LEE, C. W., PARK, N. H., KIM, J. W., UM, B. H., SHPATOV, A., SHULTS, E., SOROKINA, I. & POPOV, S. 2012. Study of skin anti-ageing and anti-inflammatory effects of dihydroquercetin, natural triterpenoids, and their synthetic derivatives. *Russian Journal of Bioorganic Chemistry*, 38, 328-334.
- LEE, W.-H., LOO, C.-Y., BEBAWY, M., LUK, F., MASON, R. S. & ROHANIZADEH, R. 2013. Curcumin and its derivatives: their application in neuropharmacology and neuroscience in the 21st century. *Current neuropharmacology*, 11, 338-378.
- LI, H.-X., ZHANG, H.-L., ZHANG, N., WANG, N., YANG, Y. & ZHANG, Z.-Z. 2014. Isolation of three curcuminoids for stability and simultaneous determination of only using one single standard substance in turmeric colour principles by HPLC with ternary gradient system. *LWT-Food Science and Technology*, 57, 446-451.
- LI, S., YUAN, W., DENG, G., WANG, P., YANG, P. & AGGARWAL, B. B. 2011. Chemical composition and product quality control of turmeric (*Curcuma longa* L.). *Pharmaceutical Crops*, 2.
- LOFTSSON, T. & MASSON, M. 2001. Cyclodextrins in topical drug formulations: theory and practice. *International journal of pharmaceuticals*, 225, 15-30.
- MAHESHWARI, R. K., SINGH, A. K., GADDIPATI, J. & SRIMAL, R. C. 2006. Multiple biological activities of curcumin: a short review. *Life sciences*, 78, 2081-2087.
- MAIZURA, M., AMINAH, A. & WAN AIDA, W. 2011. Total phenolic content and antioxidant activity of kesum (*Polygonum minus*), ginger (*Zingiber officinale*) and turmeric (*Curcuma longa*) extract. *International Food Research Journal*, 18.
- MAJEED, M. & PRAKASH, L. 2008. A Lighter Skin Tone and More... With Natural Actives.
- MANGOLIM, C. S., MORIWAKI, C., NOGUEIRA, A. C., SATO, F., BAESSO, M. L., NETO, A. M. & MATIOLI, G. 2014. Curcumin- β -cyclodextrin inclusion complex: stability, solubility, characterisation by FT-IR, FT-Raman, X-ray diffraction and photoacoustic spectroscopy, and food application. *Food chemistry*, 153, 361-370.
- MANTOVANI, A., SICA, A., ALLAVENA, P., GARLANDA, C. & LOCATI, M. 2009. Tumor-associated macrophages and the related myeloid-derived suppressor cells as a paradigm of the diversity of macrophage activation. *Human immunology*, 70, 325-330.
- MASEK, A., CHRZESCIJANSKA, E. & ZABORSKI, M. 2013. Characteristics of curcumin using cyclic voltammetry, UV-vis, fluorescence and thermogravimetric analysis. *Electrochimica Acta*, 107, 441-447.
- MATSUO, I., YOSHINO, K. & OHKIDO, M. 1983. Mechanism of skin surface lipid peroxidation. *Normal and Abnormal Epidermal Differentiation*. Karger Publishers.
- MEHDIZADEH, L. & MOGHADDAM, M. 2018. Essential Oils: Biological Activity and Therapeutic Potential. *Therapeutic, Probiotic, and Unconventional Foods*. Elsevier.
- MENG, F.-C., ZHOU, Y.-Q., REN, D., WANG, R., WANG, C., LIN, L.-G., ZHANG, X.-Q., YE, W.-C. & ZHANG, Q.-W. 2018. Turmeric: A Review of Its Chemical Composition, Quality


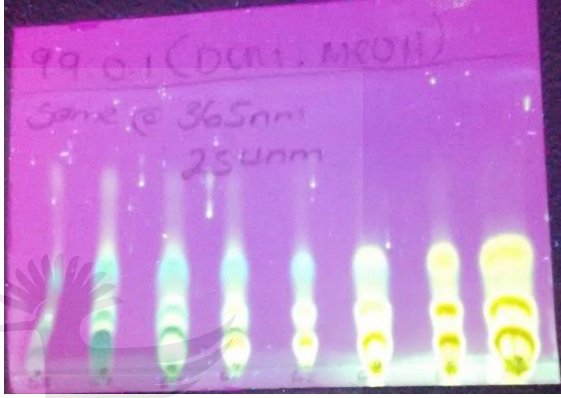
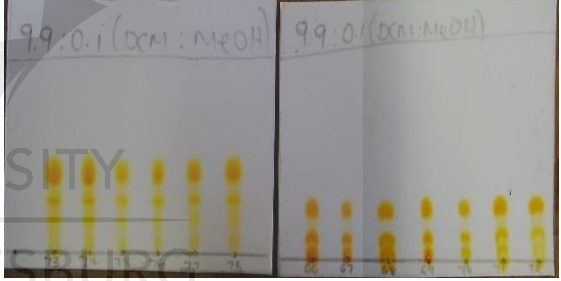
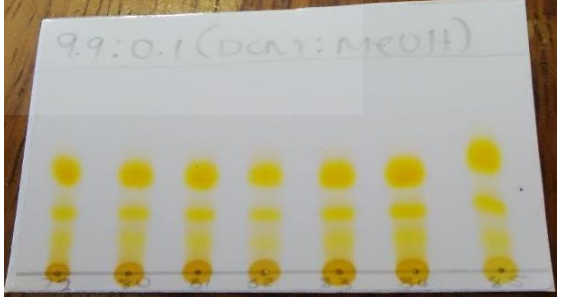

- Control, Bioactivity, and Pharmaceutical Application. *Natural and Artificial Flavoring Agents and Food Dyes*. Elsevier.
- MICHALUN, M. V. & DINARDO, J. C. 2014. *Skin Care and Cosmetic Ingredients Dictionary*, Cengage Learning.
- MODAK, S. M., SHINTRE, M. S., GAONKAR, T. & CARAOS, L. 2011. Antimicrobial compositions containing synergistic combinations of quaternary ammonium compounds and essential oils and/or constituents thereof. Google Patents.
- MONDAL, S., GHOSH, S. & MOULIK, S. P. 2016. Stability of curcumin in different solvent and solution media: UV-visible and steady-state fluorescence spectral study. *Journal of Photochemistry and Photobiology B: Biology*, 158, 212-218.
- NISAR, T., IQBAL, M., RAZA, A., SAFDAR, M., IFTIKHAR, F. & WAHEED, M. 2015. Turmeric: A promising spice for phytochemical and antimicrobial activities. *American - Eurasian Journal of Agricultural and Environmental Sciences*, 15, 1278-1288.
- NOHYNEK, G. J., ANTIGNAC, E., RE, T. & TOUTAIN, H. 2010. Safety assessment of personal care products/cosmetics and their ingredients. *Toxicology and applied pharmacology*, 243, 239-259.
- PARAMASIVAM, M., POI, R., BANERJEE, H. & BANDYOPADHYAY, A. 2009. High-performance thin layer chromatographic method for quantitative determination of curcuminoids in *Curcuma longa* germplasm. *Food Chemistry*, 113, 640-644.
- PARI, L. & AMALI, D. R. 2005. Protective role of tetrahydrocurcumin (THC) an active principle of turmeric on chloroquine induced hepatotoxicity in rats. *Journal of Pharmacy and Pharmaceutical Sciences*, 8, 115-23.
- PAULUCCI, V. P., COUTO, R. O., TEIXEIRA, C. C. & FREITAS, L. A. P. 2013. Optimization of the extraction of curcumin from *Curcuma longa* rhizomes. *Revista Brasileira de Farmacognosia*, 23, 94-100.
- PÉRET-ALMEIDA, L., CHERUBINO, A., ALVES, R., DUFOSSÉ, L. & GLORIA, M. 2005. Separation and determination of the physico-chemical characteristics of curcumin, demethoxycurcumin and bisdemethoxycurcumin. *Food Research International*, 38, 1039-1044.
- PRAKASH, L. & MAJEED, M. 2009. Multifunctional skin tone lighteners from nature: An overview. *Euro Cosmetics*, 6, 19-23.
- PREMAVALLI, K. S. 2007. Turmeric as spice and flavorant. *Turmeric. The Genus Curcuma*, 437.
- PUSHPALATHA, R., SELVAMUTHUKUMAR, S. & KILIMOZHI, D. 2018. Cross-linked, cyclodextrin-based nanosponges for curcumin delivery-Physicochemical characterization, drug release, stability and cytotoxicity. *Journal of Drug Delivery Science and Technology*, 45, 45-53.
- RACHMAWATI, H., EDITYANINGRUM, C. A. & MAULUDIN, R. 2013. Molecular inclusion complex of curcumin- β -cyclodextrin nanoparticle to enhance curcumin skin permeability from hydrophilic matrix gel. *Aaps Pharmscitech*, 14, 1303-1312.
- RAINA, V. K., SRIVASTAVA, S.K., JAIN, N., AHMAD, A., SYAMASUNDAR, K.V. & AGGARWAL, K.K. 2002. Essential oil composition of *Curcuma longa* L. cv. Roma from the plains of northern India. *Flavour and Fragrance Journal*, 17, 99-102.
- RAOOV, M., MOHAMAD, S. & ABAS, M. R. 2013. Synthesis and characterization of β -cyclodextrin functionalized ionic liquid polymer as a macroporous material for the removal of phenols and As (V). *International journal of molecular sciences*, 15, 100-119.



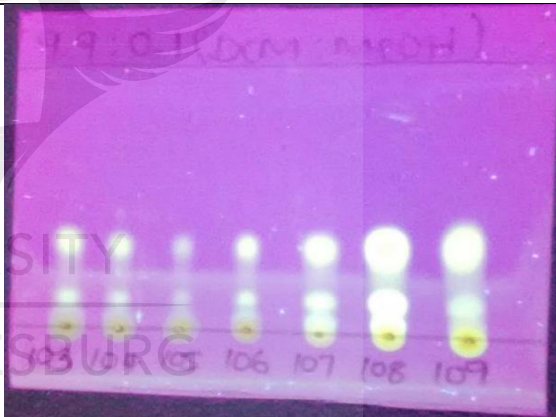

- RAVINDRAN, P., NIRMAL BABU, K. & SIVARAMAN, K. 2007. Turmeric: The golden spice of life. *Turmeric: The Genus Curcuma*. CRC Press, Boca Raton, FL, USA, 1-14.
- REMADEVI, R., SURENDRAN, E. & KIMURA, T. 2007. Turmeric in traditional medicine. *Turmeric: the genus Curcuma*, 409-436.
- REMADEVI, R. R., P.N. 2005. Turmeric: myths and traditions. *Spice India*, 18, 11-17.
- REUTER, J., MERFORT, I. & SCHEMPP, C. M. 2010. Botanicals in dermatology. *American journal of clinical dermatology*, 11, 247-267.
- REVATHY, S., ELUMALAI, S. & ANTONY, M. B. 2011. Isolation, purification and identification of curcuminoids from turmeric (*Curcuma longa* L.) by column chromatography. *Journal of Experimental sciences*, 2.
- SAIKIA, C., SARMAH, M., DAS, M. K., RAMTEKE, A. & MAJI, T. K. 8 Curcumin-Loaded Polymeric Nanoparticle.
- SAJU, K., VENUGOPAL, M. & MATHEW, M. 1998. Antifungal and insect-repellent activities of essential oil of turmeric (*Curcuma longa* L.). *Current Science*, 75, 660-662.
- SANTANA, Á. L. & MEIRELES, M. A. A. 2016. Thin-layer chromatography profiles of non-commercial turmeric (*Curcuma longa* L.) products obtained via partial hydrothermal hydrolysis. *Food and Public Health*, 6, 15-25.
- SARAF, S. 2010. Applications of novel drug delivery system for herbal formulations. *Fitoterapia*, 81, 680-689.
- SARKER, S. D. & NAHAR, L. 2007. Bioactivity of turmeric. *Turmeric: the genus Curcuma*. CRC Press, Boca Raton, 257-283.
- SHARMA, K., AGRAWAL, S. & GUPTA, M. 2012. Development and Validation of UV spectrophotometric method for the estimation of Curcumin in Bulk Drug and Pharmaceutical Dosage Forms. *International Journal of Drug Development and Research*, 4, 375-380.
- SHARMA, P. 2009. Dravyaguna vijnana Vol-2, Chaukhambha Bharathi Academy, Varanasi. Reprint.
- SHRISHAIL, D., HARISH, K., RAVICHANDRA, H., TULSIANAND, G. & SHRUTHI, S. 2013. Turmeric: Nature's precious medicine. *Asian Journal of Pharmaceutical and Clinical Research*, 6, 10-16.
- SINGH, R., CHANDRA, R., BOSE, M. & LUTHRA, P. M. 2002. Antibacterial activity of *Curcuma longa* rhizome extract on pathogenic bacteria. *Current Science*, 737-740.
- SIVAMANI, R. K., JAGDEO, J. R., ELSNER, P. & MAIBACH, H. I. 2015. *Cosmeceuticals and active cosmetics*, CRC Press.
- SKORNICKOVA, J., SABU, M. & PRASANTHKUMAR, M.G. 2004. *Curcuma mutabilis* (Zingiberaceae): a new species from South India. *Gard. Bull. Singapore*, 56, 43-54.
- SOUTO, E. & MÜLLER, R. 2008. Cosmetic features and applications of lipid nanoparticles (SLN®, NLC®). *International Journal of Cosmetic Science*, 30, 157-165.
- SRIMAL, R., KHANNA, N. & DHAWAN, B. 1971. A preliminary report on anti inflammatory activity of curcumin. *International Journal of Pharmaceutics*, 3.
- SRIVILAI, J., PHIMNUAN, P., JAISABAI, J., LUANGTOOMMA, N., WARANUCH, N., KHORANA, N., WISUITIPROT, W., SCHOLFIELD, C. N., CHAMPACHAISRI, K. & INGKANINAN, K. 2017. *Curcuma aeruginosa* Roxb. essential oil slows hair-growth and lightens skin in axillae; a randomised, double blinded trial. *Phytomedicine*, 25, 29-38.
- SUFFREDINI, I., SADER, H. S., GONÇALVES, A. G., REIS, A. O., GALES, A. C., VARELLA, A. D. & YOUNES, R. N. 2004. Screening of antibacterial extracts from plants native to

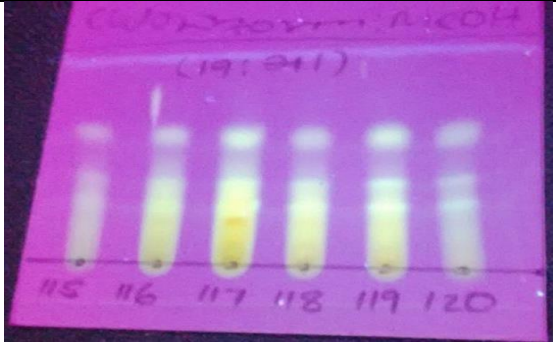

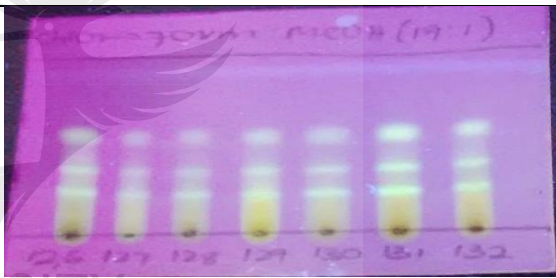

- the Brazilian Amazon Rain Forest and Atlantic Forest. *Brazilian journal of medical and biological research*, 37, 379-384.
- SURH, Y. J. 2002. Anti-tumor promoting potential of selected spice ingredients with antioxidative and anti-inflammatory activities: a short review. *Food and Chemical Toxicology*, 40, 1091-1097.
- SZEJTLI, J. 1982. Cyclodextrins in food, cosmetics and toiletries. *Starch-Stärke*, 34, 379-385.
- SZEJTLI, J. 1988. Cyclodextrin inclusion complexes. *Cyclodextrin technology*. Springer.
- TAUNGJARUWINAI, W. M., BHAWAN, J., KEADY, M. & THIELE, J. J. 2009. Differential expression of the antioxidant repair enzyme methionine sulfoxide reductase (MSRA and MSRB) in human skin. *The American Journal of Dermatopathology*, 31, 427-431.
- THAMAN, L. A. 2006. What is next in skin care cosmetic products? *Cosmetic science and technology series*, 30, 403-408.
- THIELE, J., DREHER, F. & PACKER, L. 2000. Antioxidant defense systems in skin. *Cosmetics science and technology series*, 145-188.
- THIELE, J. & ELSNER, P. 2001. *Oxidants and antioxidants in cutaneous biology*, Karger Medical and Scientific Publishers.
- THORNFELDT, C. 2006. Herbs in cosmeceuticals: Are they safe and effective? *Cosmetic science and technology series*, 30, 309-350.
- VENKATESAN, P. & RAO, M. 2000. Structure-activity relationships for the inhibition of lipid peroxidation and the scavenging of free radicals by synthetic symmetrical curcumin analogues. *Journal of pharmacy and pharmacology*, 52, 1123-1128.
- VOORHEES, J. J. 1977. Treatment of proliferating skin diseases with papaverine alkaloids. Google Patents.
- WILKEN, R., VEENA, M. S., WANG, M. B. & SRIVATSAN, E. S. 2011. Curcumin: A review of anti-cancer properties and therapeutic activity in head and neck squamous cell carcinoma. *Molecular cancer*, 10, 12.
- WOJDYŁO, A., OSZMIANŃSKI, J. & CZEMERYŚ, R. 2007. Antioxidant activity and phenolic compounds in 32 selected herbs. *Food chemistry*, 105, 940-949.
- YOSHINO, M., HANEDA, M., NARUSE, M., HTAY, H. H., TSUBOUCHI, R., QIAO, S. L., LI, W. H., MURAKAMI, K. & YOKOCHI, T. 2004. Prooxidant activity of curcumin: copper-dependent formation of 8-hydroxy-2'-deoxyguanosine in DNA and induction of apoptotic cell death. *Toxicology in vitro*, 18, 783-789.
- YUE, G. G.-L., KWOK, H.-F., LEE, J. K.-M., JIANG, L., CHAN, K.-M., CHENG, L., WONG, E. C.-W., LEUNG, P.-C., FUNG, K.-P. & LAU, C. B.-S. 2015. Novel anti-angiogenic effects of aromatic-turmerone, essential oil isolated from spice turmeric. *Journal of Functional Foods*, 15, 243-253.
- ZAMARIOLI, C. M., MARTINS, R. M., CARVALHO, E. C. & FREITAS, L. A. 2015. Nanoparticles containing curcuminoids (*Curcuma longa*): development of topical delivery formulation. *Revista Brasileira de Farmacognosia*, 25, 53-60.
- ZENGİN, H. & BAYSAL, A. H. 2014. Antibacterial and antioxidant activity of essential oil terpenes against pathogenic and spoilage-forming bacteria and cell structure-activity relationships evaluated by SEM microscopy. *Molecules*, 19, 17773-17798.
- ZHAO, R., SANDSTRÖM, C., ZHANG, H. & TAN, T. 2016. NMR Study on the Inclusion Complexes of β -Cyclodextrin with Isoflavones. *Molecules*, 21, 372.

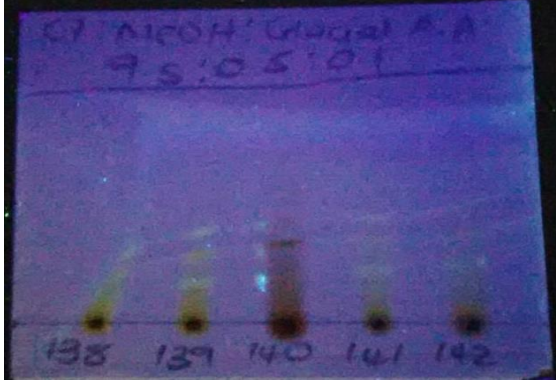
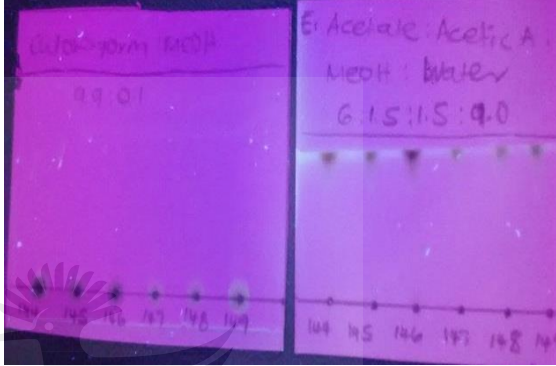

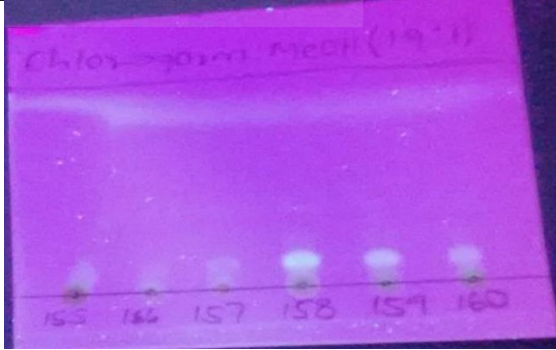
Appendix 1: TLC analysis of column chromatography (CC) fractions

TLC mobile phase	CC Polarity	Fraction	TLC results (chromatogram)
9.9:0.1 DCM: MeOH	100% Hexane	MP: 1-16	
9.9:0.1 DCM: MeOH	5% Ethyl acetate/Hex	MP: 13-20	
9.9:0.1 DCM: MeOH	10% EA/Hex	MP: 21-36	
9.9:0.1 DCM: MeOH	15% EA/Hex	MP: 43-50	

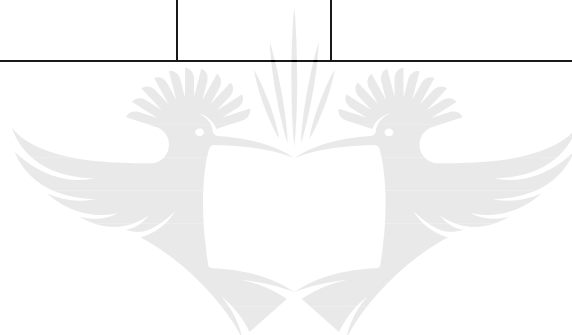
<p>9.9:0.1 DCM: MeOH</p>	<p>20% EA/Hex</p>	<p>MP: 51-7</p>	
<p>9.9:0.1 DCM: MeOH</p>	<p>25% EA/Hex</p>	<p>MP: 58-65</p>	
<p>9.9:0.1 DCM: MeOH</p>	<p>30% EA/Hex</p>	<p>MP: 66-78</p>	
<p>9.9:0.1 DCM: MeOH</p>	<p>35% EA/Hex</p>	<p>MP: 79-85</p>	
<p>9.9:0.1 DCM: MeOH</p>	<p>40% EA/Hex</p>	<p>MP: 86-92</p>	

<p>9.9:0.1 DCM: MeOH</p>	<p>45% EA/Hex</p>	<p>MP: 93-7</p>	
<p>9.9:0.1 DCM: MeOH</p>	<p>50% EA/Hex</p>	<p>MP: 98-102</p>	
<p>9.9:0.1 DCM: MeOH</p>	<p>55% EA/Hex</p>	<p>MP: 103-109</p>	
<p>19:1 CF: MeOH</p>	<p>60% EA/Hex</p>	<p>MP: 103-9, 110-4</p>	

<p>19:1 CF: MeOH</p>	<p>65% EA/Hex</p>	<p>MP: 115-20</p>	
<p>9.5:0.5:0.1 CF:MeOH:GAA GAA- Glacial acetic acid</p>	<p>70% EA/Hex</p>	<p>MP: 121-4</p>	
<p>19:1 CF: MeOH</p>	<p>75% EA/Hex 80% EA/Hex</p>	<p>MP: 126-32</p>	
<p>9.5:0.5:0.1 CF:MeOH:GAA GAA- Glacial acetic acid</p>	<p>85% EA/Hex</p>	<p>MP: 133-8</p>	

<p>9.5:0.5:0.1 CF:MeOH:GAA GAA- Glacial acetic acid</p>	<p>90% EA/Hex</p>	<p>MP: 138-42</p>	
<p>9.9:0.1 CF: MeOH 6:1.5:1.5:1 EA:AA:MeOH:Water EA- Ethyl acetate AA: Acetic acid MeOH- Methanol</p>	<p>95% EA/Hex</p>	<p>MP: 144-9</p>	
<p>9:1 PE: EA PE- Petroleum ether</p>	<p>100% EA 5% MeOH/EA</p>	<p>MP: 150-5</p>	
<p>19:1 CF: MeOH</p>	<p>10% MeOH/EA</p>	<p>MP: 156-60</p>	

19:1 CF: MeOH 9.9:0.1 DCM: MeOH 9:1 PE: EA 9.5:0.5:0.1 CF:MeOH:GAA 6:1.5:1.5:1 EA:AA:MeOH:Water	15% MeOH/EA	MP: 165- 230	No spots were visible, even when visualized with concentrated acid and under UV. The fraction collected was dark brown in color.
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Appendix 2: 2D GCxGX-TOF/MS raw data

Fraction: MP 1-6

Compound Name	Area%	Formula
Cyclocolorenone<epi->	4.4466	C15H22O
Behenic alcohol	4.2326	C22H46O
3-BUTEN-2-OL, 4-(5-METHYL-2-FURANYL)-, ACETATE	2.7546	C11H14O3
(ANTI-8)-8-PHENYLAMINOTRICYCLO[4.2.1.0(3,7)]NONANE-3-OL	2.4942	C15H19NO
1-HEXADECENE	2.2779	C16H32
4-Hydroxy-4'-methyldiphenylamine	2.2406	C13H13NO
7-ISOPROPENYL-1,4A-DIMETHYL-3-OXO-2,3,4,4A,5,6,7,8-OCTAHYDRO-2-NAPHTHALENYL ACETATE	2.1441	C17H24O3
5-Cyclohexadecen-1-one	2.0003	C16H28O
BICYCLO[3.2.1]OCTANE, 1,5-DIMETHYL-	1.9304	C10H18
FURAN, 3-[2-(2,2,6-TRIMETHYLCYCLOHEXYLIDENE)ETHYL]-, (+)-	1.9122	C15H22O
1,2,3-TRIMETHYL-2-CYCLOPENTENE-1-CARBALDEHYDE	1.9122	C9H14O
TRANS-2-METHYLCYCLOPROPANECARBALDOXIME	1.8826	C5H9NO
ZINGIBERENOL	1.8229	C15H26O
CYCLOICOSANE	1.8201	C20H40
2-CYCLOHEXEN-1-ONE, 3-(HYDROXYMETHYL)-6-(1-METHYLETHYL)-	1.624	C10H16O2
10-(1-METHYL-ALLYL)-TRICYCLO[6.3.1.0 2,7]DODECA-2(7),3,5-TRIEN-10-OL	1.6126	C16H20O
TRICYCLO[5.4.0.02,8]UNDEC-10-EN-9-ONE, 2,6,6,11-TETRAMETHYL-, STEREOISOMER	1.3826	C15H22O
HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER	1.3166	C22H42O4
1-Docosene	1.3137	C22H44
1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	1.206	C15H24
DAVANA ETHER 2	1.188	C15H22O2
1-METHYL-3-(1,3,3-TRIMETHYLBICYCLO[4.1.0]HEPT-2-YL)-1-PROPENYL ACETATE	1.1398	C16H26O2
1-[3-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-4,5-DIHYDRO-3H-PYRAZOL-4-YL]ETHANONE	1.125	C14H22N2O
3-PENTEN-2-ONE, 4-(1-HYDROPEROXY-2,2-DIMETHYL-6-METHYLENECYCLOHEXYL)-, (E)-(.+.)-	1.1032	C14H22O3
2,6,10-Undecatrien-8-ol, 2,6-dimethyl-	1.0415	C13H22O
FURAN, 5-[1-(5,5-DIMETHYL-2(5H)-FURANYLIDENE)ETHYL]-2-ETHENYLTETRAHYDRO-2-METHYL-	1.0293	C15H22O2
2-Diphenylethenylsilyloxybut-3-yne	1.0038	C18H18OSi
1-ACRYLOYLPYRROLIDINE	0.97405	C7H11NO
2-CYCLOHEXEN-1-ONE, 6-(1,5-DIMETHYL-4-HEXENYL)-3-METHYL-, [R-(R*,R*)]-	0.97286	C15H24O
PYRIDINE, 5-ETHYL-1,2,3,4-TETRAHYDRO-1-METHYL-4-[(PHENYLMETHYL)THIO]-	0.95144	C15H21NS

3-Heptyn-2-one, 5-cyclopentyl-6-hydroxy-6-methyl-5-(1-methylethyl)-	0.9272	C16H26O2
CYCLOHEXANE, BUTYLIDENE-	0.90121	C10H18
38.64 Xanthorrhizol	0.88754	C15H22O
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,3,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	0.88754	C15H24O2
PENTANOIC ACID, 2,4-DIMETHYL-, 3-METHYLBUTYL ESTER, (S)-	0.87818	C12H24O2
DIEPI-à-CEDRENEPOXIDE	0.85968	C15H24O
2,2,7,7-Tetramethyltricyclo[6.2.1.0(1,6)]undec-4-en-3-one	0.83519	C15H22O
3-Eicosyne	0.83233	C20H38
39.15 Costol<beta->	0.81812	C15H24O
7R,8R-8-Hydroxy-4-isopropylidene-7-methylbicyclo[5.3.1]undec-1-ene	0.79502	C15H24O
1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, [1ar-(1aà,4á,4á,7à,7á,7bà)]-	0.78883	C15H26O
3,5,9-Trimethyl-deca-2,4,8-trien-1-ol	0.74498	C13H22O
ETHANONE, 1-[3-METHYL-3-(4-METHYL-3-PENTENYL)OXIRANYL]-	0.70752	C11H18O2
Amantadine	0.66572	C10H17N
3H-PYRROLIZIN-3-ONE, 1-(ACETYLOXY)-1,2,5,7A-TETRAHYDRO-7-METHYL-, (1S-CIS)-	0.65748	C10H13NO3
6-METHYL-2-VINYL-5-HEPTENYL ACETATE	0.6466	C12H20O2
36.72 Nootkatol<epi->	0.64148	C15H24O
1-DODECANOL	0.63978	C12H26O
41.20 Vetivone<beta->	0.62295	C15H22O
Cyclobutane, tetrakis(1-methylethylidene)-	0.61732	C16H24
4,8,12-Tetradecatrien-1-ol, 5,9,13-trimethyl-	0.60602	C17H30O
BENZENE, (1-HEXYLHEPTYL)-	0.60305	C19H32
9-ACETYL-2,6-DIMETHYL-10-HYDROXYBICYCLO[4.4.0]DECA-1,4-DIEN-3-ONE	0.59865	C14H18O3
2H-PYRAN, 2-(7-HEPTADECYNYLOXY)TETRAHYDRO-	0.56974	C22H40O2
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4Aà,6à,8Aá)]-	0.5594	C15H22O2
31.24 Muurol-5-en-4-alpha-ol<cis->	0.55661	C15H26O
(1'S)-1-METHYL-4-(1',2',2'-TRIMETHYLCYCLOPENTYL)BENZENE [(-)-CUPARENE(2)]	0.55324	C15H22
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	0.53491	C15H24
BICYCLO[7.2.0]UNDEC-4-ENE, 4,11,11-TRIMETHYL-8-METHYLENE-, [1R-(1R*,4E,9S*)]-	0.52517	C15H24
N-7-METHYLGUANINE	0.51259	C6H7N5O
1S-à-Pinene	0.48955	C10H16
Trifluoroacetyl-lavandulol	0.47659	C12H17F3O2
3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	0.46912	C10H16O
25.19 Funebrene<beta->	0.45575	C15H24
6,11-Dimethyl-2,6,10-dodecatrien-1-ol	0.44594	C14H24O
Himachala-2,4-diene	0.44407	C15H24
1-(1,2,3-Trimethyl-cyclopent-2-enyl)-ethanone	0.44372	C10H16O

Methyl 8,11,14,17-eicosatetraenoate	0.4272	C21H34O2
2(10)-PINEN-3-ONE, (1S,5S)-(-)-	0.42052	C10H14O
22.30 Carvomenthyl acetate<neoiso->	0.42052	C12H22O2
Cyclobutanecarboxylic acid, 4-isopropylphenyl ester	0.42052	C14H18O2
9H-[1,2,4]TRIAZOLO[5,1-B][1,3]BENZOTHIAZIN-9-ONE, 2-AMINO-	0.42052	C9H6N4OS
4,7,7-Trimethylbicyclo[2.2.1]heptan-2,3-dione, 2-oxime (syn)	0.41727	C10H15NO2
Tetracyclo[6.3.2.0(2,5).0(1,8)]tridecan-9-ol, 4,4-dimethyl-	0.40653	C15H24O
3,7,11-TRIMETHYLDODECA-6,10-DIEN-1-YN-3-OL	0.40141	C15H24O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.39927	C15H22
FARNESYL ACETONE C	0.38298	C18H30O
CYCLODECA[B]FURAN-2(3H)-ONE, 3A,4,5,8,9,11A-HEXAHYDRO-3,6,10-TRIMETHYL-, [3S-(3R*,3AR*,6E,10E,11AR*)]-	0.37237	C15H22O2
Cyclohexanepropanol-	0.36742	C9H18O
1,3,7,11-Cyclotetradecatetraene, 2-methyl-	0.36245	C15H22
1,8-Cyclopentadecadiyne	0.36245	C15H22
2-Propylhept-3-enoic acid, phenylthio ester	0.35311	C16H22OS
1,2,2,6,8-Pentamethyl-7-oxabicyclo[4.3.1]dec-8-en-10-one	0.34165	C14H22O2
PROPANENITRILE, 3-(PHENYLMETHOXY)-	0.33682	C10H11NO
29.48 Himachalene<alpha-dehydro-ar->	0.32714	C15H20
1H-Indene-4-methanol, 2,3-dihydro-à,à,1,1-tetramethyl-	0.32505	C14H20O
QUINOLINE, 2-(2-THIENYL)-	0.30982	C13H9NS
BENZENE, 1,2-DIMETHYL-	0.30722	C8H10
6,10-Dodecadien-1-yn-3-ol, 3,7,11-trimethyl-	0.30616	C15H24O
endo-2-Methylbicyclo[3.3.1]nonane	0.30492	C10H18
38.52 Bisabolone <6S,7R->	0.28734	C15H24O
5-ISOPROPENYL-3,6-DIMETHYL-6-VINYL-4,5,6,7-TETRAHYDRO-1-BENZOFURAN #	0.27687	C15H20O
Tricyclo[6.3.0.0(1,5)]undecan-10-ol, 4-[(2-methoxyethoxy)methoxy]-5-methyl-	0.27394	C16H28O4
Cyclohexene, 1,2,4-trimethyl-4-(1-methylethenyl)-	0.27373	C12H20
BENZENE, 1-(1,4-DIMETHYL-4-HEXENYL)-2-METHYL-, (Z)-(.+.-)-	0.26974	C15H22
N-NITROSO-BUXTEN	0.2657	C13H18N2O3
37.62 Cryptomerione	0.2657	C15H22O
THIENO[2,3-D][1,2,3]DIAZABORINE, 1,2-DIHYDRO-2-METHYL-	0.26385	C6H7BN2S
4-(2,2-DIMETHYL-1-HYDROXYPROPYL)PHENOL	0.26203	C11H16O2
3,7,11-Trimethyl-dodeca-2,6,10-trienoic acid	0.26077	C15H24O2
1-Docosene	0.26057	C22H44
Himachala-2,4-diene	0.25743	C15H24
CYCLOHEXANONE, 2,6-DIMETHYL-4-NITRO-3-PHENYL-, (2à,3á,4á,6á)-(.+.-)-	0.25408	C14H17NO3
Caryophyllene oxide	0.24244	C15H24O
1-CYCLOPENTENCARBONSAEURE, 2-METHYL-3-VINYL-, 4'-FLUOROPHENYLESTER	0.2415	C15H15FO2
NONANE, 3,7-DIMETHYL-	0.23361	C11H24

1,4-BENZENEDIOL, 2,3,5-TRIMETHYL-	0.23354	C9H12O2
1-(2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL)-2-BUTEN-1-ONE	0.23348	C13H20O2
4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)-	0.23245	C23H34O2
á-CEDRENOXIDE	0.21903	C15H24O
Icosapent	0.21634	C20H30O2
5-Heptenal, 2,6-dimethyl-	0.21381	C9H16O
2-CYCLOHEXEN-1-ONE, 4-HYDROXY-3-METHYL-6-(1-METHYLETHYL)-, TRANS-	0.21096	C10H16O2
Chlorocyclohexyldimethylsilane	0.20954	C8H17ClSi
1-(4-HYDROXY-7-ISOPROPYL-4-METHYLOCTAHYDRO-1H-INDEN-1-YL)ETHANONE #	0.20645	C15H26O2
2,2'-BITHIAZOLE, 4,4'-BIS(1-METHYLETHYL)-	0.19496	C12H16N2S2
Cyclobutane, tetrakis(1-methylethylidene)-	0.18816	C16H24
(2E,4E,10E)-(S)-(+)-2,6-DIMETHYLDODECA-2,8,10-TRIENO-1,12-LACTONE	0.17445	C14H20O3
4-(2,7,7-TRIMETHYLBICYCLO[3.2.0]HEPT-2-EN-1-YL)-3-BUTEN-2-ONE	0.17086	C14H20O
1,2-BENZENEDIOL, 5-METHYL-3-(1,2,2-TRIMETHYLCYCLOPENTYL)-, (S)-	0.17083	C15H22O2
(1R-(1à(1S*,6S*),2á,5à))-5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ESTER OF 2-OXOBICYCLO(4.1.0)HEPTANE-1-CARBOXYLIC ACID	0.17037	C18H28O3
4A-METHYL-1,2,3,4,4A,9,10,10A-OCTAHYDRO-1-PHENANTHRENOL	0.1689	C15H20O
8,9-Dimethylbicyclo[4.4.1]undeca-2,4,8-triene	0.16536	C13H18
TRANS-2-PROPENYLDIPHENYLACETYLENE	0.16513	C17H14
6-Bromohexanoic acid, tridec-2-ynyl ester	0.15694	C19H33BrO2
(7a-Isopropenyl-4,5-dimethyloctahydroinden-4-yl)methanol	0.14695	C15H26O
2,3-BUTANEDIOL, 2,3-DIMETHYL-	0.14601	C6H14O2
2-Cyanophenyl á-phenylpropionate	0.14547	C16H13NO2
FURAN, 2-(3,7-DIMETHYL-2,6-OCTADIENYL)-3-METHYL-, (E)-	0.14429	C15H22O
d-Norpregnane (5à,14à)	0.14423	C20H34
Thujopsene	0.14251	C15H24
2H-1,4-Benzoxazine-4-acetamide, 3,4-dihydro-6-methyl-3-oxo-	0.14199	C11H12N2O3
3,6,9,12,15-PENTAOXABICYCLO[15.3.1]HENICOSA-1(21),17,19-TRIENE-2,16-DIONE #	0.1343	C16H20O7
VALERENYL HEXANOATE	0.13131	C21H34O2
1,6-OCTADIENE, 2,5-DIMETHYL-, (E)-	0.13131	C10H18
3,3,5,5-Tetramethylcyclopentene	0.13131	C9H16
37.23 Cedroxyde	0.13027	C15H24O
2-(4-P-TOLYL-THIAZOL-2-YL)-ACETAMIDE	0.1256	C12H12N2OS
LONGIFOLENALDEHYDE	0.12448	C15H24O
Phosphoric acid	0.12312	H3O4P
38.24 Bisabolone<6R,7R->	0.12214	C15H24O
Heneicosane	0.12192	C21H44
Benzene, (1,1-dimethylpropyl)-	0.12003	C11H16

3-ETHENYL-3-METHYL-4-PENTEN-1-OL	0.11743	C8H14O
38.26 Cedr-8(15)-en-9-alpha-ol, acetate	0.11565	C17H26O2
FURAN, 2-[[2,7-DIMETHYL-2,7-OCTADIENYL)OXY]METHYL]-, (Z)-	0.11487	C15H22O2
BAIMUXINAL	0.11461	C15H24O2
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.10936	C15H24
3-Buten-2-one, 4-(2,5,5-trimethyl-3,8-dioxatricyclo[5.1.0.0(2,4)]oct-4-yl)-, [1à,2à,4à(E),7à]-	0.10714	C13H18O3
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.1049	C15H24
Borneol, dimethyl(dichloromethyl)silyl ether	0.10478	C13H24Cl2OS i
2,6,10,10-TETRAMETHYLBICYCLO[7.2.0]UNDECA-1,6-DIENE	0.10333	C15H24
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.10209	C15H22
2-HEPTEN-1-OL, 2-METHYL-6-(4-METHYLPHENYL)-, (E)-(+.-)-	0.098796	C15H22O
BENZENE, 1-(1-CHLOROPROPYL)-4-METHOXY-	0.088705	C10H13ClO
6,10-DIMETHYL-3-METHYLENEUNDECA-1,9-DIEN-4-OL	0.088569	C14H24O
46.51 Occidol acetate	0.086036	C17H24O2
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-1,6-DIMETHYL-4-(1-METHYLETHYL)-, (1S-CIS)-	0.085795	C15H22
Neoisolongifolene, 8,9-epoxy-	0.084505	C15H22O
BENZOIC ACID, OCTYL ESTER	0.083362	C15H22O2
TRANS-2,2-DIMETHYL-3-(2'-METHYL-1'-PROPENYL)CYCLOBUTANOL	0.083327	C10H18O
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	0.083244	C15H22
3-METHYL-5-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-1-PENTYN-3-OL	0.082067	C15H24O
PYRIMIDINE, 2-(3-THIENYL)-	0.081962	C8H6N2S
HEPTADECANE	0.079561	C17H36
Heptane, 3-ethyl-5-methyl-	0.079561	C10H22
HEXADECANOIC ACID, 2,3-DIHYDROXYPROPYL ESTER	0.071982	C19H38O4
TRICYCLO[10.2.1.0E2,11]PENTADEC-4,8-DIEN, (E,Z)-	0.065445	C15H22
4,6,10,10-TETRAMETHYL-5-OXA-TRICYCLO[4.4.0.0 1,4]DEC-2-EN-7-OL	0.064832	C13H20O2
9-(3,3-DIMETHYL-2-OXIRANYL)-2,7-DIMETHYL-2,6-NONADIEN-1-OL	0.064084	C15H26O2
2,2,6,6-TETRAMETHYL-2H,6H-THIIN-3-ONE	0.06344	C9H14OS
2,3-Hexadienoic acid, 2-methyl-4-phenyl-, methyl ester	0.063188	C14H16O2
CYCLOHEXENE, 6-(2-BUTENYLIDENE)-1,5,5-TRIMETHYL-, (Z,E)-	0.062808	C13H20
Phosphoric acid	0.060721	H3O4P
6-(1-HYDROXYMETHYL-VINYL)-4,8A-DIMETHYL-3,5,6,7,8,8A-HEXAHYDRO-1H-NAPHTHALEN-2-ONE	0.060491	C15H22O2
[(1E)-3-ETHOXY-1,5-HEXADIENYL]BENZENE	0.058208	C14H18O
1-Adamantanecarboxylic acid, 3-pentadecyl ester	0.057775	C26H46O2
29.48 Himachalene<alpha-dehydro-ar->	0.055462	C15H20
N-[(4-CHLOROPHENYL)METHYLENE]-2-METHYL-2-PROPANAMINE N-OXIDE	0.054715	C11H14ClNO

LINALOOL FORMATE	0.052045	C11H18O2
11H-INDOLO[3,2-C]QUINOLINE	0.051521	C15H10N2
1-Hydroxy-1,7-dimethyl-4-isopropyl-2,7-cyclodecadiene	0.049619	C15H26O
7-ISOPROPENYL-1,4A-DIMETHYL-3-OXO-2,3,4,4A,5,6,7,8-OCTAHYDRO-2-NAPHTHALENYL ACETATE	0.046901	C17H24O3
3,8-à-FURANETHER	0.046451	C15H20O2
[1,1'-Bicyclohexyl]-2-one	0.045917	C12H20O
Z-THUJENOL	0.045654	C10H16O
2,2,7,7-TETRAMETHYL-TRICYCLO[6.2.1.0 1,6]UNDEC-4-EN-3-ONE	0.045612	C15H22O
Acetamide, 2-chloro-N-[2-(4,5-dihydro-5-isoxazolyl)phenyl]-	0.042447	C11H11ClN2O2
6-(P-METHOXYPHENYL)HEX-5-YN-2-ONE	0.041966	C13H14O2
Cyclopentanone, 2,5-dicyclopentylidene-	0.041556	C15H20O
2-CYCLONONEN-1-ONE, 7-(1,1-DIMETHOXYETHYL)-3-METHYL-9-(1-METHYLETHYLIDENE)-, (Z)-(+)-	0.038427	C17H28O3
3,1,2-AZAZONIABORATIN, 2,2-(1,5-CYCLOOCTANDIYL)-1,3,5-TRIDEUTERO-4,6-DIMETHYL-	0.035718	C13H20D3BN2
NAPHTHALENE, 1,2,3,4,4A,5,6,8A-OCTAHYDRO-7-METHYL-4-METHYLENE-1-(1-METHYLETHYL)-, (1à,4Aà,8Aà)-	0.034802	C15H24
2-Methyl-N-(1-methylethylidene)-4-[(1E)-1-pentadecenyl]-1,3,2-dioxaborinan-5-amine	0.033204	C22H42BNO2
Decane, 3-methyl-	0.032675	C11H24
5-BENZOFURANACETIC ACID, 6-ETHENYL-2,4,5,6,7,7A-HEXAHYDRO-7A-HYDROXY-3,6-DIMETHYL-à-METHYLENE-2-OXO-, METHYL ESTER	0.03165	C16H20O5
4-(2-Isopropyl-5-methylphenyl)-3-methylbutyric acid	0.024213	C15H22O2
DAVANA ETHER 2	0.023283	C15H22O2
1-Phenylcyclohexylamine	0.022978	C12H17N
1-(1-PROPYNYL)CYCLOPENTANOL	0.021861	C8H12O
1,5-DIMETHYL-1-VINYL-4-HEXENYL BUTYRATE	0.021841	C14H24O2
1H-Imidazole-1-octanoic acid, methyl ester	0.020526	C12H20N2O2
AMBROX	0.019575	C16H28O
AMINOUREA	0.019464	CH5N3O
41.97 Bisabolatrien-1-ol-4-one<2,7(14),10->	0.017802	C15H22O2
BENZENEMETHANESULFONAMIDOE,-4-METHYL-N-(8-OXO-3,7-DIOXATRICYCLO[4.3.1.0(2,4)]DEC-9-YL)-,	0.016811	C16H19NO5S
PENTADECANE	0.016342	C15H32
2-BUTEN-1-ONE, 1-(2-ETHENYL-1-CYCLOHEXEN-1-YL)-, (E)-	0.013628	C12H16O
2,3-Diazabicyclo[2.2.1]hept-2-ene, 7,7-dimethyl-5-phenyl-, (1à,4à,5á)-	0.013054	C13H16N2
2-Cyclohexen-1-one, 2,4,4-trimethyl-3-(3-oxo-1-butenyl)-	0.013054	C13H18O2
3-BUTEN-2-ONE, 4-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-	0.012812	C13H20O
37.63 Nuciferol<Z->	0.012254	C15H22O
BUTYRIC ACID, 3-(2,5-DIMETHYLBENZOYL)-	0.011976	C13H16O3
PROPANAL, 2-(DIMETHYLHYDRAZONO)-	0.01147	C5H10N2O

1,2,4-TRIAZOLIDINE-3,5-DIONE, 1-(1-METHYL-1-PHENYLETHYL)-4-PHENYL-	0.010998	C17H17N3O2
BENZENEMETHANOL, à-(1,1-DICHLORO-2,2,2-TRIFLUOROETHYL)-, ACETATE	0.01066	C11H9Cl2F3O 2
8-Dodecen-1-ol, acetate, (Z)-	0.010569	C14H26O2
3-PENTEN-2-OL, 4-METHYL-, (.+-.)-	0.010031	C6H12O
4-HEPTENOIC ACID, 4-ETHYL-2-(METHYLSULFONYL)-, METHYL ESTER, (E)-	0.008765	C11H20O4S
7-AZABICYCLO[4.1.0]HEPTANE, 2,2,6-TRIMETHYL-7-(4-NITROBENZOYL)-1-(3-OXO-1-BUTENYL)-, (E)-	0.007456	C20H24N2O4
Oxacyclotetradeca-4,11-diyne	0.007297	C13H18O
CYCLOHEPTANONE, 2-METHYL-2-[[[(4-METHYLPHENYL)SULFONYL]OXY]METHYL]-	0.007249	C16H22O4S
PENTANENITRILE, 2-(AMINOMETHYLENE)-3,3-DIMETHYL-, (Z)-	0.004761	C8H14N2
Bicyclo[4.1.0]heptan-2-ol, 1-phenyl-, endo-	0.004563	C13H16O
2-METHYL-2'-METHOXYBIPHENYL	0.004549	C14H14O
4A-METHYL-1,2,3,4,4A,9,10,10A-OCTAHYDRO-1-PHENANTHRENOL	0.004455	C15H20O
2-BENZYL-2-METHYL-3-OXO-PROPIONIC ACID ETHYL ESTER	0.004089	C13H16O3
2H-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-, cis-	0.003545	C13H20O
NAPHTHALENE, 1,6-DIMETHYL-4-(1-METHYLETHYL)-	0.003389	C15H18
37.21 Curcumen-15-al<ar->	0.002801	C15H20O
5-(ISOPROPYLAMINO)-1,6-DIMETHYL-2(1H)-QUINOLINONE	0.002548	C14H18N2O
27.08 Ionol<alpha-isomethyl-(E)->	0.002456	C14H24O
TRICYCLO[2.2.1.0(2,6)]HEPTAN-3-OL, 1-(METHYL-D)-7-METHYLENE-, STEREOISOMER	0.002433	C9H11DO
4-(4'-METHYLPHENYL)-4-PENTEN-1-OL	0.001712	C12H16O
2-(BENZOYLOXY)CYCLOHEXANONE	0.001601	C13H14O3
Methanone, (4-methoxyphenyl)(1,2,3-trimethyl-2-cyclopentenyl)	0.001241	C16H20O2
3-(1,3,5,7-CYCLOOCTATETRENYL)-1-PROPANOL-1,1-D2	0.001187	C11H12D2O
1-METHYL-1-(1-METHYLETHENYL)CYCLOBUTANE	0.001134	C8H14
ENDO-3-ETHYL-10,10-DIMETHYLTRICYCLO[5.2.1.0(2,6)]DECANE	0.001012	C14H24
4-(1-PHENYLETHYL)BICYCLO(3.2.1)OCT-2-ENE	0.00061	C16H20
6-HYDROXY-6,7-DIHYDROBENZO[C]FURAN	0.000355	C8H8O2
1-NAPHTHALENOL, 1,2,3,4,4A,7,8,8A-OCTAHYDRO-1,6-DIMETHYL-4-(1-METHYLETHYL)-, [1R-(1à,4á,4Aá,8Aá)]-	0.000302	C15H26O
Phendimetrazine	0.000238	C12H17NO
9H-FLUORENE	5.23E-05	C13H10
2,5-DIMETHYLTHIAZOLE-4-CARBOXYLIC ACID	2.16E-05	C6H7NO2S
NAPHTHALENE, 1,6-DIMETHYL-4-(1-METHYLETHYL)-	1.01E-05	C15H18
(4AR,9AS,9BS)-4A,6,6,9A-TETRAMETHYL-TRANS-PERHYDROINDANO[2,1-C]PYRAN	0	C16H28O
1-(7-BROMOTRICYCLO[4.1.0.0(2,7)]HEPT-1-YL)ETHANOL	0	C9H13BrO
1H-ISOINDOLE-1,3(2H)-DIONE, HEXAHYDRO-2,3A,7A-TRIMETHYL-, CIS-	0	C11H17NO2

1-TERT-BUTYL-7-METHOXY-NAPHTHALENE	0	C15H18O
Total	100	

Fraction: MP 7-13

Compound Name	Area%	Formula
1-OCTADECENE	6.7261	C18H36
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	6.2994	C15H24
1-Hexadecene	6.1935	C16H32
1-Docosene	5.4508	C22H44
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	4.5472	C15H24
CYCLOHEXENE, 1-METHYL-4-(5-METHYL-1-METHYLENE-4-HEXENYL)-, (S)-	4.5404	C15H24
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	4.415	C15H22
CYCLOTETRACOSANE	4.2827	C24H48
3,7,7-TRIMETHYL-1,3,5-CYCLOHEPTATRIENE	3.0512	C10H14
2,5-HEPTADIENE, 2-METHYL-6-(4-METHYL-3-CYCLOHEXEN-1-YL)-, (E)-	2.9987	C15H24
4,5,9,10-DEHYDRO-ISOLONGIFOLENE	2.3183	C15H20
1-HEXADECENE	2.2993	C16H32
PENTADECANE	2.0944	C15H32
PENTADECANE	2.0944	C15H32
1-TETRADECENE	1.9762	C14H28
Tetradecane	1.8655	C14H30
HEXADECANE	1.8275	C16H34
1-Docosene	1.6007	C22H44
Heptadecane	1.4571	C17H36
Octane, 3,5-dimethyl-	1.3286	C10H22
EICOSANE	1.2458	C20H42
trans-à-Bergamotene	1.2399	C15H24
29.48 Himachalene<alpha-dehydro-ar->	0.83325	C15H20
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.82742	C15H22
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	0.77498	C15H24
1,8-Cyclopentadecadiyne	0.6899	C15H22
1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (Z)-	0.6899	C15H24
1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (E)-	0.6899	C15H24
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.67976	C15H20
Nonadecane	0.63658	C19H40
HEPTACOSANE	0.62971	C27H56
Heneicosane	0.62046	C21H44
BICYCLO[7.2.0]UNDEC-4-ENE, 4,11,11-TRIMETHYL-8-METHYLENE-, [1R-(1R*,4E,9S*)]-	0.61571	C15H24

Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-	0.61571	C15H24
Octadecane	0.58059	C18H38
35.51 Turmerone<ar->	0.56728	C15H20O
1-(1-METHYL-2-PROPENYL)-4-PENTYLBENZENE	0.5577	C15H22
Cis-bicyclo[4.2.0]octane	0.52677	C8H14
NAPHTHALENE, 1,2,3-TRIMETHYL-4-PROPENYL-, (E)-	0.51769	C16H18
Tumerone	0.50903	C15H22O
2-Tridecene, (Z)-	0.48337	C13H26
1H-CYCLOPROP[E]AZULENE, DECAHYDRO-1,1,4,7-TETRAMETHYL-, [1AR-(1Aà,4á,4Aá,7á,7Aá,7Bà)]-	0.45155	C15H26
1-METHYL-4-(1,5-DIMETHYL-4-HEXENYLIDENE)-1-CYCLOHEXENE	0.41425	C15H24
BOROXIN, DIMETHYLPROPYL-	0.39963	C5H13B3O3
3-(3'-METHYL-2'-BUTENYL)-4-[(DIMETHYLAMINO)METHYL]PHENOL	0.39752	C14H21NO
PENTADECANE, 2,6,10,14-TETRAMETHYL-	0.393	C19H40
1-Docosene	0.39001	C22H44
3-FURANCARBOXYLIC ACID, 2,5-DIHYDRO-5,5-DIMETHYL-2-OXO-, ETHYL ESTER	0.36108	C9H12O4
UNDECANE, 6-ETHYL-	0.36034	C13H28
SPIRO[5.5]UNDECA-1,8-DIENE, 1,5,5,9-TETRAMETHYL-, (R)-	0.35844	C15H24
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	0.35355	C15H26
2-PROPENAL, 3-PHENYL-, (Z)-	0.34505	C9H8O
Benzenemethanamine, 3,4-dimethyl-	0.32844	C9H13N
1,4,9-Decatriene, 1-phenyl-, (E,E)-	0.31807	C16H20
3,3,5,5-Tetramethylcyclopentene	0.31444	C9H16
Octadecane, 2-methyl-	0.30904	C19H40
TRIDECANE	0.29696	C13H28
s-Indacene, 1,2,3,5,6,7-hexahydro-1,1,7,7-tetramethyl-	0.29378	C16H22
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.29358	C16H18
1-Docosene	0.29358	C22H44
3-Methyl-2-(3,7,11-trimethyldodecyl)thiophene	0.26094	C20H36S
1-METHYL-4-(1,5-DIMETHYL-4-HEXENYLIDENE)-1-CYCLOHEXENE	0.25922	C15H24
Tetradecane, 3-methyl-	0.25922	C15H32
33.20 Atlantol<beta->	0.23925	C15H24O
2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4a,7,7-trimethyl-, (R)-	0.23629	C13H20O
Spermine	0.23065	C10H26N4
Oleic Acid	0.22859	C18H34O2
TETRADECANE, 1-CHLORO-	0.22226	C14H29Cl
EICOSANE	0.20235	C20H42
HEPTANE, 6-METHYL-2-P-TOLYL-	0.19354	C15H24
TETRADECANE, 4-ETHYL-	0.18588	C16H34
2-NITRO-3-PHENYL-2-PROPENYL ACETATE	0.18588	C11H11NO4
n-Hexadecanoic acid	0.17909	C16H32O2

1,2,3-TRIMETHYL-2-CYCLOPENTENE-1-CARBALDEHYDE	0.17122	C9H14O
29.42 Curcumene<beta->	0.16991	C15H24
Curlone	0.1623	C15H22O
Pentadecane, 3-methyl-	0.16133	C16H34
1-Hexadecene	0.16087	C16H32
4-UNDECENE, 5-METHYL-, (Z)-	0.15781	C12H24
3A,9B-DIMETHYL-1,2,3A,4,5,9B-HEXAHYDRO-3H-CYCLOPENTA[A]NAPHTHALEN-3-ONE	0.15443	C15H18O
Falcarinol	0.15226	C17H24O
1,3,5-Cycloheptatriene, 6-methyl-1-(6-methyl-1,3,5-cycloheptatrien-1-yl)-	0.14762	C16H18
1b,5,5,6a-Tetramethyl-octahydro-1-oxa-cyclopropa[a]inden-6-one	0.14477	C13H20O2
2-Ethyl-1-dodecanol	0.14246	C14H30O
1-(2-METHOXY-1-METHYL-ETHYL)-2-METHYL-BENZENE	0.13847	C11H16O
NONADECANE	0.13587	C19H40
HEPTADECANE, 2,6,10,14-TETRAMETHYL-	0.13296	C21H44
1-Docosene	0.12922	C22H44
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl-	0.12796	C18H20
1,11-DODECADIENE	0.11745	C12H22
[2-METHYL-2-(4-METHYL-3-PENTENYL)CYCLOPROPYL]METHANOL	0.11745	C11H20O
(3RS,6R)-3-METHYL-6-(1'-METHYLETHENYL)DEC-9-EN-1-YL ACETATE	0.11576	C16H28O2
3-METHYL-1,1-BIS(METHYLSULFANYL)-1,3-BUTADIENE	0.11453	C7H12S2
Preg-4-en-3-one, 17à-hydroxy-17á-cyano-	0.11436	C20H27NO2
1-Hexadecene	0.11037	C16H32
Eicosane, 2-methyl-	0.10879	C21H44
2-Butyl-1-decene	0.10879	C14H28
1,9-UNDECADIEN-5-ONE, (E)-	0.10865	C11H18O
DODECANE, 2,6,10-TRIMETHYL-	0.10744	C15H32
HEXADECANE, 4-METHYL-	0.10424	C17H36
Pentadecane, 2-methyl-	0.10418	C16H34
BICYCLO[3.2.2]NONA-6,8-DIEN-3-ONE, 6,8-DIMETHYL-	0.10246	C11H14O
2-Trifluoroacetoxypentadecane	0.10243	C17H31F3O2
3(4H)-Dibenzofuranone, 4a,9b-dihydro-8,9b-dimethyl-	0.10169	C14H14O2
Imidazole, 2,4-diethyl-1-methyl-5-phenyl-	0.10169	C14H18N2
TETRADECANE, 2-METHYL-	0.10169	C15H32
1,4-Methanophthalazine, 1,4,4a,5,6,7,8,8a-octahydro-1,4,9,9-tetramethyl-, (1à,4à,4aà,8aà)-	0.099514	C13H22N2
Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)-	0.094258	C15H24
4-DECENE	0.09183	C10H20
40.70 Eudesm-11-en-4-alpha,6-alpha-diol	0.091306	C15H26O2
Cyclohexane, (1,1-dimethylpropyl)-	0.083771	C11H22
10-Heneicosene (c,t)	0.082808	C21H42

1-METHYL-4-(1,5-DIMETHYL-4-HEXENYLIDENE)-1-CYCLOHEXENE	0.080448	C15H24
1,1'-BIPHENYL, 3,4-DIETHYL-	0.080259	C16H18
2-Butyl-1-decene	0.079418	C14H28
3,5-Dimethyldodecane	0.079176	C14H30
Nonane, 5-(2-methylpropyl)-	0.078338	C13H28
2,4-Diphenyl-4-methyl-2(E)-pentene	0.07808	C18H20
6,10-DIMETHYL-5,9-UNDECADIEN-2-ONE	0.07721	C13H22O
5,9-UNDECADIEN-2-ONE, 6,10-DIMETHYL-, (Z)-	0.075933	C13H22O
24.19 Sesquithujene<7-epi->	0.075402	C15H24
2-{3'-{[(2"-ETHYNYLPHENYL)ETHYNYL]DIMETHYLSILYL}-3'-METHYLBUTOXY}TETRAHYDRO-2H-PYRAN	0.072757	C22H30O2Si
6-Methoxyharmalan	0.072159	C13H14N2O
1-IODOTETRADECANE	0.071427	C14H29I
7-Tetradecene	0.071427	C14H28
3-(4-ISOPROPYLPHENYL)-2-METHYLPROPANAL	0.070101	C13H18O
TRICYCLO[5.1.0.0(1,3)]OCT3-ENE	0.068941	C8H12
DODECANE	0.067976	C12H26
Myrtene acid bromide	0.067641	C10H13BrO
1-Docosene	0.066575	C22H44
Bicyclo[4.1.0]-3-heptene, 2-isopropenyl-5-isopropyl-7,7-dimethyl-	0.066164	C15H24
2-Hexen-1-one, 1-(2-hydroxy-5-methylphenyl)-	0.065902	C13H16O2
1-Iodo-2-methylundecane	0.063761	C12H25I
TRIDECANE, 2-METHYL-	0.059436	C14H30
Pentadecane, 4-methyl-	0.059424	C16H34
Bumetrizole	0.055969	C17H18ClN3O
1-Docosene	0.05419	C22H44
2-ETHYL-1-DECENE	0.053622	C12H24
m-Toluic acid, 2-butyl ester	0.052967	C12H16O2
EICOSANE	0.051853	C20H42
1-AZIDO-1-ETHENYLCYCLOPROPANE	0.050694	C5H7N3
NONANE, 5-BUTYL-	0.050323	C13H28
Cyclohexane, (2-nitro-2-propenyl)-	0.04761	C9H15NO2
36.03 Helifolenol C	0.044428	C15H24O
1-Decen-3-one	0.043578	C10H18O
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.043255	C15H24
BENZENE, 1,1'-[OXYBIS(METHYLENE)]BIS-	0.042929	C14H14O
HEXADECANE, 3-METHYL-	0.040454	C17H36
Pyrrolidine, 1-methyl-3,2'-spiro-benzo-1,3-dioxolane-	0.040428	C11H13NO2
n-Nonylcyclohexane	0.040255	C15H30
BENZENE, 1-ETHYL-4-(1-METHYLETHYL)-	0.040041	C11H16
Octadecane, 2-methyl-	0.039936	C19H40

OCTADECANE, 4-METHYL-	0.038846	C19H40
Benzene, 1,1'-ethylidenebis[3,4-dimethyl-	0.038293	C18H22
32.17 Tumerol<ar->	0.038114	C15H22O
7-METHYLPENTADECANE	0.036566	C16H34
HEPTADEC-8-ENE	0.035679	C17H34
DECANE, 2,2-DIMETHYL-	0.035374	C12H26
6-[2-PHENYLETHENYL]-2H-PYRAN-2,4(3H)-DIONE	0.0348	C13H10O3
Nonadecane, 2-methyl-	0.033352	C20H42
2-Piperidinone, N-[4-bromo-n-butyl]-	0.033145	C9H16BrNO
TRIDECANE, 5-METHYL-	0.032656	C14H30
CYCLOHEXANE, HEXYL-	0.032283	C12H24
PHENOL, 4-(1,1-DIMETHYLETHYL)-	0.03127	C10H14O
1-DODECENE, 2-ETHYL-	0.029926	C14H28
4,5,9,10-DEHYDRO-ISOLONGIFOLENE	0.029694	C15H20
6-(4-ISOPROPYLPHENYL)-1,5-DIAZABICYCLO[3.1.0]HEXANE	0.029231	C13H18N2
HEPTACOSANE	0.028998	C27H56
13-OXABICYCLO[10.1.0]TRIDECANE	0.028759	C12H22O
CYCLOHEXANE, OCTYL-	0.028458	C14H28
Benzene, 1,1'-ethylidenebis[4-ethyl-	0.027705	C18H22
Cyclopentadecane	0.027266	C15H30
9-Nonadecene	0.02718	C19H38
As-Indacen-1(2H)-one, 3,6,7,8-tetrahydro-3,3,6,6-tetramethyl-	0.025948	C16H20O
Curlone	0.025615	C15H22O
1-UNDECENE, 9-METHYL-	0.024604	C12H24
4-(Aminomethyl)benzoic acid	0.023272	C8H9NO2
4-Undecene, 5-methyl-, (Z)-	0.022636	C12H24
cis-Z-à-Bisabolene epoxide	0.021935	C15H24O
4-Ethylbenzoic acid, tridec-2-ynyl ester	0.021311	C22H32O2
1-HEXANOL, 2-ETHYL-	0.021133	C8H18O
TRIDECANE, 4-METHYL-	0.020656	C14H30
6,10,13-Trimethyltetradecanol	0.020452	C17H36O
2-BUTENOIC ACID, 2-METHYL-, 3-HEXENYL ESTER, (Z,Z)-	0.020193	C11H18O2
2-(2-FURYL)-N-PHENYLPROPANAMIDE	0.019574	C13H13NO2
BENZENEACETIC ACID, à,à-DIMETHYL-, 2-METHYL-2-PHENYLPROPYL ESTER	0.01864	C20H24O2
36.33 Apritone<Z->	0.018624	C15H24O
3-tert-Butylsulfanyl-3-fluoro-2-trifluoromethyl-acrylic acid methyl ester	0.017815	C9H12F4O2S
Naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S-cis)-	0.015872	C15H22
Limonen-6-ol, pivalate	0.015622	C15H24O2
BENZENEMETHANOL, 3,5-DIMETHYL-	0.015507	C9H12O
CYCLOHEXANE, 1-METHYL-2,4-BIS(1-METHYLETHENYL)-, (1à,2á,4á)-	0.015046	C13H22

TRISILOXANE, 1,1,1,5,5,5-HEXAMETHYL-3,3-BIS[(TRIMETHYLSILYL)OXY]-	0.014785	C12H36O4Si5
Tridecane, 5-propyl-	0.014112	C16H34
Benzene, 1,3,5-triethyl-	0.013779	C12H18
Cyclopentane, hexyl-	0.013513	C11H22
Cyclohexene, 3-heptyl-	0.013192	C13H24
Malonic acid, isobutyl tetradecyl ester	0.01175	C21H40O4
Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-	0.011721	C12H18
Tridecane, 3-methyl-	0.011277	C14H30
PHENOL, 4,4'-(1-METHYLETHYLIDENE)BIS-	0.011234	C15H16O2
TRIDECANE, 6-METHYL-	0.010951	C14H30
1,5,6,7-Tetramethyl-3-phenylbicyclo[3.2.0]hepta-2,6-diene	0.010611	C17H20
2-PHENYL-2-(4-HYDROXYCYCLOHEXYL)PROPANE (ISOMER B)	0.010611	C15H22O
1,8-Cyclopentadecadiyne	0.010571	C15H22
2-METHOXY-2-PHENYL-1-OXABICYCLO[5.2]OCTANE (3-ISOPROPOXY-2-METHYLPROPYL)BENZENE	0.008176	C14H18O2
OXIRANECARBOXAMIDE, 2-ETHYL-3-PROPYL-	0.007676	C8H15NO2
1-TERT-BUTYL-7-METHOXY-NAPHTHALENE	0.007449	C15H18O
1H-INDOLE-2,3-DIONE	0.006969	C8H5NO2
2-PHENYL-1-P-TOLYLETHANOL	0.00681	C14H16O
1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)-	0.005817	C14H24
Pyrido[4,3-d]pyrimidin-4(3H)-one	0.005692	C7H5N3O
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.005542	C15H24
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHOXY-	0.005037	C15H22O
BENZENE, CHLORODIETHYL-	0.004415	C10H13Cl
Naphthalene, 1,6-dimethyl-	0.003878	C12H12
ACETIC ACID, (à-METHYLSALICYLIDENE)HYDRAZIDE	0.003529	C10H12N2O2
Oxalic acid, cyclobutyl octyl ester	0.003187	C14H24O4
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.002842	C16H18
1,2-Benzenediol, O-(4-ethylbenzoyl)-O'-propargyloxycarbonyl-	0.002728	C19H16O5
UNDECANE, 3,8-DIMETHYL-	0.002692	C13H28
UNDECANE, 3,8-DIMETHYL-	0.002424	C13H28
3,3-TRIMETHYLENEDITHIOPROPIONITRILE	0.002347	C6H9NS2
Benzene, 1,1'-ethylidenebis[3,4-dimethyl-	0.002148	C18H22
Amfetamine	0.001734	C9H13N
Phenanthrene	0.001698	C14H10
ETHER, HEXYL PENTYL	0.001585	C11H24O
4,4-DIMETHYL-6-ETHYL-6-(2-METHYLPROP-2-ENYL)TETRAPYRAN-2-ONE	0.001361	C13H22O2
TRICYCLO[4.4.0.0(2,7)]DEC-3-ENE, 1,3-DIMETHYL-8-(1-METHYLETHYL)-, ST	0.001121	C15H24

1H-CYCLOPENTA[1,3]CYCLOPROPA[1,2]BENZENE, OCTAHYDRO-7-METHYL-3-METHYLENE-4-(1-METHYLETHYL)-, [3AS-(3Aà,3Bá,4á,7à,7AS*)]-	0.001082	C15H24
1,1'-BIPHENYL, 4-METHYL-	0.000905	C13H12
1-Octadecanesulphonyl chloride	0.00085	C18H37ClO2S
Furan, 3-(4,8-dimethyl-3,7-nonadienyl)-, (E)-	0.000782	C15H22O
Phenanthrene, 4-methyl-	0.000571	C15H12
Oxalic acid, isobutyl undecyl ester	0.000419	C17H32O4
1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	0.000375	C16H18
BENZENAMINE, N-(2-HYDRAZINO-1-METHYLPROPYL)-, (R*,R*)-	0.000264	C10H17N3
NAPHTHALENE, 1,2,3,4,4A,8A-HEXAHYDRO-	0.000205	C10H14
2,4-DIMETHYL-2-(2-PHENYLETHENYL)-5,6-DIHYDRO-1,2-PYRAN	0.000194	C15H18O
NAPHTHALENE-1-D, 1,2,3,4,4A,5,6,7-OCTAHYDRO-4A-METHYL-, CIS-	8.08E-05	C11H17D
IMIDOSULFUROUS DIFLUORIDE, [FLUORO[(TRIFLUOROACETYL)IMINO]METHYL]-	8.07E-05	C3F6N2OS
5-IODO-2-PENTANONE	6.19E-05	C5H9IO
FLUORANTHENE	5.65E-05	C16H10
DECANE, 3,3,5-TRIMETHYL-	3.68E-05	C13H28
2-PHENYL-2-(3,4-DIMETHYLPHENYL)PROPANE	2.98E-05	C17H20
Dodecane, 2-methyl-	2.1E-06	C13H28
BICYCLO[2.2.1]HEPTANE-2-METHANOL, 2,7-DIMETHYL-, (EXO,SYN)-	1.05E-06	C10H18O
Benzene, (1-methylundecyl)-	0	C18H30
Pyrollidine, 2,5-bis(imino)-	0	C4H7N3
Total	100	

Fraction: MP 15-16

Compound Name	Area%	Formula
ISOBUTYL ESTER OF NITROUS ACID	11.512	C4H9NO2
Octane, 2,7-dimethyl-	11.413	C10H22
1-Docosene	11.213	C22H44
1-Hexadecene	10.069	C16H32
1-Docosene	6.9548	C22H44
1-DECENE, 4-METHYL-	3.6909	C11H22
1-Docosene	3.2255	C22H44
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	2.952	C15H24
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	2.9331	C15H24
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	2.8948	C15H22
Butane, 1,3-dichloro-3-methyl-	2.8948	C5H10Cl2
24.10 Tetradecene<1->	2.0874	C14H28
1-PENTANOL, 2-PROPYL-	1.5399	C8H18O
Hexadecane	1.5399	C16H34
HEPTADECANE	1.1386	C17H36
1-METHYL-4-(5-METHYL-1-METHYLENE-4-HEXENYL)-1-CYCLOHEXENE	0.99792	C15H24
PENTADECANE	0.95402	C15H32
Heptacosane	0.93117	C27H56
1-Octene, 3,7-dimethyl-	0.88596	C10H20
Tetradecane	0.88157	C14H30
1-Docosene	0.80441	C22H44
Octadecane	0.79939	C18H38
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.65491	C15H24
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.5641	C15H22
Nonadecane	0.56289	C19H40
1-ISOPROPYL-2,2-DIMETHYL-PROPYLIDENEAMINE	0.53094	C8H17N
TRANS- ζ -BISABOLENE	0.52823	C15H24
35.51 Turmerone<ar->	0.4365	C15H20O
DODECANE, 2,6,10-TRIMETHYL-	0.42502	C15H32
Adipic acid, di(2-ethylcyclohexyl) ester	0.41023	C22H38O4
BENZENE, 1-(BROMOMETHYL)-4-(1-METHYLETHYL)-	0.38877	C10H13Br
Oxalic acid, allyl hexadecyl ester	0.33663	C21H38O4
4,8-Dioxaspiro[2.5]oct-1-ene, 6,6-dimethyl-	0.33663	C8H12O2
2-PENTANOL, 3-ETHYL-	0.32598	C7H16O
1-Docosene	0.32598	C22H44
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.32166	C15H20

1-Decene, 8-methyl-	0.3027	C11H22
Succinic acid, di(3-phenylpropyl) ester	0.29959	C22H26O4
n-Hexadecanoic acid	0.22465	C16H32O2
Hexane, 1-(hexyloxy)-3-methyl-	0.22048	C13H28O
UNDECANE, 2,6-DIMETHYL-	0.21853	C13H28
1-Docosene	0.21464	C22H44
SPIRO[2.9]DODECA-4,8-DIENE	0.20428	C12H18
Octadecane, 2-methyl-	0.20274	C19H40
2-Butyl-1-decene	0.20274	C14H28
TRICYCLO[10.2.1.0E2,11]PENTADECA-4,8-DIEN, (E,Z)-	0.18607	C15H22
3-[4'-ETHYL-2'-METHYLPHENYL]-2,2-DIMETHYLPROPANAL	0.18565	C14H20O
32.58 Helifolen-12-al B (anti-anti-anti-)	0.17673	C15H22O
1-Nonadecene	0.17544	C19H38
9-ACETYL-2,6-DIMETHYL-10-HYDROXYBICYCLO[4.4.0]DECA-1,4-DIEN-3-ONE	0.16527	C14H18O3
1-Hexadecene	0.16458	C16H32
1,4-Methanophthalazine, 1,4,4a,7,8,8a-hexahydro-9,9-dimethyl-, (1à,4à,4aà,8aà)-	0.16189	C11H16N2
1,3-BIS(PHENYLTHIO)BUT-1-ENE	0.15916	C16H16S2
4-UNDECENE, 5-METHYL-	0.15658	C12H24
Cyclooctane, 1,4-dimethyl-, trans-	0.14957	C10H20
Tetradecane, 2,6,10-trimethyl-	0.14648	C17H36
2-Butyl-1-decene	0.13958	C14H28
cis-2-Methyl-7-octadecene	0.13673	C19H38
OCTADECANE	0.13245	C18H38
TRICYCLO[5.2.1.0 1,5]DECANE-8,9-DIOL	0.12824	C10H16O2
TRANS-3-METHOXY-5-PHENY-4-METHYLCYCLOPENT-2-EN-1-ONE	0.12262	C13H14O2
Cyclohexane, (1,1-dimethylpropyl)-	0.12239	C11H22
1-Propene, 2-nitro-3-(1-cyclooctenyl)	0.12214	C11H17NO2
(3S,4S,5S)-3-BUTYL-4,5-EPOXY-5-METHYLTETRAHYDROFURAN-2-ONE	0.12046	C9H14O3
PENTADECANE, 5-METHYL-	0.12046	C16H34
4-UNDECENE, 3-METHYL-, (E)-	0.11993	C12H24
1-Nonadecene	0.11722	C19H38
cis-2-Methyl-7-octadecene	0.1119	C19H38
1-Hexadecene	0.11082	C16H32
<No Name>	0.11082	C9H13DO
1-Docosene	0.10987	C22H44
Dodecane, 2,6,10-trimethyl-	0.10831	C15H32
UNDECANE, 4,4-DIMETHYL-	0.10613	C13H28
4-DECENE, 5-METHYL-, (E)-	0.10297	C11H22
1-OCTYN-3-OL, 4-ETHYL-	0.10297	C10H18O

1,6,10-DODECATRIENE, 7,11-DIMETHYL-3-METHYLENE-, (E)-	0.097622	C15H24
Butane, 2-cyclopropyl-	0.091146	C7H14
2,5-Dimethylcyclohexanol	0.091146	C8H16O
(ñ)-2-Phenylbutyric acid	0.090843	C10H12O2
HEXADECANE, 4-METHYL-	0.090843	C17H36
Nonadecane	0.089315	C19H40
DECANE, 2,3,5,8-TETRAMETHYL-	0.088238	C14H30
TRIDECANE	0.084947	C13H28
(6,6-DIMETHYLBICYCLO[3.1.1]HEPT-2-YL)METHANOL	0.077672	C10H18O
BENZENE, (1-METHYLDECYL)-	0.077376	C17H28
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-8A-METHYL-, TRANS-	0.077376	C11H16O
BENZENE, 2,4-DIMETHYL-1-(1-METHYLPROPYL)-	0.075149	C12H18
3-EICOSENE, (E)-	0.074772	C20H40
4-UNDECENE, 5-METHYL-, (Z)-	0.074772	C12H24
CYCLOPENTANE, 1-METHYL-3-(2-METHYLPROPYL)-	0.074706	C10H20
4-Undecene, 5-methyl-, (Z)-	0.072826	C12H24
DECANE, 2,9-DIMETHYL-	0.070008	C12H26
2H-1,2-Oxazine, tetrahydro-2-methyl-6-phenyl-	0.069079	C11H15NO
Cyclooctane, 1,4-dimethyl-, trans-	0.068614	C10H20
1-PENTANOL, 3,3,4-TRIMETHYL-	0.068068	C8H18O
1-UNDECANOL	0.066773	C11H24O
DODECANE	0.066773	C12H26
38.52 Bisabolone <6S,7R->	0.06672	C15H24O
S-(4-Chlorophenyl) 3-(4-ethoxyphenyl)-2-propenethioate	0.066464	C17H15ClO2 S
1-DECEN-3-ONE	0.066055	C10H18O
2-Ethyl-1-dodecanol	0.064484	C14H30O
Octadecyl trifluoroacetate	0.063277	C20H37F3O2
3-METHYL[CARBONYL-13C]PHTHALIDE	0.063192	C9H8O2
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.061685	C13H20O2
2,6-DIMETHYLHEPTADECANE	0.060199	C19H40
DODECANE, 2,6,10-TRIMETHYL-	0.06004	C15H32
69.55 Octacosane	0.058408	C28H58
Diisoamylene	0.058408	C10H20
2-Undecene, 9-methyl-, (Z)-	0.057289	C12H24
3-EICOSENE, (E)-	0.055727	C20H40
1-PROPANONE, 2-CHLORO-1-(2,5-DIMETHYLPHENYL)-2-METHYL-	0.052132	C12H15ClO
1-Docosene	0.051462	C22H44
HEPTACOSANE	0.051222	C27H56
N-(7-OXO-7,8-DIHYDRO[1,8]NAPHTHYRIDIN-2-YL)ACETAMIDE	0.051121	C10H9N3O2

BENZENE, METHYL-	0.050047	C7H8
1-Undecene, 5-methyl-	0.049631	C12H24
Borane, diethyl(decyloxy)-	0.049245	C14H31BO
Ethanimidoyl cyanide, 2-oxo-N-(2-oxo-2-phenylethoxy)-2- [(phenylmethyl)amino]-	0.049003	C18H15N3O3
Curlone	0.049003	C15H22O
BICYCLO[7.2.0]UNDEC-4-ENE, 4,11,11-TRIMETHYL-8-METHYLENE-, [1R-(1R*,4E,9S*)]-	0.047778	C15H24
36.84 Santalol<(Z)-epi-beta->	0.047065	C15H24O
7-HEPTADECENE, 1-CHLORO-	0.047065	C17H33Cl
HEXADECANE	0.047065	C16H34
4-Undecene, 5-methyl-, (Z)-	0.046246	C12H24
3-CYCLOHEXEN-1-AMINE, 6-(4-METHYLPHENYL)-2,5-DIPHENYL-, (1à,2á,5á,6á)-	0.045722	C25H25N
5-EICOSENE, (E)-	0.045649	C20H40
7-HEXADECENE, (Z)-	0.042572	C16H32
9-Octadecene, (E)-	0.042547	C18H36
Oxalic acid, allyl octadecyl ester	0.042278	C23H42O4
1-Nonene	0.042273	C9H18
EICOSANE	0.041589	C20H42
3-HEXENE-2,5-DIONE	0.041589	C6H8O2
BIS(CYCLOPENTYLMETHYL) ETHER	0.041589	C12H22O
2-METHYLHEXADECANE	0.040634	C17H36
TRANS-7-PENTADECENE	0.040606	C15H30
CYCLOPROPANEMETHANOL, 2-(2-METHYL-1-PROPENYLIDENE)-3- (1-PROPENYL)-, [1à,3á(E)]-	0.040335	C11H16O
1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	0.039955	C16H18
Hexadecane, 3-methyl-	0.039062	C17H36
2-Naphthalenamine, 1,2,4a,5,6,7,8,8a-octahydro-4a-methyl-	0.037956	C11H19N
cis-2-Methyl-7-octadecene	0.037838	C19H38
1-Docosene	0.037591	C22H44
BENZENE, (1-METHYLDODECYL)-	0.035942	C19H32
1-Nonadecene	0.035942	C19H38
3-Heptene, 2,6-dimethyl-	0.035842	C9H18
Propane, 1-nitro-	0.035842	C3H7NO2
(E,Z)-2-METHYL-2-BUTENOIC ACID 3-HEXENYL ESTER	0.034748	C11H18O2
4-Methyl-1,5-Heptadiene	0.031191	C8H14
BENZENE, (1-ETHYLUNDECYL)-	0.031121	C19H32
DIHEXYLSULFIDE	0.030604	C12H26S
Tetradecane, 1-chloro-	0.029919	C14H29Cl
1-Docosene	0.029892	C22H44
BENZENE, 1,2-DIETHYL-4,5-DIMETHYL-	0.029132	C12H18
2,4-Decadien-1-ol	0.029126	C10H18O

UNDECANE	0.027307	C11H24
34.42 Aromadendrene epoxide-<allo->	0.027183	C15H24O
BENZENEPROPANOIC ACID, à,à-DIMETHYL-, ETHENYL ESTER	0.026159	C13H16O2
6-(3,3-Dimethyl-oxiran-2-ylidene)-5,5-dimethyl-hex-3-en-2-one	0.02562	C12H18O2
3,7-DIMETHYLDECANE	0.025296	C12H26
(Z)-3-HEXENYL PENTENOATE	0.024984	C11H18O2
BENZENE, (1-BUTYLNONYL)-	0.024745	C19H32
Tridecane, 3-methyl-	0.024136	C14H30
Benzene, (1-hexylheptyl)-	0.023555	C19H32
Undecane, 2,3-dimethyl-	0.023255	C13H28
GERMACRANE B	0.023087	C15H30
Decane, 2,9-dimethyl-	0.022931	C12H26
(E)-2-PHENY-2-BUTENE	0.021308	C10H12
1,2,4-TRIAZOLIDINE-3,5-DIONE, 4-METHYL-2-(1-METHYL-1-PHENYLETHYL)-	0.020798	C12H15N3O2
4-METHYL-4-(4-METHYLPHENYL)PENTANAL	0.020798	C13H18O
Cyclohexene, 1-octyl-	0.020754	C14H26
2-Hexyl-1-octanol	0.020614	C14H30O
(E)-2-DECENAL	0.019989	C10H18O
(E)-4,8-DIMETHYLNONA-3,7-DIEN-1-YNE	0.01993	C11H16
Benzene, 1,3,5-triethyl-	0.019444	C12H18
37.21 Curcumen-15-al<ar->	0.018949	C15H20O
TRIDECANE, 3-ETHYL-	0.018474	C15H32
2-Nonyn-1-ol	0.018474	C9H16O
Undecane, 2,8-dimethyl-	0.018304	C13H28
Sulfurous acid, hexyl pentadecyl ester	0.018221	C21H44O3S
1-DECANOL, 2-ETHYL-	0.017271	C12H26O
29.48 Himachalene<alpha-dehydro-ar->	0.017066	C15H20
DODECANE, 2-METHYL-	0.016878	C13H28
EICOSANE	0.016239	C20H42
HEXADECANE	0.016142	C16H34
2,5-DIMETHOXY-2,5-DIPHENYL-1,4-DIOXANE	0.015932	C18H20O4
DOCOSANE	0.015931	C22H46
HEPTADECANE	0.015819	C17H36
á-COPAEN-4 à-OL	0.014842	C15H24O
2,2',5,5'-TETRAMETHYL-1,1'-BIPHENYL	0.014187	C16H18
OCTANOIC ACID, 7-CHLORO-, METHYL ESTER	0.01394	C9H17ClO2
1-OCTEN-3-ONE	0.013711	C8H14O
1-DECANOL, 2-ETHYL-	0.013485	C12H26O
(O-Butyrylphenoxy)acetic acid	0.012949	C12H14O4
ETHYL-2-VINYLPYRAZINE	0.012892	C8H10N2
1-AZIDO-1-ETHENYLCYCLOPROPANE	0.01246	C5H7N3

2H-PYRAN-2-ONE, TETRAHYDRO-6-PENTYL-	0.012289	C10H18O2
(2-(2H(1)-4-METHOXYPHENYLETHYNE	0.011957	C9H7DO
UNDECANE, 3,9-DIMETHYL-	0.01051	C13H28
Cyclopentane, 1-pentyl-2-propyl-	0.0095311	C13H26
(1-METHYLCYCLOPROPYL)(PHENYL)METHANOL	0.009316	C11H14O
1H-INDOLE-2,3-DIONE	0.0088994	C8H5NO2
Benzene, (1-methylundecyl)-	0.0088167	C18H30
Cyanic acid, phenyl ester	0.0084987	C7H5NO
CYCLOHEXANE, UNDECYL-	0.0084204	C17H34
Benzene, (1-propyldecyl)-	0.0082179	C19H32
BENZENE, 1-METHYL-4-(TRIFLUOROMETHYL)-	0.007973	C8H7F3
3,4-NONADIENE	0.0077985	C9H16
Benzene, (1-ethyldecyl)-	0.0077811	C18H30
24.84 Sesquithujene	0.0076253	C15H24
37.38 Curcuphenol	0.0075958	C15H22O
Cyclopentane, 1,1'-ethylidenebis-	0.0073676	C12H22
PENTALENE, OCTAHYDRO-2-METHYLENE-3A-(PHENYLSULFONYL)-, CIS-	0.0071498	C15H18O2S
BENZENE, (1-ETHYLNONYL)-	0.0069968	C17H28
Benzene, (1-butyloctyl)-	0.0068558	C18H30
BIS-(3,5,5-TRIMETHYLHEXYL) ETHER	0.0061979	C18H38O
2-OXABICYCLO[3.3.1]NONANE, BENZENEMETHANESULFONAMIDE DERIV.	0.0061256	C16H21NO6S
Decane, 3-methyl-	0.005951	C11H24
31.02 Vetivenene<beta->	0.0054961	C15H22
HEXANOIC ACID	0.0051996	C6H12O2
2-(1H-IMIDAZOL-4-YL)ETHANAMINE DIHYDROCHLORIDE	0.0050402	C5H11Cl2N3
Undecane, 3-ethyl-	0.004893	C13H28
5,8-EPOXYISOQUINOLINE, 5,6,7,8-TETRAHYDRO-	0.0046881	C9H9NO
Benzamide, 3-methyl-N-allyl-	0.0045574	C11H13NO
1H-Inden-5-ol, 2,3-dihydro-	0.0044752	C9H10O
(+)-7-ENDO-ACEToxYMETHYL-1,4,4-TRIMETHYL-CIS-BICYCLO[3.2.0]HEPT-2-ENE	0.0041094	C13H20O2
Benzoic acid, 3-methyl-, 2-oxo-2-phenylethyl ester	0.0038323	C16H14O3
1-Dodecanol, 3,7,11-trimethyl-	0.0037603	C15H32O
Hypotaurine	0.0036936	C2H7NO2S
HEXADECANE	0.0034878	C16H34
11-TETRADECYN-1-OL, 13-METHYL-, ACETATE	0.0032947	C17H30O2
2-BUTANONE, 1-HYDROXY-1-PHENYL-	0.0029579	C10H12O2
Succinic acid	0.0027714	C4H6O4
3-Dodecene, (Z)-	0.0027555	C12H24
ETHYL-3-(4-TOLYL)ISOVALERATE	0.0023012	C14H20O2

PROPANE, 2-ISOCYANO-2-METHYL-	0.0021589	C5H9N
(1R,2S,5R)-5-METHYL-2-[1-METHYL-1-PHENYLETHYL]CYCLOHEXYL (1R,4S)-2-OXA-3-AZABICYCLO[2.2.2]OCT-5-ENE-3-CARBOXYLATE	0.0019683	C23H31NO3
HEXANE, 2,4-DIMETHYL-	0.0017779	C8H18
Benzene, (1-ethyldecyl)-	0.0015039	C18H30
METHYLENECYCLOOCTANE	0.0013806	C9H16
BENZENEPROPANOL, à,à-DIMETHYL-ç-(TRIMETHYLSILYL)-	0.0011446	C14H24OSi
2,4-DIAZA-3-METHYLBICYCLO[3.2.0]HEPTANE-1,5-DICARBONITRILE	0.001134	C8H10N4
EXO-1,2,3,4-TETRAHYDRO-9-ISOPROPYL-N-PHENYL-1,4- IMINONAPHTHALENE-2,3-DICARBOXIMIDE	0.00063072	C21H20N2O2
BENZENE, 1,1'-(1,1,2,2-TETRAMETHYL-1,2-ETHANEDIYL)BIS[4- METHYL-	0.00059275	C20H26
1-(1'-HYDROXYUNDECYL)-CYCLOPENTENE	0.00052058	C16H30O
(1S*,2S*)-2-BENZYL-4',5'-DIHYDRO-3'- METHYLSPIRO[CYCLOBUTANE-1,5'-ISOXAZOLE]	0.00051716	C14H17NO
38.64 Xanthorrhizol	0.00035048	C15H22O
Bumetrizole	0.00022278	C17H18ClN3O
Chlormequat	0.00018501	C5H13ClN
4-Methoxycinnamic acid	4.5303E-05	C10H10O3
1,1'-BIPHENYL, 3,4-DIETHYL-	4.0902E-05	C16H18
3-METHYL-3-NITRO-1-BUTANOL	0	C5H11NO3
Total	100	

Fraction: MP 17-21

Compound Name	Area%	Formula
3-Hexen-2-one	8.0341	C6H10O
3-Decen-5-one	5.1378	C10H18O
Phosphoric acid	4.2715	H3O4P
(7,7-Dimethyl-1-oxo-2,3,4,5,6,7-hexahydro-1H-inden-2-yl)acetic acid, ethyl ester	3.9868	C15H22O3
1,2-DIHYDRO-4-(4-METHYLPHENYL)NAPHTHALENE	2.7173	C17H16
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	2.0105	C20H24O5
2-Methyl-5-octyn-4-ol	1.9165	C9H16O
2,5,5,8a-Tetramethyl-6,7,8,8a-tetrahydro-5H-chromen-3-one	1.9004	C13H20O2
2-HEPTEN-4-ONE, 2-METHYL-	1.6968	C8H14O
9,12,15-OCTADECATRIENOIC ACID, METHYL ESTER	1.6968	C19H32O2
2-Pentene, 2,4-dimethyl-	1.6769	C7H14
2-PROPENYL IONONE 2	1.4587	C16H24O
Phthalic acid, 6-ethyl-3-octyl butyl ester	1.4587	C22H34O4
6-AMINO-8,9-DIHYDRO-7H-PURIN-8-OL	1.4565	C5H7N5O
2-Methyl-5-octyn-4-ol	1.4565	C9H16O
HEXANE, 1,6-DIBROMO-	1.4271	C6H12Br2
3-Decen-5-one	1.4267	C10H18O
Bicyclo[4.1.0]heptan-endo-2-ol, 1-(4-methoxyphenyl)-	1.3736	C14H18O2
2-OXABICYCLO[2.2.2]OCTANE, 1,3,3-TRIMETHYL-	1.34	C10H18O
1-Docosene	1.3262	C22H44
1-Docosene	1.2516	C22H44
2-Formyl-4,5-dimethyl-pyrrole	1.1776	C7H9NO
4H-FURO[3,2-C][1]BENZOPYRAN-4-ONE, 2,3-DIHYDRO-2,3,3-TRIMETHYL-, (+-)-	1.1582	C14H14O3
Bicyclo[2.2.1]heptane, 2-ethylidene-1,7,7-trimethyl-, (E)-	1.116	C12H20
1-Butene, 3-methyl-	1.1092	C5H10
Benzene, 1,3-dimethyl-	1.0745	C8H10
35.51 Turmerone<ar->	1.0172	C15H20O
1-(1'-METHYLCYCLOPENTYL)-2-PROPYN-1-ONE	1.0172	C9H12O
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.99384	C10H16O
BENZENE, 1,2-DIMETHYL-	0.98844	C8H10
8,8-DIMETHYL-4,6-BIS(1-METHYLETHYLIDENE)BICYCLO[5.1.0]OCTAN-2-ONE	0.95968	C16H24O
1-Docosene	0.93365	C22H44
3-Hexen-2-one	0.9244	C6H10O
6-[(2-ETHYLHEXYL)OXY]-6-OXOHEXANOIC ACID	0.9171	C14H26O4
HEXADECANOIC ACID, METHYL ESTER	0.91433	C17H34O2

ACETAMIDE, 2,2,2-TRIFLUORO-N-(3-PHENYLBUTYL)-	0.86294	C12H14F3NO
Bicyclo[3.3.0]octan-2-one, 7-neopentylidene-	0.79367	C13H20O
Undecane	0.77239	C11H24
((1,2-Diethylethylene)bis(p-phenylene))diacetate	0.75892	C22H26O4
BICYCLO[2.2.1]HEPT-2-EN-7-OL, 7-(4-METHOXYPHENYL)-, SYN-	0.75806	C14H16O2
1,3-Benzodioxole-5-methanol, 6-bromo-	0.74747	C8H7BrO3
5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.69314	C20H24O5
1-Propyne, 3,3'-[ethylidenebis(oxy)]bis-	0.67175	C8H10O2
Curlone	0.66023	C15H22O
1,3-DIOXOLANE-4-METHANOL, 2-PENTADECYL-, ACETATE, TRANS-	0.65506	C21H40O4
7-ANGELOXYBZW-9-HYDROXY-1-OXO-LONGIPINENE	0.62763	C15H22O3
38.52 Bisabolone <6S,7R->	0.60869	C15H24O
Tumerone	0.56462	C15H22O
4-BROM-DIPHENYLMETHANE	0.54471	C13H11Br
(1S*,2S*)-2-(3,5-DIMETHYL-4- HYDROXYPHENYL)CYCLOHEXANECARBOXALDEHYDE	0.50752	C15H20O2
Tumerone	0.49789	C15H22O
2-Nonen-4-one, 2-methyl-	0.4873	C10H18O
3,7,8-TRIAZATRICYCLO[4.3.0.02,5]NON-7-ENE-3-CARBOXYLIC ACID, 9,9-DIMETHYL-, METHYL ESTER, (1a,2a,5a,6a)-	0.46338	C10H15N3O2
1,3-PENTADIEN-1-AMINE, N,N,4-TRIMETHYL-, (E)-	0.42351	C8H15N
CYCLOPROP[E]INDENE-1A,2(1H)-DICARBOXALDEHYDE, 3A,4,5,6,6A,6B-HEXAHYDRO-5,5,6B-TRIMETHYL-, (1Aa,3Aa,6Aa,6Ba)- (+)-	0.41675	C15H20O2
2-OCTENOIC ACID, 7-(ACETYLOXY)-2,4,6-TRIMETHYL-8-(5- OXAZOLYL)-, [4S-(2E,4R*,6S*,7S*)]-	0.41396	C16H23NO5
BENZENE, [(1-BUTYL-1-HEXENYL)THIO]-	0.41153	C16H24S
Dicyclohexyldisulphide	0.40829	C12H22S2
1-BUTEN-3-YNE,-4-TRIMETHYLSILYL	0.40829	C7H12Si
Tumerone	0.40353	C15H22O
7-OXABICYCLO[2.2.1]HEPTANE-2-ENDO,3-EXO-DIMETHYL BIS(TRIFLUOROACETATE)	0.39647	C12H12F6O5
2-Nonadecanone	0.39216	C19H38O
3-DECEN-5-ONE	0.38832	C10H18O
4-(2-Isopropyl-5-methylphenyl)-3-methylbutyric acid	0.38154	C15H22O2
OCTANE, 3,7-DIMETHYL-1-(2,5-XYLYL)-	0.3715	C18H30
3-(1',3'-DITHIAN-2'-YL)-2-PHENYLPROPANAL	0.3715	C13H16OS2
4-PIPERIDINONE, 1-(ETHYLSULFONYL)-2,2,6,6-TETRAMETHYL-	0.3715	C11H21NO3S
2,4-DINITRO-6-(2-BUTYL)-PHENYL-à,à- DIMETHYLACRYLSAEUREESTER	0.3715	C15H18N2O6
TRICYCLO[5.3.1.0(1,5)]UNDECAN-11-ONE	0.36809	C11H16O
1-BUTYNE, 3-METHOXY-3-METHYL-	0.36648	C6H10O

BENZENE, (1-METHYLETHYL)-	0.36632	C9H12
DIDEUTERO-(E)- α -METHYLSTYRENE	0.36622	C9H8D2
1-DECEN-4-YNE, 2-NITRO-	0.3591	C10H15NO2
39.59 Atlantone<(E)-alpha->	0.35378	C15H22O
2-(4'-METHOXYBENZYL)CYCLOHEXAN-1-ONE	0.35268	C14H18O2
1,3-Benzenediol, o-(3-methylbut-2-enoyl)-o'-(isobutyryl)-	0.31397	C15H18O4
Caryophyllene oxide	0.31369	C15H24O
6,7,8,9-TETRAHYDRO-1H-PYRROLO[3,4-C]QUINOLINE-1,3,4(2H,5H)-TRIONE #	0.31297	C11H10N2O3
BENZENE, 1,3,5-TRIMETHYL-	0.31297	C9H12
4-METHYL-1-(4-METHYLBENZOYL)PIPERIDINE	0.31297	C14H19NO
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4A α ,6 α ,8A α)]-	0.29415	C15H22O2
2(3H)-Benzofuranone, 3a,4,5,6-tetrahydro-3a,6,6-trimethyl-	0.29276	C11H16O2
1,8-NONADIYNE	0.2901	C9H12
Curlone	0.2901	C15H22O
37.38 Curcuphenol	0.2901	C15H22O
37.39 Atlantone<(Z)-alpha->	0.2901	C15H22O
Norethynodrel	0.28704	C20H26O2
2H-PYRAN-2-ONE, 4-METHOXY-6-(1-OXONONYL)-	0.28204	C15H22O4
39.59 Atlantone<(E)-alpha->	0.27665	C15H22O
CARBAMIC ACID, PHENYL-, 1-METHYLETHYL ESTER	0.27384	C10H13NO2
4-FLUOROBIPHENYL-D(5)	0.26773	C12H4D5F
4A-METHYL-1,2,3,4,4A,9,10,10A-OCTAHYDRO-1-PHENANTHRENOL	0.26655	C15H20O
4-Methyl-2-heptyn-4-ol	0.26448	C8H14O
2-CYCLOHEXEN-1-ONE, 6-(1,5-DIMETHYL-4-HEXENYL)-3-METHYL-, [R-(R*,R*)]-	0.25905	C15H24O
5A-METHYL-3,8-DIMETHYLENE-2-OXODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.25585	C20H24O5
Fenfluramine	0.25579	C12H16F3N
L-Threitol	0.24755	C4H10O4
2,2'-DIIHYDROXY-4'-METHYL-5-METHOXYBIPHENYL	0.24701	C14H14O3
3-Pyridinamine, 2,6-dimethyl-	0.21532	C7H10N2
Benzene, 1,3,5-trimethyl-	0.20743	C9H12
4-(2-HYDROXY-2,6,6-TRIMETHYL-CYCLOHEXYL)-BUT-3-EN-2-ONE	0.19917	C13H22O2
BENZENAMINE, 2-METHOXY-N-2-PROPENYL-	0.18704	C10H13NO
37.63 Nuciferol<Z->	0.18268	C15H22O
4A,7-ETHANO-4AH-BENZOCYCLOHEPTENE, 1,2,3,4,7,8-HEXAHYDRO-1,1,7-TRIMETHYL-, (+.-.)-	0.18268	C16H24
Thiophene, 2-bromo-	0.17758	C4H3BrS
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4A α ,6 α ,8A α)]-	0.17742	C15H22O2

Piperidine-à-toluenesulfonic acid amide	0.17212	C12H17NO2S
á TUMERONE	0.17212	C15H22O
1,4-Dimethylindanyl acetate	0.17004	C13H16O2
Benzene, 1,3,5-trimethyl-	0.16938	C9H12
PYRROLO[3,2,1-D,E]ACRIDIN-6-ONE	0.16843	C15H9NO
n-Hexadecanoic acid	0.16373	C16H32O2
HEXADECANOIC ACID, 1-METHYLETHYL ESTER	0.15985	C19H38O2
36.51 Atlantone<(Z)-gamma->	0.15814	C15H22O
2H-1,4-Benzoxazine-6-carboxamide, N-cyclopropyl-3,4-dihydro-3-oxo-	0.15669	C12H12N2O3
37.63 Nuciferol<Z->	0.1565	C15H22O
CYCLOPENTANEUNDECANOIC ACID, METHYL ESTER	0.15524	C17H32O2
meta-Methoxybenzenethiol	0.15275	C7H8OS
1-METHYL-1H-PYRAZOLE-3-CARBOXAMIDE	0.15268	C5H7N3O
2-CYCLOHEXEN-1-ONE, 6-(1,5-DIMETHYL-4-HEXENYL)-3-METHYL-, [S-(R*,S*)]-	0.14819	C15H24O
1-(1,3-DIMETHYL-BUTA-1,3-DIENYL)-3,7,7-TRIMETHYL-2-OXA-BICYCLO[3.2.0]HEPT-3-ENE	0.14645	C15H22O
7-[1-(HYDROXYMETHYL)VINYL]-1,4A-DIMETHYL-3-OXO-2,3,4,4A,5,6,7,8-OCTAHYDRO-2-NAPHTHALENYL ACETATE	0.1464	C17H24O4
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.14282	C15H24O
3-Methyl-2-butenic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester	0.13998	C16H24O2
BENZO[B]THIOPHENE, 2-CHLORO-3-METHYL-	0.13915	C9H7ClS
2-Amino-4-(4-chloro-3-methyl)phenylthiazole	0.13908	C10H9ClN2S
1H,4H,5H,8H-3A,4A,7A,8A-TETRAAZACYCLOPENTA[DEF]FLUORENE, HEXAHYDRO-2,2,6,6-TETRAMETHYL-, CIS-	0.13908	C14H26N4
Ethylbenzene	0.13898	C8H10
NAPHTHO[1,2-B]FURAN-2,8(3H,4H)-DIONE, OCTAHYDRO-3,5A,9-TRIMETHYL-, [3S-(3à,3Aà,5Aá,9à,9Aà,9Bá)]-	0.13662	C15H22O3
BENZENE, 1-(3-CYCLOPENTYLPROPYL)-2,4-DIMETHYL-	0.13387	C16H24
Benzenemethanol, à-(1-phenylaminoethyl)-	0.13387	C15H17NO
ARTEMORIN	0.13387	C15H20O3
BENZENEMETHANAMINE, à-ETHYL-4-METHOXY-	0.13214	C10H15NO
2,5-NONADIEN-4-ONE, 9-(3-FURANYL)-2,6-DIMETHYL-, (E)-	0.13201	C15H20O2
3,3-DIETHYL-4,5-DIMETHYL-4-HEXEN-2-ONE	0.13201	C12H22O
N-(6-Methyl-8-oxo-6,7,8,9-tetrahydro-5-oxa-9-azabenzocyclohepten-3-yl)acetamide	0.13201	C12H14N2O3
Phthalic acid, butyl non-5-yn-3-yl ester	0.12936	C21H28O4
BENZENE, 1,3,5-TRIMETHYL-	0.12894	C9H12
48.44 Falcarinol<Z->	0.1282	C17H24O
35.51 Turmerone<ar->	0.12251	C15H20O
Endo-2-bornyl carbanilate	0.11918	C17H23NO2
1,2-BIS(1-METHYL-2-PROPENYL)BENZENE	0.1153	C14H18
Benzene, 1,3,5-trimethyl-	0.10296	C9H12

2-(PHENYLTHIO)-1,3-DIOXANE	0.10275	C10H12O2S
4,5,6,7-TETRAHYDRO-3A,7A-ETHANO-1H-INDENE	0.10275	C11H16
Benzene, 1,2,4-trimethyl-	0.10223	C9H12
1,4-Methano-1H-Cyclopropa[d]pyridazine, 4,4a,5,5a-tetrahydro-6,6-dimethyl-, (1à,4à,4aà,5aà)-	0.10208	C8H12N2
3-METHYLENE-4-PENTENYL ACRYLATE	0.091895	C9H12O2
3-Methylthiophene-2-carboxanilide	0.091716	C12H11NOS
2,5,7-Nonatrien-4-one, 9-(3-furanyl)-2,6-dimethyl-, (E,E)-	0.090619	C15H18O2
2-PROPENYL IONONE 3	0.089039	C16H24O
37.63 Nuciferol<Z->	0.087193	C15H22O
<No Name>	0.084919	C13H22O
2-TERT-BUTYL-6-(2-HYDROXY-2-MESITYLETHYL)-4H-1,3-DIOXIN-4-ONE	0.084919	C19H26O4
TRICYCLO[3.3.1.13,7]DECANE, 1-BROMO-	0.084919	C10H15Br
1-Ethyl-trans-2-butenyl 2,4,6-trimethylbenzoate, (ñ)-	0.083123	C16H22O2
2H,7H-10,4A-(NITRILOMETHANO)BENZOCYCLOOCTENE, 1,3,4,8,9,10-HEXAHYDRO-8,8-DIMETHYL-, TRANS-	0.082886	C15H23N
N,N'-Bis(2,6-dimethyl-6-nitrosohept-2-en-4-one)	0.079755	C18H30N2O4
Acetic acid, 2-methylene-bicyclo[3.2.1]oct-6-en-8-yl ester	0.07474	C11H14O2
ETHANONE, 1-[2-[2-METHYL-2-(5-METHYL-2-FURANYL)PROPYL]CYCLOPROPYL]-	0.068413	C14H20O2
2-n-butyladamantane	0.066278	C14H24
3,3-DIMETHOXY-2-CHLORO-1-BUTENE	0.066043	C6H11ClO2
3-PYRIDINEMETHANOL, à-(AMINOMETHYL)-	0.064916	C7H10N2O
Benzene, 1-methyl-3-(1-methylethyl)-	0.056285	C10H14
Benzene, 1-methyl-2-(1-methylethyl)-	0.056167	C10H14
1-OCTADECANOL	0.054661	C18H38O
37.63 Nuciferol<Z->	0.05428	C15H22O
Hexadecanoic acid, ethyl ester	0.052467	C18H36O2
3-(3,6-DIMETHYL-2-METHOXYPHENYL)-3-METHYLBUTANAL	0.0521	C14H20O2
29.74 Artedouglasia oxide C	0.051831	C15H22O3
2-Butanol, 4-(2,2-dimethyl-6-methylenecyclohexylidene)-	0.051831	C13H22O
FURAN, 2-(1,1-DIMETHYLETHYL)-	0.050206	C8H12O
3-METHYLENEBICYCLO[3.2.1]OCTAN-1-OL	0.050167	C9H14O
Tricyclo[5.3.0.0(2,6)]dec-3-ene-8-bromo-5,10-dioxobis(ethylene ketal)-	0.05011	C14H17BrO4
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.045654	C10H16O
1H-2-Indenone,2,4,5,6,7,7a-hexahydro-3-(1-methylethyl)-7a-methyl	0.045108	C13H20O
2-(2,5-Dimethoxyphenyl)cyclohex-2-enone	0.04235	C14H16O3
9.88 Artemisia ketone	0.041674	C10H16O
3-BUTENOIC ACID, 2-ETHYL-3-METHYL-2-(PHENYLTHIO)-, METHYL ESTER	0.040379	C14H18O2S
3(4H)-Dibenzofuranone, 4a,9b-dihydro-8,9b-dimethyl-	0.0403	C14H14O2

1,8,14-TRIOXA-13,15-DIAZATRICYCLO[7.8.0(9,17).0(11,15)]HEPTADECAN-10,12,15,17-TETRAENE-OXIDE	0.03215	C12H14N2O4
3-Methylbut-2-enoic acid, 3-methylphenyl ester	0.03215	C12H14O2
1,2-BENZENEDICARBOXYLIC ACID	0.030284	C24H38O4
1-METHYL-1-(2-OXOPROPYL)TETRAHYDROCYCLOPROPA[CD]PENTALENE-2,3(1H,2AH)-DIONE	0.029305	C12H14O3
Benzo[1,3]dioxole-5-carboxylic acid, [2-(4-cyclohexylphenoxy)ethyl]amide	0.027297	C22H25NO4
ACETIC ACID, [6,8,9-TRIMETHYL-4-(3,4-METHYLENEDIOXYPHENYL)-3-OXABICYCLO[3.3.1]NON-6-EN-1-YL)METHYL ESTER	0.026455	C21H26O5
Fenfluramine	0.026321	C12H16F3N
1H-NAPHTHO[2,1-B]PYRAN, DODECAHYDRO-7,7,10A-TRIMETHYL-, [4AR-(4Aà,6Aá,10Aà,10Bá)]-	0.025575	C16H28O
3-Heptyne, 2,2,6-trimethyl-5-chloro-6-phenyl-	0.024136	C16H21Cl
Fenfluramine	0.023456	C12H16F3N
N-MESITYL-N'-(2-PROPYNYL)THIOUREA	0.023366	C13H16N2S
35.51 Turmerone<ar->	0.023025	C15H20O
2-HEPTEN-4-ONE, 2-METHYL-6-(4-METHYLPHENYL)-, (S)-	0.022034	C15H20O
Phthalic acid, 2,7-dimethyloct-7-en-5-yn-4-yl isohexyl ester	0.021665	C24H32O4
3,4-Tetramethylene-5,5-pentamethyle-2-nepyrzoline	0.01785	C12H20N2
1,4-METHANOAZULEN-7-OL, DECAHYDRO-1,5,5,8A-TETRAMETHYL-, [1S-(1à,3Aá,	0.017758	C15H26O
2-(2,5-Dimethoxyphenyl)cyclohex-2-enone	0.016812	C14H16O3
BENZENEMETHANAMINE, à-CYCLOHEXYL-, DIDEUTERO-	0.016195	C13H17D2N
Phthalic acid, 4-fluoro-2-nitrophenyl methyl ester	0.014506	C15H10FNO6
2-Cyanoamino-4,6-dihydroxypyrimidine	0.012664	C5H4N4O2
Benzene, 1-(1,2-dimethyl-3-methylenecyclopentyl)-4-methyl-, cis-	0.012352	C15H20
2-METHYL-1,2-DIPHENYL-1-PROPANIMINE	0.011789	C16H17N
1-Butyl-3-methylimidazolium	0.01168	C8H15N2
Trimethyl(3,3-difluoro-2-propenyl)silane	0.011185	C6H12F2Si
9-Methoxycalamenene	0.011156	C16H24O
3-Methylbut-2-enoic acid, 3,4-dimethylphenyl ester	0.010552	C13H16O2
CYCLOHEXANEACETONITRILE	0.0099104	C8H13N
37.80 Curcumen-12-ol<gamma-(Z)->	0.0097746	C15H24O
1,1,4,4-TETRAMETHYL-2-HYDROXY-7-ETHYL-TETRALINE	0.0090069	C16H24O
1,2-DICYANO-4-(TOLYLTHIO)BENZENE	0.0086651	C15H10N2S
BICYCLO[2.2.1]HEPTANE-2,6-DIOL, 1,7,7-TRIMETHYL-, (ENDO,ENDO)-	0.0085033	C10H18O2
2-BUTANONE, 4-(2,2-DIMETHYL-6-METHYLENOCYCLOHEXYL)-	0.0078459	C13H22O
2-Propenal, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	0.0074607	C12H18O
7-(1,3-DIMETHYL-BUTA-1,3-DIENYL)-1,6,6-TRIMETHYL-3,8-DIOXA-TRICYCLO[5.1.0.0 2,4]OCTANE	0.0074517	C15H22O2

1H-3A,7-METHANOAZULEN-6-OL, OCTAHYDRO-3,6,8,8-TETRAMETHYL-, [3R-(3à,3Aá,6à,7á,8Aà)]-	0.0063427	C15H26O
3,8-DIHYDROXY-2-METHYLCHROMONE DIACETATE	0.0061126	C14H12O6
2-METHOXY-6-METHYLBENZAMIDE	0.0060305	C9H11NO2
D-ERYTHRO-2-PENTULOSE, 1-DEOXY-3,5-O-(PHENYLMETHYLENE)-	0.005277	C12H14O4
3-Cyclopentylpropionic acid, 3-phenylpropyl ester	0.0048304	C17H24O2
1-Bicyclo[3.3.1]non-6-en-3-yl-2-methylpropan-1-one	0.0044043	C13H20O
34.58 Cedren-3-one<2-epi-beta->	0.0044043	C15H22O
35.51 Turmerone<ar->	0.0044043	C15H20O
7à-ANGELOXYBZW-9á-HYDROXY-1-OXO-à-LONGIPINENE	0.0043468	C15H22O3
1H-Pyrrole-2-carboxamide, 5-[[5-imino-3,4-dihydro-2H-pyrrol-2-yl)carbonyl]amino]-N-(3-amino-3-iminopropyl)-	0.0042416	C13H19N7O2
(+).DELTA.4'-DEHYDROJURABIONE	0.003443	C16H24O3
1,3,2-DIOXARSOLANE, 2-METHYL-	0.0033811	C3H7AsO2
(2,4-DICHLOROPHENYL)ACETYLENE	0.0032024	C8H4Cl2
47.85 Polygodial	0.0026633	C15H22O2
3-Methylbut-2-enoic acid, 3-methylphenyl ester	0.0020226	C12H14O2
Adamantan-2-ol, 4-chloro-	0.0018403	C10H15ClO
2-METHYL-1-(4-METHYLPHENYL)-3-BUTEN-1-OL	0.0011778	C12H16O
3,6-METHANO-2H-CYCLOPENTA[B]FURAN-2-ONE, 3,3A,6,6A-TETRAHYDRO-	0.0011601	C8H8O2
AMINOUREA	0.00085308	CH5N3O
2-DEUTERIO PYRIDINE-3-CARBOXYLIC ACID-D1	0.00079583	C6H3D2NO2
5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrene	0.00063917	C15H22O3
N-Methyl-o-tolamide	0.0005807	C9H11NO
CARBAMIC ACID, [(1,4-DIHYDRO-1-METHYL-4-OXO-3-QUINOLINYL)METHYL]-, METHYL ESTER	0.00046192	C13H14N2O3
METHYL 4-METHYLENE-2-OCTYL-2-TRIMETHYLILYL-5-HEXENOATE	0.00037939	C19H36O2Si
3-Methyl-2-butenic acid, 2-methyloct-5-yn-4-yl ester	0.00035699	C14H22O2
1,2,3,4A,5,6,7,8,8A-DECAHYDROBENZ[D]INDEN-4(4H)-ONE	0.00033209	C13H18O
7-Oxabicyclo[4.1.0]heptane, 1-(2,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-, (E)-	0.00028389	C15H24O
3,3,6,6-TETRAMETHYL-9-OXA-4,5-DITHIAUNDECAN-1-OL	0.00020306	C12H26O2S2
4H-Cyclopenta[5,6]naphtho[1,2-b]thiophene, 3b,5,7,8,8a,8b,9,10-octahydro-6,10-dimethyl-	0.00015385	C17H22S
7à-ANGELOXYBZW-9á-HYDROXY-1-OXO-à-LONGIPINENE	0.00014407	C15H22O3
1-ACETYL-3-ETHYLAZULENE	0.00011657	C14H14O
4-CYANO-3-METHOXY-1,5-DIMETHYL-5,6-DIHYDROISOQUINOLINE	7.3409E-06	C13H14N2O
38.64 Xanthorrhizol	0	C15H22O
2-METHYL-1-(4-METHYLPHENYL)-3-BUTEN-1-OL	0	C12H16O
2-CYCLOHEXEN-1-ONE, 6-(4-HYDROXY-1-METHYLBUTYL)-3-METHYL-, (R*,R*)-	0	C12H20O2

2-(1-CYCLOHEXENYL)-3,3-DIMETHYLBUTAN-2-OL	0	C ₁₂ H ₂₂ O
Total	100	



Fraction: MP 22-33

Compound Name	Area%	Formula
Geranyl linalool<E,E->	5.9063	C20H34O
CYCLOICOSANE	5.0941	C20H40
CYCLOICOSANE	4.7485	C20H40
Behenic alcohol	3.5852	C22H46O
1-Docosene	3.5054	C22H44
ñ-4-Acetyl-1-methylcyclohexene	3.4207	C9H14O
7-ISOPROPENYL-4A,9-DIMETHYL-3A,4,4A,5,6,7,8,9A-OCTAHYDRONAPHTHO[2,3-D][1,3]DIOXOL-2-ONE	2.9021	C16H22O3
1-TETRADECENE	2.7993	C14H28
(Z)-3-HEXENYL (E)-2-BUTENOATE	2.6413	C10H16O2
BENZENE, 1-CHLORO-3-(4-METHYL-4-PENTENYL)-	2.2784	C12H15Cl
(-)-(1S,2R,4R)-BETA-FENCHOL	2.2727	C10H18O
9-(ETHOXYCARBONYL)-10-ETHYLIDENE BICYCLO[3.2.2]NONA-3,6-DIEN-2-ONE	2.0985	C14H16O3
D-à-Cyclohexylglycine	2.0112	C8H15NO2
Carbofurane	1.8755	C12H15NO3
n-Tetracosanol-1	1.5341	C24H50O
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	1.529	C10H16O
(S)-3-MORPHOLINOPYRROLIDINE	1.4597	C8H16N2O
2-ISOPROPENYL-5-METHYL-HEX-4-ENAL	1.3655	C10H16O
1,6-OCTADIEN-3-OL, 3,7-DIMETHYL-	1.2952	C10H18O
2-PHENYL-1-P-TOLYLETHANOL	1.2449	C14H16O
3-PENTENOIC ACID, 2,4-DIMETHYL-, 3-PHENYLPROPYL ESTER, (S)-	1.1891	C16H22O2
Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-	1.1559	C10H16O
1(2H)-NAPHTHALENONE, OCTAHYDRO-3,8A-DIMETHYL-, (3à,4Aá,8Aà)-	1.1557	C12H20O
ETHANOL, 2-(9-OCTADECENYLOXY)-, (Z)-	1.1519	C20H40O2
Benzene, 1-[1,1-dimethylethyl]-4-[2-propenyloxy]-	1.1084	C13H18O
Bicyclo[3.1.0]hex-3-en-2-one, 5-(1-methylethyl)-	1.0701	C9H12O
1,2-BENZENEDICARBOXYLIC ACID, DIBUTYL ESTER	0.98676	C16H22O4
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.9843	C15H24
2,2-DIDEUTERO OCTADECANAL	0.95383	C18H34D2O
(4Aà,8à,8Aá)-(+)-(1,4,4A,5,6,7,8,8A-OCTAHYDRO-8-HYDROXY-4A,8-DIMETHYL-2-NAPHTHALENYL)-1-ETHANONE	0.8955	C14H22O2
3-THIOPHENEACETALDEHYDE, à-ETHYL-	0.82782	C8H10OS
4-Tridecene, (Z)-	0.78862	C13H26
á-Vatirene	0.76792	C15H22
3A(1H)-AZULENOL, 2,3,4,5,8,8A-HEXAHYDRO-6,8A-DIMETHYL-3-(1-METHYLETHYL)-, [3R-(3à,3Aà,8Aà)]-	0.75003	C15H26O
33.39 Biotol <beta->	0.74309	C15H24O

SPIRO[5.5]UNDEC-2-ENE, 3,7,7-TRIMETHYL-11-METHYLENE-, (.+.)-	0.72967	C15H24
9-OCTADECENE, (E)-	0.72813	C18H36
7-ISOPROPENYL-4A,9-DIMETHYL-3A,4,4A,5,6,7,8,9A-OCTAHYDRONAPHTHO[2,3-D][1,3]DIOXOL-2-ONE	0.72705	C16H22O3
6-PROPENYL-BICYCLO[3.1.0]HEXAN-2-ONE	0.70968	C9H12O
Cyclohexanol, 2-methyl-3-(1-methylethenyl)-, (1à,2à,3à)-	0.69355	C10H18O
.DELTA.-OCTALIN EPOXIDE	0.66418	C10H16O
36.72 Himachal-4-en-1-beta-ol<11-alphaH->	0.63942	C15H26O
1-BROMO-3-METHYL-BUT-2-ENE	0.58356	C5H9Br
Phenol, 2-methyl-5-(1,2,2-trimethylcyclopentyl)-, (S)-	0.57446	C15H22O
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4Aà,6à,8Aá)]-	0.57184	C15H22O2
TETRADECANE, 1-CHLORO-	0.5661	C14H29Cl
1,3,7-Octatriene, 2,7-dimethyl-	0.56094	C10H16
3-Methyl-but-2-enoic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	0.5297	C15H24O2
2-Pentenamide, N-phenyl-	0.5203	C11H13NO
7-OXABICYCLO[4.1.0]HEPTANE, 1-(1,3-DIMETHYL-1,3-BUTADIENYL)-2,2,6-TRIMETHYL-, (E)-	0.5109	C15H24O
1-Chloro-1-n-decyloxy-1-silacyclopentane	0.49673	C14H29ClOSi
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	0.49471	C13H22O
4-Fluorobenzoic acid, 3-methylbut-2-enyl ester	0.46487	C12H13FO2
2-ETHYL-3-HYDROXYPYRIDINE	0.45709	C7H9NO
1-Docosene	0.45215	C22H44
3,7,11-Trimethyl-dodeca-2,4,6,10-tetraenal	0.40486	C15H22O
2-Pentenamide, N-phenyl-	0.40053	C11H13NO
27.38 Thujopsadiene	0.39253	C15H22
5,5,6-TRIMETHYL-6-HEPTENENITRILE	0.39172	C10H17N
7,10-PENTADECADIENOIC ACID	0.37698	C15H22O2
3-Methylbut-2-enoic acid, 4-nitrophenyl ester	0.3567	C11H11NO4
6-Tert.butyl-2,3-dicyanonaphthalen	0.34531	C16H14N2
2-PROPENYL IONONE 2	0.34531	C16H24O
N-(6-Methyl-8-oxo-6,7,8,9-tetrahydro-5-oxa-9-azabenzocyclohepten-3-yl)acetamide	0.34524	C12H14N2O3
L-(+)-Lactic acid	0.33218	C3H6O3
BICYCLO[3.3.0]OCT-2-ENE, 3-ACETOXY-8-BROMO-4-METHYL-	0.33195	C11H15BrO2
Tricyclo[4.1.0.0(2,4)]heptane, 5-(phenylthio)-, (1à,2á,4á,5à,6à)-	0.32621	C13H14S
36.72 Himachal-4-en-1-beta-ol<11-alphaH->	0.32027	C15H26O
2-CYCLOHEXEN-1-ONE, 4,4-DIMETHYL-6-METHYLENE-	0.29721	C9H12O
HEXANEDIOIC ACID, DIOCTYL ESTER	0.29364	C22H42O4
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,4A,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	0.28856	C15H24O2
1-(1,2,3-TRIMETHYL-2-CYCLOPENTEN-1-YL)ETHANONE #	0.28841	C10H16O
Dihydromyrcene	0.28386	C10H18

Propanamide, N-(3-methoxyphenyl)-2,2-dimethyl-	0.28212	C12H17NO2
2,6-DIMETHYL-2,6-OCTADIEN-1-OL	0.25741	C10H18O
47.85 Polygodial	0.25407	C15H22O2
DODECANE	0.25046	C12H26
Tridecane	0.24741	C13H28
Heptane, 3-ethyl-5-methylene-	0.24269	C10H20
3,5A,9,9-TETRAMETHYLDECAHYDROBENZO[2,3]CYCLOHEPTA[1,2-B]OXIREN-3-OL	0.24	C15H26O2
n-Hexadecanoic acid	0.23427	C16H32O2
35.53 Atlantone<beta->	0.23363	C15H22O
CYCLODECA[B]FURAN-2(3H)-ONE, 3A,4,5,8,9,11A-HEXAHYDRO-6,10-DIMETHYL-3-METHYLENE-, [3AS-(3AR*,6E,10E,11AS*)]-	0.23244	C15H20O2
LONGIPINENEPOXIDE	0.23145	C15H24O
3-OXABICYCLO[4.1.0]HEPTAN-2-ONE, 4,4,7,7-TETRAMETHYL-	0.23061	C10H16O2
36.51 Atlantone<(Z)-gamma->	0.22441	C15H22O
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.21994	C13H20O2
3-Ethyl-5-methyl-1-heptyn-3-ol	0.21807	C10H18O
CYCLOHEXENE, 4-ETHENYL-4-METHYL-3-(1-METHYLETHENYL)-1-(1-METHYLETHYL)-, (3R-TRANS)-	0.21259	C15H24
28.80 Dihydroagarofuran<4-epi-cis->	0.21259	C15H26O
1-(3,7,7-TRIMETHYLBICYCLO[4.1.0]HEPT-3-EN-2-YL)ETHANONE	0.21177	C12H18O
SPIRO[3.4]OCTAN-2-ONE, 1-ETHENYL-1-METHYL-	0.19261	C11H16O
37.63 Nuciferol<Z->	0.1881	C15H22O
4-HEXEN-3-OL, 2,2-DICHLORO-1,1,1-TRIFLUORO-5-METHYL-	0.1881	C7H9Cl2F3O
1,3-DIOXOLAN-2-ONE, 4-METHYL-5-METHYLENE-4-(2-METHYL-2-PHENYLPROPYL)-	0.1881	C15H18O3
1-SEC-BUTYL-4-METHYLBENZENE #	0.1881	C11H16
BICYCLO[5.1.0]OCTAN-2-ONE, 4,6-DIISOPROPYLIDEN-8,8-DIMETHYL-	0.18058	C16H24O
33.39 Biotol <beta->	0.17824	C15H24O
5-OXATRICYCLO[9.1.0.0(4,6)]DODEC-9-ENE-9-CARBOXALDEHYDE, 4,12,12-TRIMETHYL-, [1R-(1R*,4R*,6R*,9E,11R*)]-	0.16957	C15H22O2
1,5,5,8A-TETRAMETHYL-DECAHYDRO-1,4-METHANO-AZULEN-9-ONE	0.16678	C15H23DO
5A-METHYL-3,8-DIMETHYLENE-2-OXODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.15994	C20H24O5
2-Phenyl-l-p-toluenesulfonylaziridine	0.15994	C15H15NO2S
35.09 Atractylone	0.15924	C15H20O
Cyclopentanone, 2,5-dicyclopentylidene-	0.1588	C15H20O
Cyclopentanone, 2,5-dicyclopentylidene-	0.1588	C15H20O
Spiro[bicyclo[3.3.0]octan-6-one-3-cyclopropane]	0.15516	C10H14O
OXIRANE, 2-METHYL-3-(1-METHYL-2,3-BUTADIENYL)-, [2S-[2à,3á(R*)]]-	0.15455	C8H12O

BENZALDEHYDE, 3-HYDROXY-, OXIME	0.15095	C7H7NO2
[CARBOXY-13C]-O-TOLUIC ACID	0.15018	C8H8O2
1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hexahydro-1,4,9,9-tetramethyl-, (1à,3aà,7à,8aà)-	0.13949	C15H24
Caryophyllene	0.13737	C15H24
1-Hexadecanol	0.13482	C16H34O
3-ETHYL-2,6-DIMETHYL-4-QUINOLINETHIOL	0.13415	C13H15NS
Ylangene	0.13415	C15H24
Bergamotol, Z-à-trans-	0.13246	C15H24O
Phenacetin	0.13169	C10H13NO2
3-Methyl-2,4,10-trioxatricyclo[3.3.1.1alanan3,7alanan]decane peak 2	0.12774	C8H12O3
5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrenone	0.12461	C15H22O3
2-CYCLOHEXEN-1-ONE, 6-(1,5-DIMETHYL-4-HEXENYL)-3-METHYL-, [R-(R*,S*)]-	0.12196	C15H24O
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-5,8-DIMETHYL-1-OCTYL-	0.12173	C20H32
1-[3-(2H,3H-BENZOFURFURYL)]-2-HEPTANOL	0.12077	C15H22O2
(2E,6E)-9-(3,3-DIMETHYL-2-OXIRANYL)-3,7-DIMETHYL-2,6-NONADIENYL PHENYL SULFIDE	0.11991	C21H30OS
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-5,8-DIMETHYL-1-OCTYL-	0.11847	C20H32
36.98 Atlantone<(E)-gamma->	0.1166	C15H22O
3-METHYL-3,4,5,6,7,8,9,10,11,12,13,14-DODECAHYDRO-2H-1-OXA-BENZOCYCLODODECENE	0.11118	C16H28O
4,6,6-TRIMETHYL-2-(3-METHYL-BUTA-1,3-DIENYL)-3-OXA-TRICYCLO[5.1.0.0 2,4]OCTANE	0.10931	C15H22O
NAPHTHALENE, 1,2,3,4,4A,5,6,8A-OCTAHYDRO-4A,8-DIMETHYL-	0.10693	C12H20
3-METHYL-4-(1,3,3-TRIMETHYL-7-OXA-BICYCLO[4.1.0]HEPT-2-YL)-BUT-3-EN-2-ONE	0.10351	C14H22O2
1,6,10-DODECATRIEN-3-OL, 3,7,11-TRIMETHYL-, [S-(Z)]-	0.10351	C15H26O
1,4-BENZENEDIOL, 2,6-BIS(1,1-DIMETHYLETHYL)-	0.10155	C14H22O2
1-PROPENE, 3-CHLORO-	0.093785	C3H5Cl
BUTANE, 1,1-DIBUTOXY-	0.093426	C12H26O2
1,3-PROPANEDIOL, 2-METHYL-2-(1-METHYLPROPYL)-, DICARBAMATE	0.09227	C10H20N2O4
N-BENZYLIDENEMETHYLAMINE-N-OXIDE	0.091687	C8H9NO
2-AMINO-3-PHENYLPROPANAMIDE	0.089892	C9H12N2O
trans-Z-à-Bisabolene epoxide	0.089813	C15H24O
Bicyclo[5.1.0]octan-2-one, 4,6-diisopropylidene-8,8-dimethyl-	0.089545	C16H24O
5-HEPTEN-1-OL, 2-ETHENYL-6-METHYL-	0.089172	C10H18O
46.84 Amorpha-4,7(11)-dien-8-one<2-alpha-acetoxy->	0.0889	C17H24O3
3-Acetyl-2-hydroxy-2,4,6-cycloheptatrien-1-one	0.08845	C10H10O3
ç-HIMACHALENE	0.088362	C15H24
(-)-THUJOPSEN	0.088362	C15H24
29.70 Isobornyl isovalerate	0.088285	C15H26O2

1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester	0.087135	C16H22O4
7(1H)-QUINOLINONE, OCTAHYDRO-4A-(2-PROPENYL)-, CIS-(.-.-)-	0.08639	C12H19NO
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.086238	C13H20O2
Benzene, 1-(1,2-dimethyl-3-methylenecyclopentyl)-4-methyl-, cis-	0.083338	C15H20
3-BUTEN-2-OL, 4-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-	0.081942	C13H22O
1,4-Hexadien-3-one, 5-methyl-1-[2,6,6-trimethyl-2,4-cyclohexadien-1-yl]-	0.080856	C16H22O
1,2,3,4-TETRAKIS(1-METHYLETHYLIDENE)CYCLOBUTANE	0.080528	C16H24
1-[3,3-DIMETHYL-2-(3-METHYL-BUTA-1,3-DIENYL)-CYCLOPENTYL]-2-HYDROXY-ETHANONE	0.075442	C14H22O2
1-(3-BUTENOXY)NORBORNANE	0.074266	C11H18O
28.04 Curcumene<gamma->	0.072615	C15H24
Dodecane, 2,6,10-trimethyl-	0.071814	C15H32
BICYCLO[3.3.1]NON-2-EN-9-OL, SYN-	0.069434	C9H14O
1,3-DIOXOLANE, 2,2'-(3,7-DECADIENE-1,10-DIYL)BIS-, (E,E)-	0.067356	C16H28O
1-Docosene	0.066525	C22H44
39.01 Aristolone	0.059942	C15H22O
2-PHENYL-3-(P-TOLYL)-BUTANE	0.059288	C17H20
4-Undecene, 5-methyl-, (Z)-	0.057442	C12H24
1H-PYRAZOLE-3-CARBOXYLIC ACID, 2,5-DIHYDRO-2-METHYL-5-OXO-1-PHENYL-	0.056418	C11H10N2O3
39.59 Atlantone<(E)-alpha->	0.056053	C15H22O
2-Amino-4,6-dihydropyrimidine	0.055324	C4H5N3O2
2(5H)-FURANON, 5-(2-METHYL-3-METHYLEN-4-BUTYL)-	0.051324	C10H14O2
1,3-Benzenediol, o-(3-methylbut-2-enoyl)-o'-(2-fluorobenzoyl)-	0.051324	C18H15FO4
BENZENE, [[1-(1-CYCLOHEXEN-1-YL)ETHYL]THIO]-, (.-.-)-	0.048602	C14H18S
MESO-2-CHLORO-2'-CYANO-3,3,3',3'-TETRAMETHYL-2,2'-AZOBUTANE	0.048182	C13H24ClN3
Cyclobutanecarboxylic acid, tridec-2-ynyl ester	0.04489	C18H30O2
(5E)-3,6,10-TRIMETHYL-4,7,8,11-TETRAHYDROCYCLODECA[B]FURAN	0.043937	C15H20O
(E)-4-Hexenoic acid, 2-acetyl-2-(2-buten-1-yl)-, ethyl ester	0.043639	C14H22O3
4H-1,2,4-TRIAZOLE-3,4,5-TRIAMINE #	0.042892	C2H6N6
BENZENE, 1-METHYL-4-(1-METHYLETHYL)-	0.042733	C10H14
ç-HIMACHALENE	0.04235	C15H24
3,7-Cyclodecadien-1-one, 3,7-dimethyl-10-(1-methylethylidene)-, (E,E)-	0.039822	C15H22O
Cyclopentanone, 3,3,4-trimethyl-4-(4-methylphenyl)-	0.039148	C15H20O
PYRIMIDINE, 2-(1-BROMO-1-METHYLETHYL)-	0.038759	C7H9BrN2
4,4'-Dimethylbicyclohexyl-3,3'-diene-2,2'-dione	0.038205	C14H18O2
1-Ethyl-trans-2-butenyl 2,4,6-trimethylbenzoate, (ñ)-	0.038118	C16H22O2
1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPT-2-YL 3-METHYL-2-BUTENOATE	0.038044	C15H24O2
3-METHYL-2-PENTYL-2-CYCLOPENTEN-1-ONE	0.03512	C11H18O

36.98 Atlantone<(E)-gamma->	0.034829	C15H22O
9,12-TETRADECADIEN-1-OL, ACETATE, (E,Z)-	0.032745	C16H28O2
1H-BENZIMIDAZOLE, 1-(2-PROPENYL)-	0.031699	C10H10N2
7à-ANGELOXYBZW-9á-HYDROXY-1-OXO-à-LONGIPINENE	0.031699	C15H22O3
4-PIPERIDINONE, 1-(ETHYLSULFONYL)-2,2,6,6-TETRAMETHYL-	0.031521	C11H21NO3S
1-(2-NITRO-2-PROPENYL)-1-CYCLOOCTENE	0.030415	C11H17NO2
à-CURCUMENE, DIHYDRO-	0.029348	C15H24
ENDO-2,3-DI(METHOXYCARBONYL)- BENZO[E]BICYCLO[2.2.2]OCTANE	0.029276	C16H18O4
Pyrazole, 3,5-dimethyl-1-allyl-	0.028025	C8H12N2
1-Docosene	0.027365	C22H44
1,4-ETHENO-3H,7H-BENZO[1,2-C:3,4-C']DIPYRAN-3,7-DIONE, 9-(3-FURANYL)DECAHYDRO-4-HYDROXY-4A,10A-DIMETHYL-, [1R-(1à,4á,4Aà,6Aà,9á,10Aá,10Bà)]-	0.027018	C20H22O6
METHYL ESTER OF 3-(3,5-DI-TERT-BUTYL-4-HYDROXYPHENYL)-PROPIONIC ACID	0.026516	C18H28O3
38.24 Bisabolone<6R,7R->	0.026473	C15H24O
2,7-Dimethyl-2,6-octadien-4-ol	0.026084	C10H18O
2H-PYRAN-3(4H)-ONE, DIHYDRO-2-[(PHENYLTHIO)METHYL]-	0.025917	C12H14O2S
2,3,3-TRIMETHYLOCTANE	0.024539	C11H24
trans-Z-à-Bisabolene epoxide	0.023043	C15H24O
Mono-TMS of (pyridoxine-H2O)	0.02264	C11H17NO2Si
5,8,11,14,17-Eicosapentaenoic acid, methyl ester, (all-Z)-	0.021102	C21H32O2
2-METHYL-3-METHYLENE-1-HEPTEN-5-YNE	0.020882	C9H12
BENZO[1,2-B:5,4-B']DIFURAN-2-CARBOXYLIC ACID, 5,6-DIHYDRO-8-METHOXY-	0.020816	C12H10O5
ACETAMIDE, N-[(DIMETHYLAMINO)METHYLENE]-, (E)-	0.018813	C5H10N2O
(4AR,10AS,10BS)-7,7,10A-TRIMETHYL-TRANS-PERHYDRONAPHTHO[2,1-C]PYRAN	0.017364	C16H28O
ç-DODECADIENOLACTONE (Z-Z OR E-Z)	0.016669	C12H18O2
7-OXABICYCLO[2.2.1]HEPT-5-ENE-2-CARBOXYLIC ACID, 1-METHYL-3-PROPYLIDENE-, ETHYL ESTER, (1à,2à,3E,4à)-	0.016095	C13H18O3
4,5-DIMETHYL-2-PHENYL-2-PHOSPHABICYCLO[3.1.0]HEX-3-ENE-2-OXIDE	0.015999	C13H15OP
NONADECANE	0.0148	C19H40
Oxirane, tetramethyl-	0.0148	C6H12O
Bicyclo[11.3.0]hexadecane-2,14-dione	0.014791	C16H26O2
46.51 Occidol acetate	0.014369	C17H24O2
PYRIDINE, 2-[(TRIMETHYLSILYL)METHYL]-	0.014009	C9H15NSi
1,8-CYCLOTETRADECADIYNE	0.012723	C14H20
5,5,6-TRIMETHYL-6-HEPTENENITRILE	0.012225	C10H17N
1-PENTYN-3-OL, 3-METHYL-	0.012225	C6H10O
4A-METHYL-1,2,3,4,4A,9,10,10A-OCTAHYDRO-1-PHENANTHRENOL	0.011674	C15H20O

BENZENE BUTANENITRILE, à,à'-AZOBIS[à,ç,ç-TRIMETHYL-, [R*,S*-(E)]-	0.011366	C26H32N4
Coumarin-6-ol, 3,4-dihydro-4,4,5,8-tetramethyl-	0.010952	C13H16O3
2,4-HEXADIEN-1-OL	0.010747	C6H10O
OXIRANECARBOXAMIDE, 2-ETHYL-3-PROPYL-	0.010747	C8H15NO2
Bicyclo[4.1.0]heptan-3-ol, 3,7,7-trimethyl-, [1S-(1à,3à,6à)]-	0.010044	C10H18O
3-(3,5-DI-TERT-BUTYL-4-HYDROXYPHENYL)PROPIONIC ACID	0.0093798	C17H26O3
30.56 Sesquisabinene hydrate <cis-->(IPP vs. OH)	0.0086513	C15H26O
cis-3-Hexenyl isovalerate	0.0081764	C11H20O2
4,8-CYCLODODECADIEN-1-ONE	0.0074386	C12H18O
4-(3-METHOXYPHENYL)-4-METHYLCYCLOHEXANONE	0.0073766	C14H18O2
3-BUTEN-2-ONE, 4-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-	0.0070215	C13H20O
35.85 Occidenol	0.0066974	C15H24O2
(11S)-12-ACETOXY-4á,5à,7à-EUDESMAINE-3,6-DIONE	0.0062562	C17H26O4
Bumetizole	0.0060961	C17H18ClN3O
Glaucyl alcohol	0.0046298	C15H24O
2,4,6-CYCLOHEPTATRIEN-1-ONE, 2-[(4-CHLOROPHENYL)METHYL]-	0.0045183	C14H11ClO
Silane, 2-cyclohexen-1-yltrimethyl-	0.0042836	C9H18Si
4-HEXEN-2-OL, 3-ETHENYL-2,5-DIMETHYL-, ACETATE, (S)-	0.0042734	C12H20O2
DIMETHYL-BIS[1-METHYL-2-PYRROLYL] GERMANE	0.0037012	C12H18GeN2
T-BUTYL (2-METHYL-4-NITROBENZIMIDAZOL-1-YL)ACETATE	0.0033131	C14H17N3O4
METHYL [METHYL-3-CHLORO-5-O-(3'-CHLOROBENZOYL)-2,3-DIDEOXY-à-DL-ARABINO-HEXAFURANOSIDE]URONATE	0.0031007	C15H16Cl2O6
2H-PYRROLE, 5-(5-CHLORO-2-METHOXYPHENYL)-3,4-DIHYDRO-	0.0030195	C11H12ClNO
4-Ethyl-3-octanol	0.0021572	C10H22O
5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrone	0.0019607	C15H22O3
1,2-NAPHTHALENEDIOL, 1-ETHYL-1,2,3,4-TETRAHYDRO-, CIS-	0.001948	C12H16O2
1,3-Cyclopentadiene, 1,2-dimethyl-	0.0015576	C7H10
1-Methyl-5-phenylsulfanyl-1H-pyrazole-4-carbonitrile	0.0013561	C11H9N3S
PENTADECANE	0.0011078	C15H32
48.09 Isopropyl hexadecanoate	0.0010201	C19H38O2
METHYL CIS-3-HYDROXYCYCLOPENTANEACETATE	0.00099194	C8H14O3
1H-NAPHTHALIN-2-ON, 3,4,5,6,7,8-HEXAHYDRO-4A,8A-DIMETHYL-(CIS/TRANS)	0.00061513	C12H20O
Galactonic phenylhydrazide	0.00049303	C12H18N2O6
CIS-8-BROMOBICYCLO[4.2.0]OCTA-1,3,-TRIEN-7-OL	0.00046909	C8H7BrO
Tetracyclo[6.2.1.1(3,6).0(2,7)]dodec-4-ene, 11-isopropylidene-	0.00014173	C15H20
Silane, trimethylphenyl-	0.000022404	C9H14Si
Total	100	

Fraction: MP 33-37

Compound Name	Area%	Formula
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	3.8278	C15H24
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	3.8207	C15H24
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	3.7482	C15H24
5-(4-METHYLPHENYL)CYCLOHEXANE-1,3-DIONE	3.4461	C13H14O2
25.79 Dictamnol	3.3368	C12H18O
40.59 Amorpha-4,7(11)-diene<2-alpha-acetoxy->	2.6914	C17H26O2
1,2-Di(prop-2-ynyl)cyclohexane	2.6914	C12H16
2,4,6,8-NONATETRAENE, (E,Z,E)-	2.2688	C9H12
E-15-Heptadecenal	2.2169	C17H32O
2-PROPENYL IONONE 2	2.1917	C16H24O
3-Methyl-but-2-enoic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	2.0804	C15H24O2
2-PROPENYL IONONE 2	2.0311	C16H24O
1-Docosene	2.0153	C22H44
28.04 Curcumene<gamma->	1.9608	C15H24
1-TETRADECENE	1.8469	C14H28
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	1.7575	C20H24O5
1-Docosene	1.7301	C22H44
Oxalic acid, heptyl propyl ester	1.6825	C12H22O4
7-HEXADECENE, (Z)-	1.6762	C16H32
Fumaric acid, dimyrtanyl ester	1.4843	C24H32O4
1H-3A,7-METHANOAZULENE, 2,3,4,7,8,8A-HEXAHYDRO-3,6,8,8-TETRAMETHYL-, [3R-(3à,3Aá,7á,8Aà)]-	1.4754	C15H24
TRICYCLO[5.4.0.0(3,9)]UNDECA-4,10-DIENE, 4,7,9-TRIMETHYL-8-METHYLENE-	1.3737	C15H20
1H-CYCLODECAPYRAZOLE, 4,5,6,7,8,9,10,11-OCTAHYDRO-	1.3559	C11H18N2
CODIMER OF NORBORNADIENE AND DICYCLOPENTADIENE	1.2997	C17H20
IMIDAZOLIDINETRIONE, METHYLPHENYL-	1.2604	C10H8N2O3
2-(4a,8-Dimethyl-2,3,4,4a,5,6-hexahydro-naphthalen-2-yl)-prop-2-en-1-ol	1.2132	C15H22O
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	1.1684	C15H24
1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPT-2-YL 3-METHYL-2-BUTENOATE	1.0499	C15H24O2
29.48 Himachalene<alpha-dehydro-ar->	0.97439	C15H20
5,7-DIMETHYL-2-METHYLENEADAMANTANE	0.96844	C13H20
1H-BENZIMIDAZOLE, 2-METHYL-	0.89899	C8H8N2
27.38 Thujopsadiene	0.89007	C15H22
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.85842	C15H22

ALLYL IONONE 1	0.8353	C16H24O
3-(3-HYDROXY-4-METHYL-PHENYL)-3,4,4-TRIMETHYL-CYCLOPENTANONE	0.80053	C15H20O2
24.84 Sesquithujene	0.79769	C15H24
PYRIMIDINE, 4-CYCLOPROPYL-	0.7438	C7H8N2
ETHANONE, 2-BROMO-1-(4-METHYLPHENYL)-	0.74125	C9H9BrO
1-CHLOROOCCTADECANE	0.73307	C18H37Cl
BICYCLO[3.3.1]NONAN-9-ONE, 1,2,4-TRIMETHYL-3-NITRO-, (2-ENDO,3-EXO,4-EXO)-(.+.-)-	0.72182	C12H19NO3
1-HEXADECENE	0.71363	C16H32
38.52 Bisabolone <6S,7R->	0.71328	C15H24O
Tetradecane	0.70958	C14H30
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.70348	C10H16O
Benzofuran, 7-cyclohexyl-2,3-dihydro-2-methyl-	0.69828	C15H20O
2-Hexene, 4,4,5-trimethyl-	0.67663	C9H18
2-(Chloromethyl)tetrahydropyran	0.64801	C6H11ClO
1,3,5-Cycloheptatriene, 7-ethyl-	0.63607	C9H12
1,5-Cyclooctadiene, 3-(1-methyl-2-propenyl)-	0.61619	C12H18
1-Docosene	0.60325	C22H44
Thymol	0.60102	C10H14O
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.60009	C13H20O2
31.44 Bornyl angelate	0.59871	C15H24O2
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4Aà,6à,8Aá)]-	0.55122	C15H22O2
2-NAPHTHALENEMETHANOL, DECAHYDRO-à,à,4A-TRIMETHYL-8-METHYLENE-, [2R-(2à,4Aà,8Aá)]-	0.5297	C15H26O
BENZENE, [(2,5-DIMETHYL-2-HEXENYL)THIO]-, (E)-	0.52562	C14H20S
1,9-Dichlorononane	0.51864	C9H18Cl2
3,3,5,5-Tetramethylcyclopentene	0.48499	C9H16
Pantothenic acid	0.48156	C9H17NO5
33.39 Biotol <beta->	0.47576	C15H24O
2,5-HEPTADIENE, 2-METHYL-6-(4-METHYL-3-CYCLOHEXEN-1-YL)-, (E)-	0.44688	C15H24
Hexadecane	0.42857	C16H34
2-Methyl-5-octyn-4-ol	0.41744	C9H16O
4-(3',4'-METHYLENEDIOXYPHENYLETHYL)-2-METHOXY-1,2-BUTADIENE	0.40572	C14H16O3
4-(2,2-DIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL)-3-BUTYN-2-ONE	0.40517	C12H16O2
2,3,7-TRIMETHYL-3-VINYLOCT-6-ENOIC ACID	0.39926	C13H22O2
35.51 Turmerone<ar->	0.39649	C15H20O
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-	0.38216	C15H26O

9-(ETHOXYCARBONYL)-10-ETHYLIDENE BICYCLO[3.2.2]NONA-3,6-DIEN-2-ONE	0.37036	C14H16O3
1(2H)-NAPHTHALENONE, 3,4,4A,5,6,8A-HEXAHYDRO-4-HYDROXY-4A,8-DIMETHYL-2-(1-METHYLETHYLIDENE)-, (4À,4AÀ,8AÀ)-(.+.)-	0.36705	C15H22O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.34719	C20H24O5
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4AÀ,6À,8AÀ)]-	0.32124	C15H22O2
Bicyclo[4.4.0]dec-5-ene, 1,5-dimethyl-3-hydroxy-8-(1-methylene-2-hydroxyethyl-1)-	0.31982	C15H24O2
TRICYCLO[2.2.1.0(2,6)]HEPTAN-3-OL, 1-(METHYL-D)-7-METHYLENE-, STEREOISOMER	0.31431	C9H11DO
1,3,9,9-TETRAMETHYL-4-OXATETRACYCLO[5.5.0.0~2,8~.0~3,5~]DODECANE	0.31346	C15H24O
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,4A,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	0.30331	C15H24O2
2-PROPENYL IONONE 2	0.30167	C16H24O
(.+.)-2-METHYL-6-P-TOLYL-2-HEPTEN-4-OL (DIASTEREOISOMER II)	0.27591	C15H22O
Methamphetamine-D5	0.26353	C10H10D5N
38.24 Bisabolone<6R,7R->	0.26237	C15H24O
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.26053	C12H18
3-Ethyl-5-methyl-1-heptyn-3-ol	0.25629	C10H18O
2-(2-ACETYLPHENYL)CYCLOPENTANONE	0.25626	C13H14O2
SILANE, TRIMETHYL[(2-PHENYLETHENYL)OXY]-, (Z)-	0.24622	C11H16OSi
(2,4-DIMETHYL-PHENYL)-HYDRAZINE	0.24411	C8H12N2
Bicyclo[3.1.1]heptane-2-methanol, 6,6-dimethyl-, [1S-(1À,2À,5À)]-	0.24047	C10H18O
N-[2-(METHYLTHIO)ISOPROPYL]ANILINE	0.23899	C10H15NS
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4AÀ,6À,8AÀ)]-	0.23606	C15H22O2
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.23571	C15H24O
40.80 Vetivenic acid	0.23444	C15H22O2
[(3S, P(RS))-3-(PHENYLPHOSPHANYL) PYRROLIDINE	0.23342	C10H14NP
4,4'-DIMETHYL-BICYCLOHEXYL-3,3'-DIENE-2,2'-DIONE	0.23306	C14H18O2
Benzenepropanoic acid, Á,Á-dimethyl-, methyl ester	0.22855	C12H16O2
2(3H)-FURANONE, 3-(2-(DECAHYDRO-6-HYDROXY-5-(HYDROXYMETHYL)-5,8A-DIMETHYL-2-METHYLENE-1-NAPHTHALENYL)ETHYLIDENE)DIHYDRO-4-HYDROXY-, (1R-(1-ALPHA(E(S*)),4A-BETA,5-ALPHA,6-ALPHA,8A-ALPHA))-	0.21877	C20H30O5
3,3,5,5-Tetramethylcyclopentene	0.21776	C9H16
2À,8À-DICYANO-4,6-DIMETHYL-3,5,7-TRIOXATETRACYCLO[7.2.1.0(4,11).0(6,10)]DODECANE	0.20854	C13H14N2O3
Tridecane	0.20664	C13H28

27.38 Thujopsadiene	0.203	C15H22
Oxalic acid, cyclohexyl dodecyl ester	0.19494	C20H36O4
45.70 Columellarin	0.19494	C15H20O2
6-TRIDECEN-4-YNE, (Z)-	0.19255	C13H22
Eicosane	0.18942	C20H42
33.20 Atlantol<beta->	0.18043	C15H24O
(1,3-Dimethyl-2-methylene-cyclopentyl)-methanol	0.17952	C9H16O
BUTANE, 2-BROMO-2-METHYL-	0.17913	C5H11Br
35.51 Turmerone<ar->	0.1787	C15H20O
Tumerone	0.17372	C15H22O
1-Docosene	0.1707	C22H44
MEGASTIGMA-3,5-DIEN-9-OL	0.16837	C13H22O
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.15861	C13H20O2
5,5-DIMETHYLCYCLOPENTADIENE-1,2,4-(2)H(3) (3-D4)	0.15839	C7H6D4
METHYL 4-(1-METHOXY-2-HYDROXY-5-METHYLBICYCLO[2.2.2]OCT-5-EN-2-YL)-3-OXOBUTAONOATE	0.15795	C15H22O5
D-Asparagine	0.15784	C4H8N2O3
OCTADECANE	0.15332	C18H38
HEXADECANOIC ACID	0.15223	C16H32O2
32.70 Turmerone<ar-dihydro->	0.14771	C15H22O
2-[(2E,6Z)-7-(DIDEUTEROHYDROXYMETHYL)-3,11-DIMETHYL-2,6,10-DODECATRIENYL]BENZO-1,4-QUINONE	0.14521	C21H26D2O3
4-METHOXY-6-AZABICYCLO[3.1.0]HEX-3-ENE-6-PROPANOL	0.14106	C9H15NO2
46.84 Amorpha-4,7(11)-dien-8-one<2-alpha-acetoxy->	0.14013	C17H24O3
2-AMINO-6-ETHYL-3-METHYLPYRIDINE	0.13654	C8H12N2
Bergamotol, Z-à-trans-	0.13089	C15H24O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.13074	C20H24O5
ACETIC ACID, DICHLORO-, 2-METHYL-1-NAPHTHALENYL ESTER	0.13029	C13H10Cl2O2
(3R,3AS,4S)-3-HYDROXY-3-ISOPROPYL-6,8A-DIMETHYL-1,2,3,3A,4,5,8,8A-OCTAHYDRO-4-AZULENYL 4-METHOXYBENZOATE	0.13015	C23H32O4
2-Naphthalenemethanol, decahydro-à,à,4a-trimethyl-8-methylene-, [2R-(2à,4aà,8aá)]-	0.12358	C15H26O
9-OCTADECENOIC ACID (Z)-	0.12341	C18H34O2
2,4-Pentadien-1-ol, 3-pentyl-, (2Z)-	0.11403	C10H18O
SPIRO[4,5]DECAN-7-ONE, 1,8-DIMETHYL-8,9-EPOXY-4-ISOPROPYL-	0.11385	C15H24O2
12-Oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl-, [1R-(1R*,3E,7E,11R*)]-	0.11358	C15H24O
48.09 Isopropyl hexadecanoate	0.11253	C19H38O2
SILANE, 2-HEPTENYLDIMETHYLPHENYL-, (Z)-	0.11109	C15H24Si
5-ETHYL-3,12-DIOXATRICYCLO[4.4.2.0(1,6)]DODECAN-4-ONE	0.10643	C12H18O3

6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,3,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	0.10168	C15H24O2
Curlone	0.097124	C15H22O
á-Cyano-L-alanine	0.087975	C4H6N2O2
5,11-DIMETHYL-7,10-DIOXOTETRACYCLO[7.3.0.0(3,8).0(4,12)]DODEC-5-ENE	0.086211	C14H16O2
2-Methyl-4-octenal	0.082445	C9H16O
HEXADECANOIC ACID, METHYL ESTER	0.082158	C17H34O2
ISOPROPYL TETRADECANOATE	0.081121	C17H34O2
1-METHYL-4-(1,5-DIMETHYL-4-HEXENYLIDENE)-1-CYCLOHEXENE	0.079904	C15H24
27.73 Acoradiene<10-epi-beta->	0.07767	C15H24
3-Ethyl-5-methyl-1-heptyn-3-ol	0.074977	C10H18O
EICOSANE	0.074977	C20H42
Hexanedioic acid, bis(2-ethylhexyl) ester	0.072898	C22H42O4
CYCLOHEXENE, 3,4-DIETHENYL-1,6-DIMETHYL-	0.07212	C12H18
1,2-Benzenedicarboxylic acid, diisooctyl ester	0.066578	C24H38O4
BENZENEMETHANOL, à,à,4-TRIMETHYL-	0.065427	C10H14O
4,4-Diallyl-cyclohex-2-enone	0.062685	C12H16O
Dodecane, 2,6,10-trimethyl-	0.060954	C15H32
1,3-DITHIANE, 2-PHENYL-, 1-OXIDE, CIS-	0.058766	C10H12OS2
1,2-BENZISOTHIAZOLIN-3-ONE, 2-(PROPOXYMETHOXY)-, 1,1-DIOXIDE	0.058333	C11H13NO4S
1H-INDENE-4-ACETIC ACID, 6-(1,1-DIMETHYLETHYL)-2,3-DIHYDRO-1,1-DIMETHYL-	0.057874	C17H24O2
38.02 Eremophilone	0.055454	C15H22O
1,4,9-TRIOXA-8,10-DIAZATRICYCLO[7.4.0(5,13).0(7,11)]TRIDECA-5,7,10,12-TETRAENE	0.055403	C8H6N2O3
9-UNDECEN-2-ONE, 6,10-DIMETHYL-	0.051805	C13H24O
2-BUTENOIC ACID, 2-METHYL-, 3-METHYL-6-(1-METHYLETHYL)-2-OXO-3-CYCLOHEXEN-1-YL ESTER, [1R-[1à(Z),6à]]-	0.051753	C15H22O3
Benzene, 1,1'-[3-(3-cyclopentylpropyl)-1,5-pentanediy]bis-	0.051447	C25H34
BORANE, CHLOROBIS(1-METHYLETHYL)-	0.04466	C6H14BCl
Dodecane	0.043968	C12H26
ETHANOL, 2-(3,3-DIMETHYLBICYCLO[2.2.1]HEPT-2-YLIDENE)-	0.043798	C11H18O
19.42 Necrodol acetate<trans-alpha->	0.039642	C12H20O2
29.48 Himachalene<alpha-dehydro-ar->	0.038322	C15H20
1-Docosene	0.034354	C22H44
TRANS-1-HYDROXY-2,5,6-TRIMETHOXYDIHYDROBENZOCYCLOBUTENE	0.032274	C11H14O4
Murolan-3,9(11)-diene-10-peroxy	0.032108	C15H24O2
2-Butyl-1-decene	0.031038	C14H28
BUTANE, 1,1-DIBUTOXY-	0.030897	C12H26O2
2-(1-Methyl-1,2,3,4-tetrahydro-isoquinolin-1-yl)-butan-2-ol	0.030724	C14H21NO

2(4H)-BENZOFURANONE, 5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-	0.029358	C11H16O2
1-CYCLOPENTYLACETONE	0.028816	C8H14O
4-[3-(P-T-BUTYLPHENYL)-2-METHYLPROPYLTHIO]PENTAN-1-OL	0.026862	C19H32OS
4-Undecene, 5-methyl-, (Z)-	0.026565	C12H24
Cyclopentane, 1,2,4-trimethyl-	0.026366	C8H16
CYCLOPROPANE, 1-METHYL-1-(2-METHYLPROPYL)-2-NONYL-	0.026328	C17H34
Fenretinide	0.025076	C26H33NO2
1-Heptyne, 3-methoxy-3,4-dimethyl-	0.025076	C10H18O
2.90 Cyclohexadiene<1-methyl-1,3->	0.024905	C7H10
Propanoic acid, 2-propenyl ester	0.024601	C6H10O2
N-[3-CHLORO-3-METHYL-5-((TRIMETHYLSILYL)OXY)-2-PENTYLIDENE]CYCLOHEXYLAMINE	0.02354	C15H30CINOSi
OCTANE, 2,3,7-TRIMETHYL-	0.022987	C11H24
Benzenemethanol, à-(1-phenylaminoethyl)-	0.022747	C15H17NO
36.98 Atlantone<(E)-gamma->	0.021413	C15H22O
Khellin	0.019998	C14H12O5
1-Nonadecene	0.019915	C19H38
29.48 Himachalene<alpha-dehydro-ar->	0.018117	C15H20
6-Tridecene	0.018042	C13H26
Phenol, 2-(2-propenyl)-, acetate	0.017782	C11H12O2
2-Methyl-5-octyn-4-ol	0.017031	C9H16O
19.83 Verbenyl acetate<trans->	0.015965	C12H18O2
cis-3-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane	0.015409	C11H18
4H-4a,7-Methanooxazirino[3,2-I][2,1]benzothiazole, tetrahydro-9,9-dimethyl-, 3,3-dioxide, [4as-(4aà,7à,8ar*)]-	0.014856	C10H15NO3S
BENZENE, 1-METHYL-3-(1,2,2-TRIMETHYLCYCLOPENTYL)-, (S)-	0.014662	C15H22
DIBENZOFURAN	0.012421	C12H8O
38.52 Bisabolone <6S,7R->	0.010994	C15H24O
Selegiline	0.01093	C13H17N
Methylmalonic acid	0.010905	C4H6O4
Histidine	0.010843	C6H9N3O2
5-Undecene, 3-methyl-, (Z)-	0.010707	C12H24
(.+-.)-2-METHYL-6-P-TOLYL-2-HEPTEN-4-OL (DIASTEREOISOMER II)	0.010601	C15H22O
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.010356	C15H24O
Tricyclo[3.3.1.1(3,7)]decane, 2-nitro-	0.0087197	C10H15NO2
3-Methylbut-2-enoic acid, 4-nitrophenyl ester	0.008293	C11H11NO4
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,4A,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	0.0082423	C15H24O2
1-METHYL-4-METHYLENEBICYCLO[3.2.0]HEPTAN-6-ONE	0.0075942	C9H12O
[CARBOXY-13C]-O-TOLUIC ACID	0.0071909	C8H8O2
3-Oxabicyclo[3.3.0]octan-2-one, 7-neopentylidene-	0.0066459	C12H18O2

2,4-Diphenyl-4-methyl-2(E)-pentene	0.0057684	C18H20
2-sec-Butyl-4,6-dinitrophenyl 3-methylcrotonate (binapacryl)	0.005474	C15H18N2O6
36.48 Germacrone	0.0050236	C15H22O
BENZENE, 1,1'-[[1-(2-PROPENYL)HEXYLIDENE]BIS(THIO)]BIS-	0.0046085	C21H26S2
6,10-DIMETHYL-5,9-UNDECADIEN-2-ONE	0.004527	C13H22O
2,3,4-TRIMETHYL-1-PENTANOL	0.0042144	C8H18O
Bumetrizole	0.0039685	C17H18ClN3O
2,3,6-Trimethylacetophenone	0.0035981	C11H14O
HEPTADECANOIC ACID, 16-METHYL-, METHYL ESTER	0.0034176	C19H38O2
(+)-(4-HYDROXYPHENYL)METHYLPHENYLPHOSPHINE OXIDE	0.0033443	C13H13O2P
3-BUTEN-2-ONE, 4-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-	0.0031849	C13H20O
Butanamide, N-(3-methylphenyl)-	0.0031578	C11H15NO
4A-METHYL-1,2,3,4,4A,9,10,10A-OCTAHYDRO-1-PHENANTHRENOL	0.0030205	C15H20O
5-ETHENYL-3-METHYL-2-CYCLOHEXEN-1-ONE	0.0027783	C9H12O
3-(3,3-DIMETHYL-1-BUTYNYL)-2,2-DIMETHYL-1-PHENYLCYCLOPROPYL METHYL ETHER	0.0026186	C18H24O
2-BUTANAMINE, HYDROCHLORIDE	0.0025453	C4H11N
3-(3,5-Dimethylphenyl)adamantanol-1	0.0025279	C18H24O
Nonane, 2,2,4,4,6,8,8-heptamethyl-	0.0023188	C16H34
4-Aminophthalhydrazide	0.0020738	C8H7N3O2
(3Z)-3-HEXENYL 2-AMINOBENZOATE	0.0020402	C13H17NO2
Selenofenchone	0.0018755	C10H16Se
2,2,6-TRIMETHYL-6-(BUT-1,3-DIENYL)-CYCLOHEX-4-EN-1-ONE	0.0016804	C13H18O
28.53 Muurolo-4(14),5-diene<trans->	0.0015466	C15H24
PHENACYL PHENYLACETATE	0.0014784	C16H14O3
7-OXABICYCLO[4.1.0]HEPTAN-2-OL, 1,5,5-TRIMETHYL-6-(3-METHYL-1,3-BUTADIENYL)-, [1à,2á,6à(E)]-	0.0013386	C14H22O2
CYCLODECA[B]FURAN-2(3H)-ONE, 3A,4,5,6,7,8,9,11A-OCTAHYDRO-3,6,10-TRIMETHYL-	0.0013317	C15H24O2
1-HEPTANOL	0.0013145	C7H16O
DILL ETHER	0.0010495	C10H16O
Divinylbis(cyclopropyl)silane	0.0010008	C10H16Si
1H-1,2,4-TRIAZOLE, 1-(1-ETHYL-1-PROPENYL)-3-(METHYLTHIO)-, (E)-	0.00096305	C8H13N3S
CEDR-8-EN-15-OL	0.00073994	C15H24O
1,3-CYCLOHEPTADIENE	0.00044696	C7H10
1-PHENOXY-7-1-NONANOL	0.00038501	C15H24O2
3-[[1-(2-PHENYLETHYL)-2-PROPYNYL]OXY]BUTANOIC ACID	0.00036361	C15H18O3
7à-ANGELOXYBZW-9á-HYDROXY-1-OXO-à-LONGIPINENE	0.00014091	C15H22O3
1-(P-ETHYLPHENYL)-2-CYANOPROPANE	0.0001142	C12H15N
2-TRIDECANONE	3.7951E-05	C13H26O
2-TRIDECANONE	1.0762E-06	C13H26O

2-Naphthalenemethanol, decahydro-à,à,4a-trimethyl-8-methylene-, [2R-(2à,4aà,8aá)]-	0	C15H26O
2-CYCLOHEXEN-1-ONE, 4-(1,5-DIMETHYL-4-HEXENYL)-	0	C14H22O
1-(4-METHOXYPHENYL)-1-METHOXYPROPANE	0	C11H16O2
TRANS-8-ETHYLBICYCLO[4.3.0]-3-NONENE	0	C11H18
BENZO[C]CINNOLINE, 5,6-DIHYDRO-2,5,6,9-TETRAMETHYL-	0	C16H18N2
4,5-CIS-4,6-DIMETHYL-2,5-DIPHENYL-1,3-DIOXA-2-BORACYCLOHEXANE	0	C17H19BO2
Total	100	



Fraction: MP 38

Compound Name	Area%	Formula
2-PROPENYL IONONE 2	2.9134	C16H24O
2,4-DIAZA-3-METHYLBICYCLO[3.2.0]HEPTANE-1,5-DICARBONITRILE	2.8235	C8H10N4
25.58 Phenyl hexan-3-one<1->	2.8235	C12H16O
33.39 Biotol <beta->	2.737	C15H24O
1-Nonadecene	2.542	C19H38
[1,2,4]TRIAZOLO[5,1-C][1,2,4]TRIAZIN-4(1H)-ONE, 1,3,7-TRIMETHYL-	2.401	C7H9N5O
25.79 Dictamnol	2.3056	C12H18O
25.79 Dictamnol	2.3056	C12H18O
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	2.0597	C15H24
CYCLOHEXENE, 1-METHYL-4-(5-METHYL-1-METHYLENE-4-HEXENYL)-, (S)-	1.9531	C15H24
(+.-)-2-METHYL-6-P-TOLYL-2-HEPTEN-4-OL (DIASTEREOISOMER II)	1.9269	C15H22O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	1.8731	C20H24O5
5-Methylthieno[3,2-b]pyridine	1.8705	C8H7NS
2,4,6,8-NONATETRAENE, (E,Z,E)-	1.8195	C9H12
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	1.7868	C15H24
27.38 Thujopsadiene	1.7401	C15H22
1-Docosene	1.6367	C22H44
Behenic alcohol	1.6367	C22H46O
1-HENEICOSENE	1.6367	C21H42
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,3,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	1.6024	C15H24O2
4,4-Diallyl-cyclohex-2-enone	1.6024	C12H16O
CYCLOHEXENE, 1-METHYL-4-(5-METHYL-1-METHYLENE-4-HEXENYL)-, (S)-	1.5176	C15H24
27.05 Sesquisabinene	1.4993	C15H24
1-Hexadecene	1.3751	C16H32
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-, [1S-(1à,4à,5á)]-	1.2149	C15H24O
1-HYDROXY-4,6-DIMETHYL-7-OXO-4-VINYL-2,3-DIOXABICYCLO[4.3.0]NONANE	1.1459	C11H16O4
Spiro[4.5]decan-7-one, 1,8-dimethyl-8,9-epoxy-4-isopropyl-	1.1239	C15H24O2
3-CHLORO-3-FLUORO-2-THIABICYCLO[2.2.1]HEPT-5-ENE	1.1158	C6H6ClFS
(+)-9-EOI-18-NORAMBROX	1.0675	C15H26O
1-Docosene	1.0307	C22H44

3-Cyclopentylpropionic acid, phenyl ester	1.0208	C14H18O2
Dibutyl phthalate	0.93623	C16H22O4
BICYCLO[2.2.1]HEPTAN-2-OL, 1,7,7-TRIMETHYL-, ACETATE, EXO-	0.93571	C12H20O2
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester	0.9196	C16H22O4
5,1-Benzothiazepine-2-one, 3-acetylamino-	0.89176	C11H12N2O2S
(S)-1-METHYL-9-PHENYLBICYCLO[4.3.0]NONA-6,8-DIENE	0.88867	C16H18
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4Aà,6à,8Aá)]-	0.88316	C15H22O2
2-(3-Chloro-propyl)-1,1-dimethyl-3-methylene-cyclohexane	0.87626	C12H21Cl
4,5-DIMETHYL-2-PHENYL-2-PHOSPHABICYCLO[3.1.0]HEX-3-ENE-2-OXIDE	0.87484	C13H15OP
31.44 Bornyl angelate	0.8578	C15H24O2
à-Benzylphenethylamine	0.77783	C15H17N
TRANS-1,2-DIFLUORO-3,3-DIMETHYLBUT-1-ENE	0.77322	C6H10F2
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.75997	C15H22
Tricyclo[5.4.0.0(2,8)]undec-9-ene, 2,6,6,9-tetramethyl-	0.75024	C15H24
Propiolonitrile	0.7332	C3HN
24.84 Sesquithujene	0.73264	C15H24
7-(1,3-Dimethylbuta-1,3-dienyl)-1,6,6-trimethyl-3,8-dioxatricyclo[5.1.0.0(2,4)]octane	0.72995	C15H22O2
2-CYCLOHEXEN-1-ONE, 3-METHYL-6-(1-METHYLETHYL)-	0.71167	C10H16O
cis-Z-à-Bisabolene epoxide	0.71011	C15H24O
ç-Isosparteine	0.71011	C15H26N2
2-(4A,8-DIMETHYL-2,3,4,4A,5,6-HEXAHYDRO-2-NAPHTHALENYL)-2-PROPEN-1-OL	0.67898	C15H22O
3-BUTENOIC ACID, 4-PHENYL-, METHYL ESTER	0.67459	C11H12O2
CYCLOPENTANONE, 3-METHYL-2-(2-PENTENYL)-	0.65774	C11H18O
PHENOL, 5-METHYL-2-(1-METHYLETHYL)-	0.65774	C10H14O
1-Decen-4-yne, 2-nitro-	0.65774	C10H15NO2
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-	0.56984	C15H26O
NAPHTHALENE, 1,2,3-TRIMETHYL-4-PROPENYL-, (E)-	0.56984	C16H18
19.73 Sabinyl acetate<trans-> (Ac vs. IPP)	0.54235	C12H18O2
29.05 Premnaspirodiene	0.53031	C15H24
7-Methyl-1,2,3,5,8,8a-hexahydronaphthalene	0.49796	C11H16
4,5,9,10-DEHYDRO-ISOLONGIFOLENE	0.48743	C15H20
1-Docosene	0.48611	C22H44
29.42 Curcumene<beta->	0.47409	C15H24
3,7,7-TRIMETHYL-1,3,5-CYCLOHEPTATRIENE #	0.45398	C10H14
1-DODECENE	0.45148	C12H24
8,8-DIMETHYL-2H,8H-PYRANO[2,3-F]CHROMEN-2-ONE	0.44207	C14H12O3
1,8-Cyclopentadecadiyne	0.44042	C15H22
2-PROPENYL IONONE 2	0.4049	C16H24O

Tumerone	0.40483	C15H22O
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-	0.40062	C15H24O
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.40062	C13H20O2
Dodecane, 1,12-dibromo-	0.39019	C12H24Br2
BENZENE, 4-ETHENYL-1,2-DIMETHYL-	0.38209	C10H12
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.38209	C15H22
38.52 Bisabolone <6S,7R->	0.35325	C15H24O
3A(1H)-AZULENOL, 2,3,4,5,8,8A-HEXAHYDRO-6,8A-DIMETHYL-3-(1-METHYLETHYL)-, [3R-(3à,3Aà,8Aà)]-	0.33454	C15H26O
1-Chloro-2-methyl-2-phenylpropane	0.32787	C10H13Cl
PHENOL, 4-OCTYL-	0.30092	C14H22O
7-(1,3-DIMETHYL-BUTA-1,3-DIENYL)-1,6,6-TRIMETHYL-3,8-DIOXA-TRICYCLO[5.1.0.0 2,4]OCTANE	0.30002	C15H22O2
1-DOCOSANOL, FORMATE	0.29878	C23H46O2
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.29028	C10H16O
Bicyclo[4.4.0]dec-5-ene, 1,5-dimethyl-3-hydroxy-8-(1-methylene-2-hydroxyethyl-1)-	0.28759	C15H24O2
9-TRICOSENE, (Z)-	0.27027	C23H46
NONADECANE	0.26711	C19H40
BENZENE, 1,3-DIETHYL-5-METHYL-	0.26466	C11H16
Tricyclo[6.3.3.0]tetradec-4-ene,10,13-dioxo-	0.26171	C14H18O2
Benzene, 1-(1,3-dimethyl-3-butenyl)-3-methoxy-	0.25834	C13H18O
Bicyclo[3.2.2]non-8-en-6-ol, (1R,5-cis,6-cis)-	0.25819	C9H14O
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.258	C10H16O
Cyclopropanemethanol, à,2-dimethyl-2-(4-methyl-3-pentenyl)-, [1à(R*),2à]-	0.24696	C12H22O
Ar-tumerone	0.23712	C15H20O
2-(Phenylthio)acetonitrile	0.23109	C8H7NS
THREO-PENTONIC ACID, 2,4-DIDEOXY-2,2,4-TRIMETHYL-5-C-PHENYL-, .DELTA.-LACTONE, (5S*)-	0.22916	C14H18O3
Propanenitrile, 3-[(2-methylpropyl)amino]-	0.22844	C7H14N2
2,6,10-DODECATRIEN-1-OL, 3,7,11-TRIMETHYL-	0.22454	C15H26O
2-AZA-HEXAMETHYLTRICYCLO-(3.3.0.0)OCTAN-3-ONE	0.22382	C13H21NO
1,2-DI(2-PROPYNYL)CYCLOHEXANE	0.22306	C12H16
2,4-Hexadien-1-ol	0.21644	C6H10O
HYDROPEROXIDE, 1-METHYLPENTYL	0.21085	C6H14O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.20462	C20H24O5
2(3H)-BENZOTHIAZOLETHIONE	0.19495	C7H5NS2
BENZENE, 1-ETHENYL-3-ETHYL-	0.18929	C10H12
BICYCLO[4.3.0]-2,9-NONADIENE	0.18895	C9H12
Cyclotetradecane	0.18765	C14H28

15.21 Terpeneol<alpha->	0.18594	C10H18O
CEDR-8-EN-15-OL	0.18132	C15H24O
1-(1H-INDOL-3-YL)-2-[4-(3-PHENYL-ALLYL)-PIPERAZIN-1-YL]-ETHANOL	0.17995	C23H27N3O
2-BUTANONE, 3-METHYL-3-PHENYL-	0.17944	C11H14O
(R,R)-3,8-DIMETHYLDECANE	0.17405	C12H26
L-(+)-Threose	0.17196	C4H8O4
6-Octen-1-yn-3-ol, 3,7-dimethyl-	0.16691	C10H16O
Tetradecane	0.16674	C14H30
BUTYRONITRILE	0.16599	C4H7N
2-ISONONENAL	0.16423	C9H16O
NONADECANE	0.15992	C19H40
19.83 Verbenyl acetate<trans->	0.1554	C12H18O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.14778	C20H24O5
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.14712	C13H20O2
14.32 Mentha-1,5-dien-8-ol<para->	0.14465	C10H16O
2-BORNANONE, 5-BROMO-	0.1435	C10H15BrO
BENZENEETHANOL, à,à,á,á-TETRAMETHYL-	0.1434	C12H18O
HEXADECANOIC ACID	0.14257	C16H32O2
OXACYCLOTETRADECA-4,11-DIYNE	0.14164	C13H18O
Z-11,13-Dimethyl-11-tetradecen-1-ol acetate	0.14139	C18H34O2
1-HEPTANETHIOL	0.13905	C7H16S
11.69 Fenchocamphorone<alpha->	0.13597	C9H14O
1S-à-Pinene	0.12638	C10H16
5-ISOPROPENYL-3,6-DIMETHYL-6-VINYL-4,5,6,7-TETRAHYDRO-1-BENZOFURAN	0.1252	C15H20O
CYCLOPROPANECARBOXALDEHYDE, 2-METHYL-2-(4-METHYL-3-PENTENYL)-, TRANS-(.+.)-	0.1252	C11H18O
1-Octene, 3,7-dimethyl-	0.11914	C10H20
1-Docosene	0.11878	C22H44
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,4A,5,6,7,8,8A-OCTAHYDRO-2-NAPHTHALENOL	0.11341	C15H24O2
EICOSANE	0.11341	C20H42
1-OCTADECANOL	0.11257	C18H38O
1,8-CYCLOTETRADECADIYNE	0.11252	C14H20
4,8,13-Cyclotetradecatriene-1,3-diol, 1,5,9-trimethyl-12-(1-methylethyl)-	0.10704	C20H34O2
6-Tridecen-4-yne, (E)-	0.1059	C13H22
5-DECYLMETHYL-URACYL	0.10039	C15H26N2O3
CIS-2-METHYLENEBICYCLO[3.3.0]OCTAN-3-ONE	0.098565	C9H12O
2,5-Dimethyl-3-isopropylpyrazine	0.096413	C9H14N2

26.71 Amorpha-4,11-diene	0.094622	C15H24
9-OCTADECENOIC ACID (Z)-	0.093834	C18H34O2
2,6,11-Tridecatrien-10-ol, 2,6,10-trimethyl-	0.093256	C16H28O
3-[2-(3-Methyl-2-butenyl)phenylthio]propanal	0.092579	C14H18OS
HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.092237	C22H42O4
Hexadecanoic acid, methyl ester	0.091737	C17H34O2
4-(2,4-Dimethylcyclohex-4-enyl)but-3-en-2-one	0.090126	C12H18O
12-METHYLENE-5,6,7,12-TETRAHYDRODIBENZO[A,D]CYCLOOCTEN-6-ONE	0.08984	C17H14O
2-PROPENYL IONONE 2	0.08875	C16H24O
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	0.088313	C15H26O
HEPTADECANE	0.087769	C17H36
BENZENE, 1-METHYL-4-(1,2,2-TRIMETHYLCYCLOPENTYL)-, (R)-	0.085915	C15H22
3,3,5,5-Tetramethylcyclopentene	0.082334	C9H16
PHENOL, 5-METHYL-2-(1-METHYLETHYL)-	0.080469	C10H14O
Sulfoxide, methyl phenethyl	0.080309	C9H12OS
3,3,5,5-Tetramethylcyclopentene	0.079759	C9H16
Ethanone, 1-(7-hydroxy-5-methoxy-2,2-dimethyl-2H-1-benzopyran-8-yl)-	0.078991	C14H16O4
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.078679	C12H18
3,5-METHANO-6H-CYCLOPENTA[B]FURAN-6-ONE, HEXAHYDRO-7-METHYL-, [3R-(3à,3Aá,5à,6Aá,7R*)]-	0.073042	C9H12O2
(S)-4-HEXANOLIDE	0.071711	C6H10O2
CYCLOPENTANE, BROMO-	0.069038	C5H9Br
35.51 Turmerone<ar->	0.068922	C15H20O
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.068574	C15H20
PENTADECANE	0.067272	C15H32
Benzenepropanoic acid, 2-propenyl ester	0.064392	C12H14O2
9-EICOSENE, (E)-	0.063183	C20H40
2,5-CYCLOHEXADIENE-1-CARBOXYLIC ACID, 1-METHYL-, METHYL ESTER	0.058907	C9H12O2
29.97 Octenyl cyclopentanone<E->	0.058177	C13H22O
Hexadecane	0.05454	C16H34
38.52 Bisabolone <6S,7R->	0.052772	C15H24O
HYDROPEROXIDE, 1-METHYL-1-PHENYLETHYL	0.050516	C9H12O2
OCTANE, 3,7-DIMETHYL-1-(2,5-XYLYL)-	0.049507	C18H30
BENZOFURAN, 7-CYCLOHEXYL-2,3-DIHYDRO-2-METHYL-	0.047167	C15H20O
(-)-3-BETA-ACETOXY-5-ETIENIC ACID	0.046257	C22H32O4
39.26 Bisabolonal<beta->	0.045496	C15H22O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.045303	C15H22
Picolinic acid N-oxide	0.044449	C6H5NO3
1,1,4,4-TETRAMETHYL-2-TETRALONE	0.043442	C14H18O
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-1,4-DIMETHYL-	0.042892	C12H16

Spiro[4.5]dec-7-ene, 1,8-dimethyl-4-(1-methylethenyl)-, [1S-(1à,4á,5à)]-	0.042325	C15H24
14.82 Isocitral<E->	0.041268	C10H16O
2-METHYL-2-(3-METHYL-2-OXOBUTYL)CYCLOHEXANONE	0.040462	C12H20O2
PROPANE, 2-METHOXY-2-METHYL-	0.039508	C5H12O
32.94 Guaia-3,10(14)-diene <9,11-epoxy->	0.039175	C15H22O
Methyl 10,12-heptadecadiynoate	0.037719	C18H28O2
1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester	0.037021	C16H22O4
6-Octen-1-yn-3-ol, 3,7-dimethyl-	0.035946	C10H16O
ACETAMIDE, N-(4-AMINOPHENYL)-	0.034085	C8H10N2O
1-Docosene	0.03074	C22H44
2,5-FURANDIONE, 3-ETHENYLDIHYDRO-3-METHYL-4-(1-METHYLETHYLIDENE)-, (.+.)-	0.029481	C10H12O3
2,3,4,5,6,7-HEXAHYDRO-2,2,3-TRIMETHYL-4-BENZOFURANONE	0.029456	C11H16O2
27.05 Sesquisabinene	0.028877	C15H24
5-OCTADECENE, (E)-	0.028702	C18H36
48.09 Isopropyl hexadecanoate	0.028577	C19H38O2
2,4-Pentadien-1-ol, 3-pentyl-, (2Z)-	0.027893	C10H18O
2-BENZOYL-3-PHENYL-1-AZIRINE	0.02735	C15H11NO
BICYCLO[3.1.0]HEXAN-3-OL, 4-METHYLENE-1-(1-METHYLETHYL)-, [1S-(1à,3á,5à)]-	0.026853	C10H16O
4a(2H)-Naphthalenol, octahydro-, trans-	0.02625	C10H18O
2-Propenal, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	0.025205	C12H18O
1-(1,2-DIFLUORO-1-PHENYLETHYL)-3-METHYLBENZENE	0.021631	C15H14F2
3-N-BUTYL[1]STAFFANE-1-CARBOXYLIC ACID	0.020934	C10H16O2
2,4,6-Trimethyl-1,3,6-heptatriene	0.020591	C10H16
3(5)-D1-1,2,4-TRIAZOLE	0.020054	C2H2DN3
1-DIMETHYL(PHENYL)SILYLPROPAN-2-OL	0.019706	C11H18OSi
5-ISOPROPENYL-2-METHYL-7-OXA-BICYCLO[4.1.0]HEPTAN-2-OL	0.017765	C10H16O2
1-DODECENE, 2-ETHYL-	0.01767	C14H28
3-BUTYN-2-ONE, 1-(4-METHYL-3-CYCLOHEXEN-1-YL)-4-(TRIMETHYLSILYL)-	0.017148	C14H22OSi
BENZENE, 1,3,5-TRIMETHYL-	0.0167	C9H12
PENTACOSANE	0.016494	C25H52
Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)-	0.016122	C15H24O
1-Nonanol	0.012344	C9H20O
5,9-Undecadien-1-yne, 6,10-dimethyl-	0.012302	C13H20
DODECANE, 2,6,10-TRIMETHYL-	0.011388	C15H32
ETHANOL, 2-XYLYL-	0.0098458	C10H14O
TRIDECANE	0.0090037	C13H28
Eudesma-5,11(13)-dien-8,12-olide	0.0087675	C15H20O2
2-BENZOTHIAZOLAMINE, 6-METHYL-	0.0085928	C8H8N2S
2-Decene, 3-methyl-, (Z)-	0.0079274	C11H22

2-TRIDECANONE	0.0071007	C13H26O
2-CYCLOHEXEN-1-ONE, 4-(1,5-DIMETHYL-4-HEXENYL)-	0.0068136	C14H22O
19.83 Verbenyl acetate<trans->	0.0067542	C12H18O2
35.53 Atlantone<beta->	0.0065165	C15H22O
BUTANOIC ACID, 2,3,3-TRIMETHYL-, METHYL ESTER	0.0063485	C8H16O2
1-(METHYLTHIO)-1-CYCLOHEXYLAMINO-2-NITROETHYLENE	0.0059441	C9H16N2O2S
3-CYCLOHEXENE-1-METHANOL, à,à,4-TRIMETHYL-, (S)-	0.0058561	C10H18O
1,2-Ethanediamine, N'-ethyl-N,N-dimethyl-	0.0046391	C6H16N2
3-Buten-2-one, 4-(4-hydroxy-3-methoxyphenyl)-	0.0041356	C11H12O3
CHLORODIVINYL BORANE	0.0034854	C4H6BCl
1-Dimethylamino-4-trimethylsilylmethoxy-benzene	0.0034788	C12H21NOSi
2-UNDECENE, 3-METHYL-, (Z)-	0.003273	C12H24
1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPT-2-YL 3-METHYL-2-BUTENOATE	0.0032569	C15H24O2
1,2-BIS(3-METHYL-1,2-BUTADIENYL)BENZENE	0.0029085	C16H18
Bumetrizole	0.0026916	C17H18ClN3O
Citronellic acid	0.0025251	C10H18O2
4-Methyl-2-octyn-4-ol	0.0018339	C9H16O
2-METHYL-1-PHENYL-3-(P-TOLYL)-1,3-PROPANDIOL	0.001826	C17H20O2
Cyclopentane, 1,2,4-trimethyl-	0.00096237	C8H16
6-(2-METHYLPROP-2-ENYL)-4,4,6-TRIMETHYLTETRAPYRAN-2-ONE	0.0007049	C12H20O2
1,3-Dimethyl-5-n-propyl-adamantane	0.00032046	C15H26
2-UNDECENAL, (Z)-	0.00023635	C11H20O
Naphthalene, 1-(1,1-dimethylethyl)-7-methoxy-	0.00016096	C15H18O
Cyclopropane, 1,1,2,2-tetramethyl-	9.0823E-05	C7H14
BENZAMIDINE, N,N'-DIMETHYL-	7.3211E-05	C9H12N2
Benzene, 1,1'-ethylidenebis[3,4-dimethyl-	0.00003213	C18H22
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	2.5427E-05	C18H28O3
Benzenebutanal, ç,4-dimethyl-	1.9992E-06	C12H16O
4H-INDEN-4-ONE, 5-BUTYL-1,2,5,6,7,7A-HEXAHYDRO-6-METHYL-, (5à,6á,7Aá)-(+.-)-	1.6538E-06	C14H22O
3,4-Dihydrocoumarin, 4,4-dimethyl-6-hydroxy-	7.2444E-07	C11H12O3
2-(4'-METHOXYBENZYL)CYCLOHEPTAN-1-ONE	0	C15H20O2
15-BROMO-2-PENTADECANONE	0	C15H29BrO
Total	100	

Fraction: MP 39

Compound Name	Area%	Formula
2-Butenoic acid, 3-methyl-, 4a,5,8,9-tetrahydro-9,9-dimethyl-5-oxobenzo[1,2-b:4,3-b']dipyran-8-yl ester	4.0082	C19H20O5
5A-METHYL-3,8-DIMETHYLENE-2-OXODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	3.6514	C20H24O5
1(4H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-3,4A,8,8-TETRAMETHYL-4-METHYLENE-, (4AS-TRANS)-	3.5202	C15H22O
CIS-2,3-EPOXYOCTAN-1-OL	3.4875	C8H16O2
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	3.4875	C15H26O
37.62 Cryptomerione	3.1105	C15H22O
Tumerone	2.5245	C15H22O
2-HEPTEN-4-ONE, 2-METHYL-6-(4-METHYLPHENYL)-, (S)-	2.3157	C15H20O
2-PENTANONE, 4-METHYL-4-PHENYL-	2.1481	C12H16O
2-PROPENYL IONONE 2	1.9244	C16H24O
38.24 Bisabolone<6R,7R->	1.785	C15H24O
2-Methyl-5-octyn-4-ol	1.5906	C9H16O
30.56 Sesquisabinene hydrate <cis-->(IPP vs. OH)	1.4588	C15H26O
Cyclohexane, (2-ethyl-1-methyl-1-butenyl)-	1.449	C13H24
27.38 Thujopsadiene	1.4316	C15H22
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	1.3578	C15H24
Cyclohexene, 1-methyl-4-(5-methyl-1-methylene-4-hexenyl)-, (S)-	1.3544	C15H24
2,4,6,8-NONATETRAENE, (E,Z,E)-	1.2589	C9H12
à-Benzylphenethylamine	1.2589	C15H17N
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	1.2476	C15H24
33.39 Biotol <beta->	1.198	C15H24O
6,7-Dioxabicyclo[3.2.2]non-8-ene	1.198	C7H10O2
39.59 Atlantone<(E)-alpha->	1.197	C15H22O
1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	1.1474	C15H24
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	1.1474	C15H24
LONGIFOLENALDEHYDE	1.1405	C15H24O
Curlone	1.0847	C15H22O
Curlone	1.0847	C15H22O
28.04 Curcumene<gamma->	1.0804	C15H24
3-PENTEN-1-OL, 2-METHYL-	1.0739	C6H12O
29.70 Sesquiphellandrene<beta->	1.055	C15H24
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	1.0306	C12H18
7-(1,3-DIMETHYL-BUTA-1,3-DIENYL)-1,6,6-TRIMETHYL-3,8-DIOXA-TRICYCLO[5.1.0.0 2,4]OCTANE	1.0008	C15H22O2

6-(3,3-DIMETHYL-2-OXIRANYLIDENE)-5,5-DIMETHYL-3-HEXEN-2-ONE	0.96027	C12H18O2
2-Pentenoic acid, 2-methyl-	0.95574	C6H10O2
14.35 Coahuilensol	0.92575	C9H10O
36.51 Atlantone<(Z)-gamma->	0.791	C15H22O
6-Isopropyl-1,2-dimethyl-4-oxo-bicyclo[3.3.1]non-2-ene-9-carboxaldehyde	0.78729	C15H22O2
BENZENE, 1-BUTYL-4-METHOXY-	0.77442	C11H16O
Bi-1-cycloocten-1-yl	0.7707	C16H26
1-CYCLOHEXENE-1-BUTANOL, 2,6,6-TRIMETHYL-	0.7485	C13H24O
HEPTADECANE	0.74813	C17H36
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.7455	C20H24O5
6-Isopropyl-1,2-dimethyl-4-oxo-bicyclo[3.3.1]non-2-ene-9-carboxaldehyde	0.73643	C15H22O2
(.+-)-AR-TURMERONE	0.73241	C15H20O
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4Aà,6à,8Aá)]-	0.73153	C15H22O2
3-PENTENOIC ACID, 2,4-DIMETHYL-, 3-PHENYLPROPYL ESTER, (S)-	0.69685	C16H22O2
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	0.6962	C16H22O4
1,3,6-OCTATRIENE, 3,7-DIMETHYL-	0.6861	C10H16
1,2-Benzenediol, o-(4-butylbenzoyl)-o'-(2-methylbenzoyl)-	0.6805	C25H24O4
24.19 Sesquithujene<7-epi->	0.60828	C15H24
1-Hexadecene	0.60584	C16H32
Tumerone	0.59059	C15H22O
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	0.58239	C15H22
2-(1,2-EPOXYCYCLOHEXYL)-1-PENTENE	0.57558	C11H18O
Tumerone	0.57339	C15H22O
3-Methylbut-2-enoic acid, 4-isopropylphenyl ester	0.55248	C14H18O2
5-OCTADECENE, (E)-	0.547	C18H36
2,6-Octadiene, 2,4-dimethyl-	0.5458	C10H18
Vanillin	0.51734	C8H8O3
1,2-BIS(3-METHYL-1,2-BUTADIENYL)BENZENE	0.51486	C16H18
TRANS-2-BROMOPHENYLCYCLOPROPANE-CIS-1,3-D2	0.5096	C9H7D2Br
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.43943	C20H24O5
2(3H)-FURANONE, 4-[(3,4-DIMETHOXYPHENYL)METHYL]DIHYDRO-, (.+-)-	0.42681	C13H16O4
PENTANOIC ACID, 2,4-DIMETHYL-, 3-PHENYLPROPYL ESTER, (S)-	0.41727	C16H24O2
2-BUTANONE, 4-(4-HYDROXY-3-METHOXYPHENYL)-	0.41377	C11H14O3
3-Octyn-2-ol	0.4124	C8H14O
n-Hexadecanoic acid	0.40046	C16H32O2
1,5-Decadiyne	0.40013	C10H14

1-BUTYNE, 3-METHOXY-3-METHYL-	0.37301	C6H10O
6,7,8,9-Tetrahydro-1H-benzo[e]indole-1,2(3H)-dione	0.3665	C12H11NO2
BENZENE, (1-ETHYLOCTYL)-	0.35415	C16H26
CYCLOPENTANEMETHANOL, 2-METHYL-5-(1-METHYLETHENYL)-, (1à,2à,5á)-	0.35187	C10H18O
1-(2,4-Dimethylphenyl)-3-(tetrahydrofuryl-2)propane	0.3427	C15H22O
1-Docosene	0.33667	C22H44
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	0.32129	C15H26O
TRICYCLO[6.6.0.0(3,6)]TETRADECA-1(8),4,11-TRIENE	0.32054	C14H18
CYCLOOCTANE	0.30897	C8H16
Bicyclo[4.4.0]dec-5-ene, 1,5-dimethyl-3-hydroxy-8-(1-methylene-2-hydroxyethyl-1)-	0.30246	C15H24O2
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	0.29187	C15H26O
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.2911	C12H18
32.70 Turmerone<ar-dihydro->	0.27531	C15H22O
ZINGIBERENOL	0.26713	C15H26O
BICYCLO[7.2.0]UNDEC-4-ENE, 4,11,11-TRIMETHYL-8-METHYLENE-, [1R-(1R*,4E,9S*)]-	0.26713	C15H24
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.26663	C10H16O
<No Name>	0.26431	C14H20O
4,6-DIMETHYL-2-PYRIMIDINECARBAMONITRILE	0.26241	C7H8N4
BICYCLO[2.2.1]HEPTAN-2-ONE, 1,3,3,4-TETRAMETHYL-	0.25271	C11H18O
S-(4-Chlorophenyl) 3-(4-ethoxyphenyl)-2-propenethioate	0.24023	C17H15ClO2S
32.17 Tumerol<ar->	0.23482	C15H22O
27.73 Acoradiene<10-epi-beta->	0.23362	C15H24
á-Ethylphenethyl alcohol	0.23102	C10H14O
trans-à-Bergamotene	0.22942	C15H24
7-HYDROXY-7,8-DIHYDRO-ATLANTONE	0.22503	C15H24O2
BENZENE, (1-NITROETHYL)-	0.22215	C8H9NO2
5',6',7',8'-Tetrahydro-2'-acetonaphthone	0.2218	C12H14O
3,7,7-TRIMETHYL-1,3,5-CYCLOHEPTATRIENE #	0.22172	C10H14
1-Oxaspiro[4.5]deca-3,6-diene, 2,6,10,10-tetramethyl-	0.21846	C13H20O
2-BUTENAL	0.21601	C4H6O
n-Octyl phenyl ketone	0.21228	C15H22O
BENZENEETHANOL, à,à-DIMETHYL-, ACETATE	0.20972	C12H16O2
1,8-Cyclopentadecadiyne	0.20542	C15H22
39.31 Squamulosone	0.20542	C15H22O
2-METHYLENEBICYCLO[3.2.1]OCT-6-EN-8-YL ACETATE	0.20538	C11H14O2
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.19951	C12H18
(Z)-2-FLUORO-3-METHYL-2,6-HEPTADIENAL	0.19917	C8H11FO
Inosine, 2'-deoxy-	0.19736	C10H12N4O4
4-HEXOXYBENZALDEHYDE	0.19608	C13H18O2

6-TRIDECEN-4-YNE, (E)-	0.18987	C13H22
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.18452	C15H20
1-Docosene	0.18344	C22H44
38.52 Bisabolone <6S,7R->	0.18207	C15H24O
1,1'-BIPHENYL, 3,4-DIETHYL-	0.17854	C16H18
2-PROPENYL IONONE 2	0.17793	C16H24O
25.79 Dictamnol	0.17421	C12H18O
Linalool, methyl ether	0.17002	C11H20O
N,N-DIISOPROPYL-3-METHYLENE-4-(TRIMETHYLSILYL)BUTYLAMINE	0.16967	C14H31NSi
30.56 Sesquisabinene hydrate <cis-->(IPP vs. OH)	0.16776	C15H26O
Tumerone	0.16749	C15H22O
6-BUTYL-3,5-DICHLORO-2,4-DIMETHYLPHENOL	0.16017	C12H16Cl2O
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-	0.14839	C15H24O
1H-BENZIMIDAZOL-2-YLMETHYL 4-ISOPROPYLBENZYL SULFIDE	0.14808	C18H20N2S
1,4-Cyclohexadiene, 1-methyl-	0.14784	C7H10
Tetradecane	0.14354	C14H30
2,6,10-DODECATRIEN-1-OL, 3,7,11-TRIMETHYL-	0.14262	C15H26O
30.03 Bisabolene<(E)-gamma->	0.14123	C15H24
1,8-Cyclopentadecadiyne	0.13313	C15H22
PROPANE, 1-NITRO-	0.13158	C3H7NO2
D-à-Cyclohexylglycine	0.12746	C8H15NO2
Cyclotetradecane	0.1239	C14H28
Thiourea, N-(3-methoxyphenyl)-N'-(2-propenyl)-	0.12274	C11H14N2OS
2(1H)-Naphthalenone, octahydro-1,4a-dimethyl-, (1à,4aà,8aà)-	0.1129	C12H20O
Bergamotol, Z-à-trans-	0.1087	C15H24O
42.84 Flourensadiol	0.10784	C15H26O2
2'-Deoxyadenosine	0.10418	C10H13N5O3
1-METHYL-4-(1,5-DIMETHYL-4-HEXENYLIDENE)-1-CYCLOHEXENE	0.10415	C15H24
2,2,4-TRIMETHYL-3A,7A-DIHYDRO-1,3-BENZODIOXOLE #	0.10178	C10H14O2
[CARBOXY-13C]-O-TOLUIC ACID	0.10079	C8H8O2
Benzene, (chloromethyl)pentamethyl-	0.10024	C12H17Cl
Tumerone	0.10024	C15H22O
1-Silacyclo-2,4-hexadiene	0.088929	C5H8Si
HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.088031	C22H42O4
1-Docosene	0.088031	C22H44
N-Methylallylamine	0.082597	C4H9N
Ibuprofen	0.082431	C13H18O2
Benzene, 1-(1-ethylpropyl)-2-propyl-	0.081912	C14H22
METHYL 2-PHENYLETHENYL CARBAMATE	0.081413	C10H11NO2
Sebacic dihydrazide	0.080958	C10H22N4O2
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.079469	C12H18

5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6- YL 2-METHYL-2-BUTENOATE	0.079071	C20H24O5
21.70 Presilphiperfol-7-ene	0.078492	C15H24
CIS,CIS - CYCLOPENTENE OXIDE ETHER	0.077884	C10H14O3
2-[(2-METHYLBICYCLO[2.2.1]HEPT-2-YL)OXY]TETRAHYDRO-2H- PYRAN	0.072064	C13H22O2
1-METHYL-4-(2-METHYL-2-OXIRANYL)-7- OXABICYCLO[4.1.0]HEPTANE	0.070709	C10H16O2
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.069508	C12H18
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.069123	C15H22
1-(4-HYDROXY-7-ISOPROPYL-4-METHYLOCTAHYDRO-1H-INDEN-1- YL)ETHANONE	0.06908	C15H26O2
5-ISOPROPYL-6-METHYL-HEPTA-3,5-DIEN-2-OL	0.068051	C11H20O
BENZOFURAN, 7-CYCLOHEXYL-2,3-DIHYDRO-2-METHYL-	0.067936	C15H20O
Methanesulfonyl fluoride, trifluoro-	0.067504	CF4S
NAPHTHALENE, 1-METHYL-	0.066085	C11H10
1,1'-Biphenyl, 3,4-diethyl-	0.065057	C16H18
3,3,5,6,8,8-HEXAMETHYLTRICYCLO[5.1.0.0~2,4~]OCT-5-ENE	0.064522	C14H22
2-PHENYL[CARBOXY-13C]ACETIC ACID	0.064462	C8H8O2
2-ETHYL-6-METHYL-4-PYRIDINOL	0.063543	C8H11NO
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,4A,5,6,7,8,8A- OCTAHYDRO-2-NAPHTHALENOL	0.060388	C15H24O2
3,6-Octadecadiynoic acid, methyl ester	0.059851	C19H30O2
23.69 Dictamnol<8-epi->	0.053913	C12H18O
5,6-AZULENEDICARBOXALDEHYDE, 1,2,3,3A,8,8A-HEXAHYDRO- 2,2,8-TRIMETHYL-, (3Aà,8à,8Aà)-(-)-	0.051545	C15H20O2
3-CYCLOHEXENE-1-METHANOL, à,à,4-TRIMETHYL-, (S)-	0.051199	C10H18O
1-BUTENE, 2-(O-ANISYL)-	0.049681	C11H14O
35.51 Turmerone<ar->	0.048101	C15H20O
7-TERT-BUTYL-1,2-DICYANONAPHTHALENE	0.048064	C16H14N2
BENZENE, 1,2,3,4-TETRAMETHYL-	0.046229	C10H14
27.38 Thujopsadiene	0.045467	C15H22
CYCLOHEXENE, 1-(2-NITRO-2-PROPENYL)-	0.045381	C9H13NO2
BORANE, CHLOROBIS(1-METHYLETHYL)-	0.044868	C6H14BCl
2H-PYRAN, 2-(BICYCLO[2.2.1]HEPT-2-YLOXY)TETRAHYDRO-, (1à,2á,4à)-	0.044721	C12H20O2
1,1-DIMETHYL-2-(1-PROPENYL)CYCLOPROPANE	0.044392	C8H14
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-	0.044301	C15H24O
1,2,3-TRIMETHOXYBENZENE	0.0433	C9H12O3
2-PROPANONE, 1-PHENYL-	0.039409	C9H10O
4,5-DEHYDRO-ISOLONGIFOLENE	0.039303	C15H22
TRIDECANE	0.038892	C13H28
Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-	0.038283	C12H16

Longiverbenone	0.036572	C15H22O
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.035688	C15H24
1-INDANONE, 4-HYDROXY-7-METHYL-	0.034887	C10H10O2
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.03378	C15H22
Benzoic acid, 3-(acetylamino)-2-hydroxy-	0.032527	C9H9NO4
Dodecyl acrylate	0.032527	C15H28O2
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-	0.031586	C15H24O
TETRADECANOIC ACID, ETHYL ESTER	0.031359	C16H32O2
6-Isopropyl-1,2-dimethyl-4-oxo-bicyclo[3.3.1]non-2-ene-9-carboxaldehyde	0.031262	C15H22O2
9-OCTADECENOIC ACID (Z)-	0.029456	C18H34O2
Pyrrolidine-2-carboxamide, 1-cyclohexyl-N-mesityl-	0.028444	C20H30N2O
BICYCLOELEMENE	0.02687	C15H24
3-[2-METHOXY-1-METHYLETHENYL]-3-METHYL-1-CYCLOPENTENE	0.025369	C10H16O
Bicyclo[3.1.1]hept-3-en-2-ol, 4,6,6-trimethyl-, [1S-(1à,2à,5à)]-	0.021639	C10H16O
1,3-BIS(PHENYLTHIO)-2-PROPANOL	0.021422	C15H16OS2
3-Decen-5-one	0.021028	C10H18O
2-BUTENOIC ACID, 2-METHYL-, 2-PROPENYL ESTER, (E)-	0.020026	C8H12O2
1-METHYL-5-(1-METHYLETHYL)-1H-PYRAZOL-3-OL	0.019346	C7H12N2O
Pentadecane	0.018909	C15H32
3,3,5,5-Tetramethylcyclopentene	0.017992	C9H16
3-Cyclopentylpropionic acid, phenyl ester	0.017949	C14H18O2
N,N'-Bis(2,6-dimethyl-6-nitrosohept-2-en-4-one)	0.016886	C18H30N2O4
BENZENAMINE, 2-METHYL-	0.016886	C7H10CN
Furan, 2-ethyl-5-methyl-	0.016688	C7H10O
1-CYCLOHEXENE-1-ACROLEIN, 2,6,6-TRIMETHYL-	0.016589	C12H18O
1-Methyl-6-(3-methylbuta-1,3-dienyl)-7-oxabicyclo[4.1.0]heptane	0.016365	C12H18O
Benzene, 1,3-bis(1-methylethyl)-	0.016139	C12H18
2-NONANONE, 9-HYDROXY-	0.015327	C9H18O2
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.015164	C15H20
DODECANE	0.014356	C12H26
2-BUTANONE	0.012709	C4H8O
Benzene, (3-nitrobutyl)-	0.012444	C10H13NO2
9.88 Artemisia ketone	0.012385	C10H16O
10-HYDROXY-1,4,5,8-TETRAMETHYLANTHRONE	0.012163	C18H18O2
.DELTA.-TERPINEOL	0.011222	C10H18O
1,4-HEXADIENE, 2,5-DIMETHYL-3-VINYL-	0.010976	C10H16
27.05 Sesquisabinene	0.010927	C15H24
Phenol, 2-(1-methylethyl)-	0.010908	C9H12O
2-NORPINENE, 2,6-DIMETHYL-6-(4-METHYL-3-PENTENYL)-, TRANS-(-)-	0.010151	C15H24
2-Hexanone, 5-methyl-5-phenyl-	0.0091542	C13H18O

2,6-DIMETHYL-1-ISOPROPYLPYRIDIN-4-ONE	0.0077226	C10H15NO
5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-	0.0067194	C18H30O
2-PROPENAL, 3-(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)-, (E)-	0.0062816	C12H18O
3-CYCLOHEXENE-1-METHANOL, 1-HYDROXY-à,à,4-TRIMETHYL-, (.+.-)-	0.0053783	C10H18O2
DISPIRO[2.1.2.1]OCTAN-4-ONE	0.0053337	C8H10O
1,1-DIMETHYL-1,2,3,5,7,8,9,9A-OCTAHYDRO-6H-BENZO[A]CYCLOHEPTEN-6-ONE	0.0043178	C13H20O
HISTAMINIUMDICHLORID	0.003439	C5H11Cl2N3
19.90 Undecanone<2->	0.0033963	C11H22O
Benzene, 2-methoxy-4-(2-propenyl)-1-(1-propynyloxy)-	0.003275	C13H14O2
4(1H)-PYRIMIDINONE, 5-METHOXY-, HYDRAZONE	0.002498	C5H8N4O
METHYL (2R,3S)-3-HYDROXY-2-METHYLBUTANOATE	0.0023072	C6H12O3
FURAN, TETRAHYDRO-2,5-DIPHENYL-, CIS-	0.0022774	C16H16O
1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester	0.0019462	C16H22O4
1-TERT-BUTYL-7-METHOXY-NAPHTHALENE	0.0013382	C15H18O
HEPTADECANE	0.0012827	C17H36
TRICYCLO[5.2.1.0(2,6)]DECANE, 3-METHYLEN-4-PHENYL-, SYN	0.0012823	C17H20
2-Cyclohexylamino-1-phenylethanol	0.00078882	C14H21NO
5-HEPTEN-1-OL, 2-[2-(2,3,3A,4,5,7A-HEXAHYDRO-3,6-DIMETHYL-2-BENZOFURANYL)ETHYLIDENE]-6-METHYL-, [2R-[2à(E),3á,3Aà,7Aà]]-	0.00061694	C20H32O2
BENZOFURAN, 2,3,3A,4,5,7A-HEXAHYDRO-3,6-DIMETHYL-	0.00059178	C10H16O
PYRIDINE, 4-(2,4-CYCLOPENTADIEN-1-YLIDENE)-1,4-DIHYDRO-1-METHYL-	0.00032823	C11H11N
2H,7H-10,4A-(NITRILOMETHANO)BENZOCYCLOOCTENE, 1,3,4,8,9,10-HEXAHYDRO-8,8-DIMETHYL-, TRANS-	0.00026919	C15H23N
2-METHYL-5,6-TETRAMETHYLENETHIENO[2,3-D]THIAZOLE	0.0001863	C10H11NS2
8-Dihydroantidesmone	0.00010604	C19H31NO3
(ETHYLSILYL)GERMANE	0.00005552	C2H10GeSi
Phenyldimethylvinylsilane	1.6579E-06	C10H14Si
Total	100	

Fraction: MP 40-45

Compound Name	Area%	Formula
(6E)-2,4-DIMETHYL-2,6-OCTADIENE	5.6818	C10H18
2,7,11-Trimethyl-4-phenylthiododeca-2,6,10-triene	5.5412	C21H30S
2,7,11-TRIMETHYL-4-PHENYLSULFANYL-DODECA-2,6,10-TRIENE	5.0829	C21H30S
3-Methyl-2-butenoic acid, 3-phenylpropyl ester	3.6554	C14H18O2
Corymbolone	3.5275	C15H24O2
Tyr-Ala	2.1561	C12H16N2O4
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	2.1046	C15H26O
36.98 Atlantone<(E)-gamma->	1.9803	C15H22O
39.59 Atlantone<(E)-alpha->	1.9799	C15H22O
1-Decen-4-yne, 2-nitro-	1.8767	C10H15NO2
2,5-HEPTADIEN-4-ONE, 2,6-DIMETHYL-	1.8656	C9H14O
36.51 Atlantone<(Z)-gamma->	1.8473	C15H22O
(4AR,6R,8AR)-4-ACETYL-1,1,3,6-TETRAMETHYL-4A,5,6,7,8,8A-HEXAHYDRO-1H-2-BENZOPYRAN	1.8408	C15H24O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	1.7453	C20H24O5
7à-ANGELOXYBZW-9á-HYDROXY-1-OXO-à-LONGIPINENE	1.7453	C15H22O3
35.51 Turmerone<ar->	1.5615	C15H20O
2-BUTANONE, 4-(4-HYDROXY-3-METHOXYPHENYL)-	1.4946	C11H14O3
Tumerone	1.4742	C15H22O
Benzenemethanol, 2,5-dimethyl-	1.4586	C9H12O
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	1.1969	C12H18
n-Hexadecanoic acid	1.1518	C16H32O2
Methyl 2-hydroxy-octadeca-9,12,15-trienoate	1.1518	C19H32O3
36.81 Sesquicineol-2-one	1.137	C15H24O2
Dihydromyrcene	1.133	C10H18
1,5-HEPTADIEN-4-ON, 3,3,6-TRIMETHYL- (ARTEMISIAKETON)	1.0731	C10H16O
39.59 Atlantone<(E)-alpha->	1.0437	C15H22O
12-Azabicyclo[9.2.2]pentadeca-1(13),11,14-trien-13-ylamine	0.99721	C14H22N2
9-Oxabicyclo[6.1.0]nonane, 1-methyl-, cis-	0.96504	C9H16O
CYCLOPENTANEACETIC ACID, 2-(2-HYDROXY-4-METHOXYBENZOYL)-2-METHYL-, CIS-(.+.)-	0.95804	C16H20O5
L-Deprenyl	0.9247	C13H17N
CYCLOHEXADECANE	0.91959	C16H32
1-OCTADECENE	0.90851	C18H36
2-PENTANONE, 4-METHYL-4-PHENYL-	0.8875	C12H16O

5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6- YL 2-METHYL-2-BUTENOATE	0.87522	C20H24O5
Curlone	0.86696	C15H22O
2(1H)-NAPHTHALENONE, 7-ETHYNYL-4A,5,6,7,8,8A-HEXAHYDRO- 1,4A-DIMETHYL-, (1à,4Aá,7á,8Aà)-	0.86105	C14H18O
10,12-Octadecadiynoic acid	0.86105	C18H28O2
4-HYDROXY-6-METHYL-2- (CYCLOHEXYLIDENEHYDRAZINO)PYRIMIDINE	0.84091	C11H16N4O
2-CYCLOHEXEN-1-ONE, 3-METHYL-6-(1-METHYLETHYL)-	0.83951	C10H16O
2-ACETYL-3-(2-CINNAMIDO)ETHYL-7-METHOXYINDOLE	0.80434	C22H22N2O3
Patchouli alcohol	0.7744	C15H26O
[1,2,4]TRIAZOLO[5,1-C][1,2,4]TRIAZIN-4(1H)-ONE, 1,3,7-TRIMETHYL-	0.7703	C7H9N5O
1-Adamantanecarboxylic acid, 3-phenylpropyl ester	0.75715	C20H26O2
37.22 Farnesal<2E, 6Z->	0.75541	C15H24O
PENTADECANOIC ACID	0.7275	C15H30O2
3-Methyl-2-butenoic acid, 2-isopropoxyphenyl ester	0.66073	C14H18O3
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	0.65835	C15H26O
Selegiline	0.64645	C13H17N
p-Methoxy-à-phenethylamine	0.64284	C9H13NO
4,8,8-TRIMETHYLBICYCLO[4.2.0]OCT-4-ENE-7,7-DICARBONITRILE	0.54653	C13H16N2
Oleic Acid	0.54228	C18H34O2
PSEUDOSCOPINE BENZYL ETHER	0.53625	C15H19NO2
3-AMINO-2-METHYL-3-(4-METHYLPHENYL)-1-PHENYL-1- PROPANOL	0.5268	C17H21NO
2,7-Bis(spirocyclopropane)bicyclo[2.2.1]heptan-5-one	0.52568	C11H14O
1-Docosene	0.52447	C22H44
1,5-DIMETHYL-4-HYDROXYMETHYLPYRAZOLE	0.51616	C6H10N2O
9-OCTADECENOIC ACID (Z)-	0.51199	C18H34O2
29.42 Curcumene<beta->	0.50632	C15H24
BENZENEPROPANOL, ACETATE	0.50023	C11H14O2
2,2,6-TRIMETHYL-10- METHYLENETRICYCLO[5.3.1.0~1,6~]UNDECAN-9-OL	0.4652	C15H24O
8,9-DIMETHYLBICYCLO[4.4.1]UNDECA-2,4,8-TRIENE	0.40506	C13H18
(E)-5-ISOPROPYL-8-HYDROXY-8-METHYL-NON-6-EN-2-ONE	0.40506	C13H24O2
1,1,4A,7,8A-PENTAMETHYL-1,2,3,4,4A,5,8,8A- OCTAHYDRONAPHTHALENE	0.40204	C15H26
Curlone	0.39384	C15H22O
4-METHYL-2-(1-METHYL-2-BUTYNYL)PHENOL	0.33983	C12H14O
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	0.33489	C15H24
6-[1-(HYDROXYMETHYL)VINYL]-4,8A-DIMETHYL-1,2,4A,5,6,7,8,8A- OCTAHYDRO-2-NAPHTHALENOL	0.32208	C15H24O2

5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6- YL 2-METHYL-2-BUTENOATE	0.31802	C20H24O5
Dibutyl phthalate	0.31802	C16H22O4
2-PROPENYL IONONE 2	0.30381	C16H24O
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.30316	C15H24
1-Nonene	0.29779	C9H18
Vanillin	0.29334	C8H8O3
à-TUMERONE	0.2857	C15H22O
2-PENTEN-1-OL, 2-METHYL-5-(2-METHYL-3- METHYLENEBICYCLO[2.2.1]HEPT-2-YL)-, [1R-[1à,2á(Z),4à]]-	0.28407	C15H24O
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	0.28189	C15H22
5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6- YL 2-METHYL-2-BUTENOATE	0.27914	C20H24O5
{2-[1-PROPENYL]CYCLOPROPYL}METHANOL	0.27579	C7H12O
8-OXABICYCLO[5.1.0]OCTANE	0.27579	C7H12O
Tumerone	0.27129	C15H22O
(2E)-2-BUTENOYL CHLORIDE #	0.26797	C4H5ClO
1-NAPHTHALENOL, 4,7-DIMETHYL-2-(1-METHYLETHYL)-	0.26433	C15H18O
(+)-2-CAREN, 4-ALPHA-ISOPROPENYL-	0.25765	C13H20
1-Docosene	0.25633	C22H44
4-(2,4,4-Trimethyl-cyclohexa-1,5-dienyl)-but-3-en-2-one	0.25423	C13H18O
Cyclohexanecarboxylic acid, 3-phenylpropyl ester	0.25119	C16H22O2
Tetradecyl trifluoroacetate	0.2487	C16H29F3O2
7,10-Epoxy-6H-azepino[1,2-e]purine-8,9-diol, 4-amino-7,8,9,10-tetrahydro-, [7R-(7à,8à,9à,10à)]-	0.24794	C10H11N5O3
Tumerone	0.24378	C15H22O
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(2-methyloxiranyl)-	0.22998	C10H16O2
28.04 Curcumene<gamma->	0.22796	C15H24
Binapacryl	0.22281	C15H18N2O6
Phosphoric acid	0.22072	H3O4P
2á,8á-DICYANO-4,6-DIMETHYL-3,5,7- TRIOXATETRACYCLO[7.2.1.0(4,11).0(6,10)]DODECANE	0.21661	C13H14N2O3
N-Morpholinomethyl-isopropyl-sulfide	0.21366	C8H17NOS
2-(4-METHYL-2-CYCLOHEXEN-1-YL)-1-PROPANOL	0.21284	C10H18O
1,1'-Bicyclohexyl, 2-(1-methylethyl)-, trans-	0.21078	C15H28
Cyclohexane, 1,2,4-tris(methylene)-	0.20538	C9H12
[1-(3-METHYL-1,2- BUTADIENYL)CYCLOPROPYL](PHENYL)METHANOL	0.20094	C15H18O
BENZENE, 1,3,5-TRIMETHYL-	0.19527	C9H12
5,9-Undecadien-2-one, 6,10-dimethyl-	0.18279	C13H22O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.18247	C15H22

N-(3-METHYL-1,3-BUTADIENYL)-2-PYRROLIDINONE	0.18004	C9H13NO
4,6,6-TRIMETHYLBICYCLO[3.1.1]HEPT-3-EN-2-OL	0.17336	C10H16O
2,6-Octadiene, 2,4-dimethyl-	0.17239	C10H18
BUTYL 1-(PHENYLTHIO)ETHYLCARBONATE	0.16787	C13H18O3S
2-ALLYL-1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-OL	0.16585	C13H22O
6-Octen-1-yn-3-ol, 3,7-dimethyl-	0.16104	C10H16O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.15405	C15H22
DIHYDROFRAXINELLONE	0.15068	C14H18O3
1,8-Cyclopentadecadiyne	0.14463	C15H22
1-METHYL-4-METHYLENE-2-(2-METHYL-1-PROPENYL)-1-VINYLCYCLOHEPTANE	0.14445	C15H24
27.05 Sesquisabinene	0.14128	C15H24
6-PROPENYL-BICYCLO[3.1.0]HEXAN-2-ONE	0.13633	C9H12O
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.13206	C12H18
1,1,4,7-TETRAMETHYLDECAHYDRO-4AH-CYCLOPROPA[E]AZULEN-4A-OL	0.1308	C15H26O
30.56 Sesquisabinene hydrate <cis-->(IPP vs. OH)	0.1308	C15H26O
1-Isopropenyl-3,3-dimethyl-5-(3-methyl-1-oxo-2-butenyl)cyclopentane	0.12574	C15H24O
CYCLOTETRADECANE	0.12361	C14H28
24.19 Sesquithujene<7-epi->	0.12276	C15H24
2,3,7-TRIMETHYL-3-VINYL-OCT-6-ENOIC ACID	0.11242	C13H22O2
3-PENTEN-2-ONE, 4-METHYL-1-[4-(1-METHYLETHYL)PHENYL]-	0.11223	C15H20O
à-Bromomesitylene	0.11045	C9H11Br
Hexanedioic acid, bis(2-ethylhexyl) ester	0.11026	C22H42O4
1-Docosene	0.11026	C22H44
Pyrazine, isopropenyl-	0.10761	C7H8N2
46.51 Occidol acetate	0.10517	C17H24O2
5-Methyl-5-hexen-3-yn-2-ol	0.10303	C7H10O
TRICYCLO[3.1.0.02,6]HEXANE, 1-BUTYL-	0.10155	C10H16
35.52 Dihydroatlantone<(E)-10,11->	0.10155	C15H24O
6-TRIDECEN-4-YNE, (E)-	0.096637	C13H22
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.0962	C20H24O5
Curlone	0.0962	C15H22O
(2-Methyl-cyclohex-2-enylidene)-acetaldehyde	0.092859	C9H12O
Spiro[4.5]dec-7-ene, 1,8-dimethyl-4-(1-methylethenyl)-, [1S-(1à,4á,5à)]-	0.092859	C15H24
Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-	0.091528	C18H22
1-METHYL-4-(1,5-DIMETHYL-4-HEXENYLIDENE)-1-CYCLOHEXENE	0.084481	C15H24
3-METHYL-1-PHENYL-1,4-BUTANEDIOL #	0.083434	C11H16O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.081661	C20H24O5

2H-PYRAN-2-CARBOXALDEHYDE, 3,4-DIHYDRO-	0.074629	C6H8O2
2-Methyl-Z,Z-3,13-octadecadienol	0.069666	C19H36O
5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrene	0.069418	C15H22O3
SILANE, TRIMETHYL(3-METHYL-1-BUTYNYL)-	0.067209	C8H16Si
1H-IMIDAZOLE, 4,5-DIHYDRO-2-(PHENYLMETHYL)-	0.066827	C10H12N2
DISPIRO[2.1.2.4]UNDECANE, 8-METHYLENE-	0.066827	C12H18
BENZENE, 1-METHYL-4-(1-METHYLETHYL)-	0.065146	C10H14
2,4-DINITRO-6-(2-BUTYL)-PHENYL-à,à-DIMETHYLACRYLSAEUREESTER	0.063819	C15H18N2O6
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.063227	C15H20
2-NORPINENE, 2,6-DIMETHYL-6-(4-METHYL-3-PENTENYL)-, TRANS-(-)-	0.063051	C15H24
Ethanol, 2-butoxy-	0.06173	C6H14O2
HYDRAZINECARBOXAMIDE, 2-[2,2-DIMETHYL-5-(1-METHYLETHYL)BICYCLO[3.1.0]HEX-3-YLIDENE]-, (1S)-	0.060881	C12H21N3O
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.060881	C13H20O2
TETRADECANOIC ACID, ETHYL ESTER	0.056577	C16H32O2
4-(4-METHYLPHENYL)PENTANAL	0.055821	C12H16O
3-Isopropyl-4-methyl-1-pentyn-3-ol	0.055701	C9H16O
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-	0.055595	C15H24O
(BUT-3-EN)-2,3,5-TRIMETHYL-CYCLOPENTA-2,4 -DIEN	0.055171	C12H18
2-PENTEN-1-ONE, 1-(2-HEXYLCYCLOPROPYL)-	0.05459	C14H24O
36.51 Atlantone<(Z)-gamma->	0.054569	C15H22O
2-(2-HYDROXY-CYCLOHEXYLMETHYL)-PYRIDIN-1-OL	0.054482	C12H17NO2
29.48 Himachalene<alpha-dehydro-ar->	0.054298	C15H20
DISPIRO[3.0.3.1]NONANE	0.054152	C9H14
1-BUTANONE, 3-METHYL-1-PHENYL-	0.051264	C11H14O
42.84 Flourensadiol	0.049591	C15H26O2
36.98 Atlantone<(E)-gamma->	0.049023	C15H22O
1,2,3,1',2',3'-Hexamethyl-bicyclopentyl-2,2'-diene	0.047165	C16H26
6-(HYDROXY)-1-(5-HEXENYL)BICYCLO[3.3.0]OCTAN-2-ONE	0.047053	C14H22O2
FARNESYL ACETONE C	0.046118	C18H30O
37.23 Cedroxyde	0.04574	C15H24O
AROMADENDRENOXID-(2)	0.044356	C15H24O
7-Oxabicyclo[4.1.0]heptane, 1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-, (E)-	0.042134	C15H24O
1-BUTANONE, 1-[2-(3-FURANYL)-2-HYDROXY-5-METHYLCYCLOPENTYL]-3-METHYL-	0.04186	C15H22O3
1,2-Benzenedimethanol	0.037195	C8H10O2
3,3,5,5-Tetramethylcyclopentene	0.03705	C9H16
34.58 Cedren-3-one<2-epi-beta->	0.036637	C15H22O

DODECAHYDRO-8A-METHYL-3,5-BIS(METHYLENE)-2-OXONAPHTHO[2,3-B]FURANE ??? EPOXY?	0.035129	C15H20O3
29.44 Sesquicineole	0.03383	C15H26O
TRIDECANE	0.032486	C13H28
2-(4a,8-Dimethyl-2,3,4,4a,5,6-hexahydro-naphthalen-2-yl)-prop-2-en-1-ol	0.032182	C15H22O
3-[2-METHOXY-1-METHYLETHENYL]-3-METHYL-1-CYCLOPENTENE	0.030662	C10H16O
3-CYCLOHEXENE-1-METHANOL, 1-HYDROXY-à,à,4-TRIMETHYL-, (.+.)-	0.029759	C10H18O2
Tetradecane	0.029383	C14H30
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.029052	C20H24O5
11.09 Cymenene<para->	0.028977	C10H12
Tetradecane	0.027562	C14H30
BENZALDEHYDE-3-D	0.027046	C7H5DO
Benzeneacetamide, N-methyl-	0.025948	C9H11NO
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.025218	C12H18
HEXADECANE	0.024148	C16H34
1-BUTANAMINE	0.023591	C4H11N
2á,8á-DICYANO-4,6-DIMETHYL-3,5,7-TRIOXATETRACYCLO[7.2.1.0(4,11).0(6,10)]DODECANE	0.023403	C13H14N2O3
Furan, 2-ethyl-5-methyl-	0.023339	C7H10O
trans-2,3-Dimethylacrylic acid	0.023338	C5H8O2
Benzene, 1,3-bis(1-methylethyl)-	0.02288	C12H18
1-SEC-BUTYL-4-METHYLBENZENE	0.022079	C11H16
BENZENE, [[(4-METHYL-3-PENTENYL)OXY]METHYL]-	0.020051	C13H18O
1,1,7-TRIMETHYL-4-METHYLENE-1A,2,3,4,6,7,7A,7B-OCTAHYDRO-1H-CYCLOPROPA[E]AZULENE	0.019977	C15H22
3-ETHYLIDENE-1-CYCLOHEPTENE	0.018952	C9H14
27.38 Thujopsadiene	0.018494	C15H22
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.018417	C13H20O2
2-BUTANONE, 4-(2,2,6-TRIMETHYLCYCLOHEXYL)-, CIS-	0.016342	C13H24O
36.51 Atlantone<(Z)-gamma->	0.015549	C15H22O
PENTADIENAL, 2-METHYL-	0.015418	C6H8O
Benzenepropanol, 4-methoxy-à-methyl-	0.015014	C11H16O2
2-METHYL-1-D-BENZIMIDAZOLE	0.013273	C8H7DN2
s-Indacene, 1,2,3,5,6,7-hexahydro-1,1,7,7-tetramethyl-	0.012875	C16H22
1,2,3,4-TETRAKIS(1-METHYLETHYLIDENE)CYCLOBUTANE	0.01247	C16H24
1H-INDENE, 2,3-DIHYDRO-1,1,3-TRIMETHYL-3-PHENYL-	0.011734	C18H20
METHYL 3à,4.APHA.-ISOPROPYLIDENEDIOXY-5á-(FLUOROMETHYL)CYCLOHEX-1-ENE-1-CARBOXYLATE	0.011564	C12H17FO4
D,L-p-Fluorophenylalanine	0.011315	C9H10FNO2
L-(+)-Lactic acid	0.011132	C3H6O3

Cycloisolongifolene, 8,9-dehydro-9-formyl-	0.010723	C16H22O
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.009981	C16H18
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.009948	C20H24O5
6-Methoxy-1-indanone	0.009777	C10H10O2
35.89 Helifolenol B	0.009333	C15H24O
DODECANOIC ACID, ETHYL ESTER	0.009115	C14H28O2
6-ACETOXY-BICYCLO[2.2.1]HEPT-2-ENE-1-CARBOXYLIC ACID METHYL ESTER	0.008972	C11H14O4
Adenosine	0.008078	C10H13N5O4
(+/-)-5-METHYL-1-á-[(4-METHYLPHENYL)SULFONYL]-4-NITRO-2,3,3Aá,4á,5á,7Aá-HEXAHYDRO-1H-INDENE	0.008047	C17H21NO4S
3-NITRO-4-HYDROXYPYRIDINE	0.007811	C5H4N2O3
Benzene, 2-methyl-1,4-bis(1-methylethyl)-	0.007696	C13H20
Bicyclo[4.3.0]nonan-2-one, 8-isopropylidene-	0.007641	C12H18O
1,3-ISOBENZOFURANDIONE, 4,5,6,7-TETRAHYDRO-4,4,7-TRIMETHYL-	0.005362	C11H14O3
(Z)-HEX-3-EN-2,5-DIONE	0.005291	C6H8O2
2-OXABICYCLO[2.2.2]OCTAN-6-OL, 1,3,3-TRIMETHYL-	0.005271	C10H18O2
CHLORODIVINYLBORANE	0.004594	C4H6BCl
ISOLONGIFOLEN, 4,5-DEHYDRO-	0.004472	C15H22
DECANE, 2,9-DIMETHYL-	0.004308	C12H26
4-METHYL-4-[(TRIMETHYLSILYL)OXY]HEXAHYDRO-2(1H)-PENTALENONE	0.004176	C12H22O2Si
2,3,5-TRIMETHYLFURAN	0.0037	C7H10O
FURAN, 5-[1-(5,5-DIMETHYL-2(5H)-FURANYLIDENE)ETHYL]-2-ETHENYLTETRAHYDRO-2-METHYL-	0.002678	C15H22O2
Acetaldehyde, (1-methylethyl)(2-propenyl)hydrazone	0.002205	C8H16N2
1,1'-BIPHENYL, 3,4-DIETHYL-	0.001962	C16H18
S-INDACENE, 1,2,3,5,6,7-HEXAHYDRO-1,1,4,8-TETRAMETHYL-	0.001922	C16H22
6H-PURIN-6-ONE, 1,7-DIHYDRO-	0.001785	C5H4N4O
1,2-Benzenediol, O-dichloroacetyl-O'-(3-methylbut-2-enoyl)-	0.001654	C13H12Cl2O4
(S)-1-METHYL-9-PHENYLBICYCLO[4.3.0]NONA-6,8-DIENE	0.001383	C16H18
1-INDANONE, 5-METHYL-	0.0012	C10H12O
1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester	0.001176	C16H22O4
2(5H)-FURANONE, 5,5-DIMETHYL-	0.000894	C6H8O2
3,3,5,5-Tetramethylcyclopentene	0.000848	C9H16
(+)-á-ATLANTONE	0.000846	C15H22O
METHYL 2-PHENYLETHENYL CARBAMATE	0.000154	C10H11NO2
PENTANOIC ACID	0.000119	C5H10O2
10-(2-NITROPHENYL)-4,10-DIHYDRO-1H,3H-FURO[3,4-C][1,5]BENZOTHIAZEPIN-1-ONE	5.94E-05	C17H12N2O4S
1-BUTANONE, 1-(4H-1,4-BENZOTHIAZIN-2-YL)-	3.62E-05	C12H13NOS

1-BUTYL-1,2,3,4-TETRAHYDROISOQUINOLINE	4.18E-07	C13H19N
2-METHYL-5,6-TETRAMETHYLENETHIENO[2,3-D]THIAZOLE	0	C10H11NS2
2H,7H-10,4A-(NITRILOMETHANO)BENZOCYCLOOCTENE, 1,3,4,8,9,10-HEXAHYDRO-8,8-DIMETHYL-, TRANS-	0	C15H23N
Total	100	



Fractions: MP 46-49

Compound Name	Area%	Formula
3-Methyl-2-butenic acid, 3-phenylpropyl ester	5.0224	C14H18O2
(4AR,6R,8AR)-4-ACETYL-1,1,3,6-TETRAMETHYL-4A,5,6,7,8,8A-HEXAHYDRO-1H-2-BENZOPYRAN	3.3196	C15H24O2
(6E)-2,4-DIMETHYL-2,6-OCTADIENE	3.3196	C10H18
2-Butanone, 4-(4-hydroxyphenyl)-	3.1935	C10H12O2
2-CYCLOHEXYL-2-(1-CYCLOHEXYLETHYL)MALONONITRILE	3.0282	C17H26N2
E-15-Heptadecenal	2.9642	C17H32O
35.51 Turmerone<ar->	2.5112	C15H20O
1-HEXADECANOL	2.4261	C16H34O
1-HEXADECENE	2.3994	C16H32
3-Methylene-bicyclo[3.2.1]oct-6-en-8-ol	2.2914	C9H12O
4,8,8-TRIMETHYLBICYCLO[4.2.0]OCT-4-ENE-7,7-DICARBONITRILE	2.1912	C13H16N2
2-PROPENYL IONONE 4	2.1912	C16H24O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	2.1333	C20H24O5
1-Nonadecene	1.8957	C19H38
Patchouli alcohol	1.8846	C15H26O
1,2,4-TRIAZOLO(4,3-A)PYRIMIDINE	1.748	C5H4N4
Curlone	1.748	C15H22O
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	1.4865	C13H22O
36.98 Atlantone<(E)-gamma->	1.4586	C15H22O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	1.4288	C20H24O5
CYCLOHEXANEACETONITRILE	1.2669	C8H13N
NEROLIDOL-EPOXYACETATE	1.2539	C17H28O4
1-TETRADECENE	1.1302	C14H28
Tumerone	1.1203	C15H22O
3-Methylbut-2-enoic acid, 4-nitrophenyl ester	1.0678	C11H11NO4
1-Docosene	1.0328	C22H44
4-N-BUTYL-5-AZACINNOLINE	1.0069	C11H14N4
3-PENTENOIC ACID, 2,4-DIMETHYL-, 3-PHENYLPROPYL ESTER, (S)-	0.97211	C16H22O2
36.51 Atlantone<(Z)-gamma->	0.94115	C15H22O
Bergamotol, Z-à-trans-	0.93165	C15H24O
27.38 Thujopsadiene	0.92296	C15H22
trans-Z-à-Bisabolene epoxide	0.90405	C15H24O
Benzenemethanol, 2,5-dimethyl-	0.87064	C9H12O

But-2-ynoic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	0.84537	C14H20O2
3-Methyl-2-butenic acid, pent-2-en-4-ynyl ester	0.83932	C10H12O2
38.75 Nuciferol<E->	0.79409	C15H22O
Bicyclo[3.1.1]heptan-2-one, 3,6,6-trimethyl-	0.76571	C10H16O
BENZALDEHYDE, 4-HYDROXY-3-METHOXY-	0.7158	C8H8O3
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.69524	C20H24O5
n-Hexadecanoic acid	0.69524	C16H32O2
36.98 Atlantone<(E)-gamma->	0.69206	C15H22O
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.68929	C13H20O2
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.67938	C15H24O
1-Propanone, 1-cyclohexyl-	0.67205	C9H16O
4,4'-Dimethylbicyclohexyl-3,3'-diene-2,2'-dione	0.58927	C14H18O2
1-ISOPROPENYL-3-PROPENYL-CYCLOPENTANE	0.57043	C11H18
3-PENTENOIC ACID, 2,4-DIMETHYL-, 3-PHENYLPROPYL ESTER, (S)-	0.54673	C16H22O2
9-CYCLOHEPTADECEN-1-OL	0.53763	C17H32O
3,7,7-TRIMETHYLBICYCLO[4.1.0]HEPT-3-EN-2-OL	0.53681	C10H16O
CYCLOHEXANE, BROMO-	0.50696	C6H11Br
39.19 Curcumen-15-al<gamma->	0.48642	C15H22O
PENTANE, 1-NITRO-	0.48509	C5H11NO2
2-PROPENYL IONONE 2	0.4702	C16H24O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.46589	C15H22
BENZENE, 1,2,4,5-TETRAKIS(1-METHYLETHYL)-	0.46085	C18H30
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	0.45939	C15H22
1-Hexadecanol	0.45311	C16H34O
7-N-PROPYL-7-HYDROXY-PERHYDROINDOLIZINE /EPIMER B	0.43445	C11H21NO
2,6-DIMETHYL-1,7-OCTADIENE-3,6-DIOL #	0.42556	C10H18O2
SPIRO[4,5]DECAN-7-ONE, 1,8-DIMETHYL-8,9-EPOXY-4-ISOPROPYL-	0.40544	C15H24O2
Hexadecane-1,2-diol	0.39465	C16H34O2
BENZENEPROPANOIC ACID, ã,ã-DIMETHYL-, ETHENYL ESTER	0.39082	C13H16O2
9(2H)-ANTHRACENONE, 1,3,4,4A,9A,10-HEXAHYDRO-9A-METHYL-, (4AR-TRANS)-	0.3872	C15H18O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.38663	C20H24O5
39.59 Atlantone<(E)-alpha->	0.38493	C15H22O
35.51 Turmerone<ar->	0.38461	C15H20O
2-CYANO-3,5-DIMETHYL-1-HYDROXY PYRROLE	0.38383	C7H8N2O
[1-(3-METHYL-1,2-BUTADIENYL)CYCLOPROPYL](PHENYL)METHANOL	0.37387	C15H18O
1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	0.37382	C15H24

Benzyl isobutyl ketone	0.35944	C12H16O
1-HYDROXY-6-(3-ISOPROPENYL-1-CYCLOPROPEN-1-YL)-6-METHYL-2-HEPTANONE	0.35499	C14H22O2
(6E)-2,4-DIMETHYL-2,6-OCTADIENE #	0.35022	C10H18
1-Docosene	0.34709	C22H44
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R*,S*)]-	0.33374	C15H24
TETRADECANOIC ACID, ETHYL ESTER	0.33334	C16H32O2
4,12,12-TRIMETHYL-9-METHYLENE-5-OXATRICYCLO[8.2.0.0~4,6~]DODECANE	0.33067	C15H24O
29.48 Himachalene<alpha-dehydro-ar->	0.33067	C15H20
Bicyclo[4.1.0]heptan-endo-2-ol, 1-(4-methoxyphenyl)-	0.31979	C14H18O2
1(2H)-Naphthalenone, octahydro-4a,8a-dimethyl-7-(1-methylethyl)-, [4aR-(4aà,7á,8aà)]-	0.31979	C15H26O
1-Hexene, 4,5-dimethyl-	0.31604	C8H16
1-METHYL-3-(1-METHYLETHYL)-1H-PYRAZOL-5-OL	0.30692	C7H12N2O
trans(2-Chlorovinyl)triethylsilane	0.29274	C8H17ClSi
N-(3',3'-DIDEUTERO-ALLYL)ANILINE	0.29125	C9H9D2N
Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-	0.28836	C18H22
6-PROPENYL-BICYCLO[3.1.0]HEXAN-2-ONE	0.28047	C9H12O
10,12-Octadecadiynoic acid	0.27768	C18H28O2
9-OCTADECENOIC ACID (Z)-	0.26789	C18H34O2
2-Methoxybenzoic acid, 3-phenylpropyl ester	0.25454	C17H18O3
36.98 Atlantone<(E)-gamma->	0.25108	C15H22O
BENZENE, METHYL(1-METHYLETHYL)-	0.24976	C10H14
11-Hydroxy-11-methyl-tricyclo[4.3.1.1(2,5)]undecan-10-one	0.24333	C12H18O2
Cyclobutanecarboxylic acid, tridec-2-ynyl ester	0.23445	C18H30O2
Dodecyl acrylate	0.23317	C15H28O2
trans-Z-à-Bisabolene epoxide	0.23278	C15H24O
Propanoic acid, 3-chloro-, 4-formylphenyl ester	0.23066	C10H9ClO3
5-cis-Methyl-1R,3-cis-cyclohexanediol	0.22842	C7H14O2
32.44 Hexadecene<1->	0.21956	C16H32
Dibutyl phthalate	0.21865	C16H22O4
2-CYCLOBUTEN-1-ONE, 2-BUTYL-4-HYDROXY-3-METHOXY-4-(2-PROPENYL)-	0.21073	C12H18O3
4,4'-DIMETHYL-BICYCLOHEXYL-3,3'-DIENE-2,2'-DIONE	0.21002	C14H18O2
3-CYCLOHEXENE-1-METHANOL, à,à,4-TRIMETHYL-	0.20244	C10H18O
Tumerone	0.19934	C15H22O
11-METHYLDODECA-1,10-DIENE	0.19452	C13H24
32.70 Turmerone<ar-dihydro->	0.19291	C15H22O
Curlone	0.19291	C15H22O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.19249	C20H24O5

3-Cyclohexene-1-methanol, à,à4-trimethyl-	0.19102	C10H18O
AZULENE	0.19035	C10H8
Benzene, (1,1-dimethylpropyl)-	0.18937	C11H16
BICYCLO[3.1.1]HEPT-2-ENE-2-ETHANOL, 6,6-DIMETHYL-	0.18914	C11H18O
Decyloxybenzene	0.17133	C16H26O
Tetradecane	0.17063	C14H30
31.99 Sesquisabinene hydrate<trans->(IPP vs. OH)	0.16747	C15H26O
1-METHYL-YL-3-(PROP-2'-EN-1'-YL)PIPERIDIN-2-ONE	0.16545	C9H15NO
2-METHYL-1,3-CYCLOHEXADIENE	0.15587	C7H10
THUJOL	0.15458	C10H16O
6-(1-Hydroxymethylvinyl)-4,8a-dimethyl-3,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one	0.15245	C15H22O2
4-Methyl-2-octyn-4-ol	0.15066	C9H16O
2-FURANMETHANOL, 5-ETHENYLTETRAHYDRO-à,à,5-TRIMETHYL-, CIS-	0.15034	C10H18O2
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.14868	C16H18
1-METHOXY-3,5-DIMETHYL-CYCLOHEXENE	0.14864	C9H16O
[CARBOXY-13C]-P-TOLUIC ACID	0.14628	C8H8O2
1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	0.14402	C16H18
29.40 Italicene epoxide<iso->	0.14288	C15H24O
ETHANONE, 1-(METHYLPHENYL)-	0.14021	C9H10O
1,8-Cyclopentadecadiyne	0.13738	C15H22
8-METHYL-6A-(2-PROPYNYL)-1A,2,2A,2B,3,4,6A,7A,8,8A-DECAHYDRO-7H-FLUORENO[2,3-B]OXIREN-7-ONE	0.13726	C17H20O2
2,4,6-TRIMETHYL-BENZOIC ACID 5-METHYLENE-1,3A,4,5,6,6A-HEXAHYDRO-PENTALEN-1-YL ESTER	0.13585	C19H22O2
Bicyclo[4.1.0]heptan-2-one, 3,4,4-trimethyl-3-(3-methyl-1,3-butadienyl)-, [1à,3à(E),6à]-(.+-)-	0.13479	C15H22O
(1R,CIS)-3-AMINOMETHYL-1,2,2-TRIMETHYLCYCLOPENTYLMETHANOL	0.13308	C10H21NO
5-Methyl-5-hexen-3-yn-2-ol	0.13203	C7H10O
2-PENTANONE, 4-METHYL-4-PHENYL-	0.12802	C12H16O
1,4-Benzenedimethanol	0.12745	C8H10O2
28.04 Curcumene<gamma->	0.12722	C15H24
TRANS-2-DODECENAL	0.12722	C12H20O
3-Methylbut-2-enoic acid, 4-cyanophenyl ester	0.12617	C12H11NO2
36.98 Atlantone<(E)-gamma->	0.1189	C15H22O
1,2,3,4-TETRAKIS(1-METHYLETHYLIDENE)CYCLOBUTANE	0.11799	C16H24
9.88 Artemisia ketone	0.10994	C10H16O
2-PENTEN-1-OL, 2-METHYL-5-(2-METHYL-3-METHYLENE-2-NORBORNYL)-	0.10945	C15H24O
Benzenemethanol, à-[1-(dimethylamino)ethyl]-, [R-(R*,S*)]-	0.10907	C11H17NO
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.10506	C15H24O

TRIDECANE	0.10482	C13H28
Benzene, undecyl-	0.10242	C17H28
(R,R)-3,8-DIMETHYLDECANE	0.097067	C12H26
35.51 Turmerone<ar->	0.095793	C15H20O
(E)-1,2-(2H(2)-4-METHOXYPHENYLETHENE	0.092306	C9H8D2O
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.086393	C12H18
3-[2-METHOXY-1-METHYLETHENYL]-3-METHYL-1-CYCLOPENTENE	0.084816	C10H16O
1-Docosene	0.082281	C22H44
Cyclohexene, 1-(3-ethoxy-1-propenyl)-, (Z)-	0.077656	C11H18O
Pentadecane	0.077102	C15H32
8-Heptadecene	0.076605	C17H34
2-HEXENE, 2,3-DIMETHYL-	0.075317	C8H16
HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.074749	C22H42O4
1-METHYLENE-3-VINYLCYCLOHEXANE	0.069168	C9H14
2(3H)-FURANONE, 3-(1-CYCLOHEXEN-1-YL)DIHYDRO-	0.068954	C10H14O2
Ethanol, 2-butoxy-	0.06884	C6H14O2
12-Oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl-, [1R-(1R*,3E,7E,11R*)]-	0.065102	C15H24O
CYCLOOCTANONE	0.064889	C8H14O
5,9-Undecadien-2-ol, 6,10-dimethyl-	0.064162	C13H24O
2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (Z)-	0.06083	C9H14O3
Bicyclo[2.2.1]heptane-3-methylene-2,2-dimethyl-5-ol acetate	0.059776	C12H18O2
PENTADECANE	0.05972	C15H32
40.01 Bisabolol<beta->	0.058369	C15H24O
Isolongifolene, 4,5,9,10-dehydro-	0.055138	C15H20
BENZENEETHANOL, à,à-DIMETHYL-, ACETATE	0.05497	C12H16O2
Glutaric acid	0.053858	C5H8O4
1,3-CYCLOPENTADIENE, 5-(ETHOXYFLUOROMETHYLENE)-	0.053536	C8H9FO
1-Docosene	0.052358	C22H44
BETA-CEDREN-9-ALPHA-OL	0.052321	C15H24O
3,3,5,5-Tetramethylcyclopentene	0.051304	C9H16
1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPT-2-YL 3-METHYL-2-BUTENOATE	0.050071	C15H24O2
HEXADECANE	0.047545	C16H34
N-(TRIDEC-1-YL)CYCLOHEXYLAMINE	0.047327	C19H39N
24.84 Sesquithujene	0.046822	C15H24
3-ETHOXY-4-METHYL-3-CYCLOBUTENE-1,2-DIONE	0.04668	C7H8O3
2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1,1-dimethylpropyl)-	0.044756	C16H24O2
1-NONANONE, 1-PHENYL-	0.042222	C15H22O
SILANE, TRIMETHYL[(3,7,11-TRIMETHYL-2,6,10-DODECATRIENYL)OXY]-	0.040221	C18H34OSi
3-ACETYLBICYCLO[2.2.1]HEPT-2-ENE	0.038519	C9H12O

ETHANONE, 1-[3-[2-METHYL-2-[3-(1-METHYLETHENYL)-1-CYCLOPROPEN-1-YL]PROPYL]OXIRANYL]-	0.035184	C14H20O2
Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-	0.0348	C16H26O
1,1-DICHLORO-2,2-DIFLUORO-PROPANE	0.034251	C3H4Cl2F2
4,6-OCTADIENOIC ACID	0.034107	C8H12O2
(5E)-6,10-DIMETHYL-5,9-UNDECADIEN-1-YNE	0.034045	C13H20
11-OXO-12-PHENYLDODECANENITRILE	0.030043	C18H27NO
1,2,3-BENZOTHIADIAZOLE	0.030011	C6H4N2S
2-(2-METHYLPROPYL)PHENOL	0.029788	C10H14O
Benzene, 1,3-bis(1-methylethyl)-	0.029217	C12H18
SPIRO[BICYCLO[3.3.0]OCTAN-6-ON-3-CYCLOPROPANE]	0.029094	C10H14O
6-OXABICYCLO[3.2.1]OCT-2-ENE-8-CARBOXYLIC ACID, 1,8-DIMETHYL-7-OXO-, METHYL ESTER, ANTI-(.-.-)-	0.02747	C11H14O4
3-Methyl-2-butenic acid, tridec-2-ynyl ester	0.027201	C18H30O2
2(3H)-Naphthalenone, 4,4a,5,6-tetrahydro-7-methyl-	0.025962	C11H14O
4,7-Methanobenzofuran, 2,2'-oxybis[octahydro-7,8,8-trimethyl-, [2à(2'R*,3'aS*,4'R*,7'R*,7'aS*),3aà,4à,7à,7aà]-	0.025843	C24H38O3
DODECANOIC ACID, ETHYL ESTER	0.02491	C14H28O2
1,2-BIS(3-METHYL-1,2-BUTADIENYL)BENZENE	0.024034	C16H18
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.023493	C20H24O5
BENZENE, 1-[[[(1-ETHENYL-5-ETHOXY-2-METHOXY-4-PENTYNYL)OXY]METHYL]-4-METHOXY-, [S-(R*,S*)]-	0.022393	C18H24O4
35.75 Isobornyl isobutanoate<8-hydroxy->	0.021554	C14H24O3
23.02 Decanoic acid	0.018488	C10H20O2
N-METHYL-4,5-INDOLOQUINONE	0.018467	C9H7NO2
2-UNDECANONE	0.017925	C11H22O
3,4-Octadiene, 7-methyl-	0.01764	C9H16
Flurbiprofen	0.017208	C15H13FO2
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	0.016924	C15H26
3,3,5-TRIMETHYL-2-(3-METHYLPHENYL)-2-HEXANOL #	0.016585	C16H26O
4,5-HEPTADIEN-2-ONE, 3,3,6-TRIMETHYL-	0.016158	C10H16O
2,4,4-TRIMETHYL-8-METHYLENE-1-OXA-SPIRO[2.5]OCTANE	0.016131	C11H18O
2'-Hydroxybutyrophenone oxime	0.015142	C10H13NO2
2-ISOBUTYLIDENEAMINO-3-METHYL-BUTYRONITRILE	0.014299	C9H16N2
Benzenepropanoic acid, 2-propenyl ester	0.013233	C12H14O2
2-(DIETHOXYPHOSPHANYL)-4,5-DIMETHYLPHOSPHININE	0.013023	C11H18O2P2
3-Pentanol	0.012755	C5H12O
DODECANE, 2,7,10-TRIMETHYL-	0.011003	C15H32
4-Hydroxyproline	0.010956	C5H9NO3
2-HYDROXY-2-PHENYLPROPYL 4-METHYLBENZOATE	0.010858	C17H18O3
METHYLNAPHTHALENE	0.010377	C11H10

2,4-Azetidinedione, 3-ethyl-3-phenyl-	0.010064	C11H11NO2
DIBENZOFURAN	0.009439	C12H8O
4-Methylbenzoic acid, 3-pentyl ester	0.008589	C13H18O2
1,2-Benzenedicarboxylic acid, diisooctyl ester	0.008354	C24H38O4
4-(4-METHYLPHENYL)PENTANAL	0.007898	C12H16O
2,2,5-Trimethyl-1-phenylhexa-3,4-dien-1-one	0.007808	C15H18O
1,1-BIS(P-TOLYL)ETHANE	0.007783	C16H18
6-(p-Tolyl)-2-methyl-2-heptenol	0.007678	C15H22O
1,1'-Biphenyl, 2,2'-diethyl-	0.007084	C16H18
3-Methyl-2-butenic acid, cyclobutyl ester	0.00595	C9H14O2
BIS(2-METHYLPENTYL) PROPYLPHOSPHONATE	0.005441	C15H33O3P
2',4',6'-Triisopropylacetophenone	0.004476	C17H26O
Butane, 1,1-dibutoxy-	0.004121	C12H26O2
2-BUTANAMINE, HYDROCHLORIDE	0.004121	C4H11N
2(3H)-BENZOFURANONE, HEXAHYDRO-7A-METHYL-3-METHYLENE-, CIS-(.+.)-	0.00393	C10H14O2
2-TERT-BUTYL-6-(2-HYDROXY-1-METHYL-4-PHENYL-BUT-3-ENYL)-[1,3]DIOXIN-4-ONE	0.00365	C19H24O4
2-PROPN-1-ONE-3-D, 1-(1-METHYLCYCLOPENTYL)-	0.003201	C9H11DO
6,8-DECADIEN-5-OL, (Z,E)-	0.00246	C10H18O
2-FLUORO-5-METHOXYBENZYL BROMIDE	0.002411	C8H8BrFO
BICYCLO[2.2.1]HEPTANE-7-ACETIC ACID, METHYL ESTER	0.002104	C10H16O2
METHYLENECYCLOOCTANE	0.002063	C9H16
NAPHTHALENE, 1-METHYL-	0.002023	C11H10
2-FLUORO-4,5-DICYANOIMIDAZOLE	0.002002	C5HFN4
1,2-PROPANEDIOL, 3,3-BIS(ETHYLTHIO)-1-(4-METHOXYPHENYL)-, (R*,R*)-(.+.)-	0.000825	C14H22O3S2
5',6',7',8'-Tetrahydro-2'-acetonaphthone	0.000554	C12H14O
2-PROPANAMINE, 2-METHYL-N-[(4-NITROPHENYL)METHYLENE]-	0.000185	C11H14N2O2
ETHANONE, 1-(2,4,6-TRIMETHYLPHENYL)-	0.000166	C11H14O
2,8-DICYANO-4,6-DIMETHYL-3,5,7-TRIOXATETRACYCLO[7.2.1.0(4,11).0(6,10)]DODECANE	0.000148	C13H14N2O3
1,4-Naphthalenedione, 2-hydroxy-3-(2-methyl-1-propenyl)-	9.2E-05	C14H12O3
1-PROPANONE, 1-(4-HYDROXYPHENYL)-	0	C9H10O2
N-Methyl-N-methoxy-5,6,7,8-tetrahydro-1-naphthamide	0	C13H17NO2
1,3,5-TRIS(TRIMETHYLSILYL)HEXENE	0	C15H36Si3
Total	100	

Fraction: MP 50

Compound Name	Area%	Formula
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	6.0325	C13H20O2
35.51 Turmerone<ar->	4.9436	C15H20O
3-Methyl-2-butenic acid, pent-2-en-4-ynyl ester	3.9137	C10H12O2
Oleic Acid	3.1821	C18H34O2
7-Hexadecyn-1-ol	3.1821	C16H30O
trans-13-Octadecenoic acid	3.1821	C18H34O2
BICYCLO[3.2.2]NONA-6,8-DIEN-3-ONE, 1,5-DIMETHYL-	3.081	C11H14O
BENZENEACETIC ACID, à-HYDROXY-2-METHOXY-	2.532	C9H10O4
2-sec-Butyl-4,6-dinitrophenyl 3-methylcrotonate (binapacryl)	2.4597	C15H18N2O6
HYDROSORBIC ACID, 4-HYDROXY-, ç-LACTONE	2.4028	C6H8O2
1-(CYCLOPROPYLAZO)-1-SPIROPENTANECARBONITRILE	1.9998	C9H11N3
1-METHYL-2-ISOPROPYL-3-PHENYLCYCLOPROPENE	1.865	C13H16
27.38 Thujopsadiene	1.7857	C15H22
Cyclopropanecarboxylic acid, isobornyl ester	1.7455	C14H22O2
27.04 Prenyl limonene<trans->	1.7455	C15H24
Curlone	1.7455	C15H22O
2-Octenoic acid, 7-(acetyloxy)-2,4,6-trimethyl-8-(5-oxazolyl)-, [4s-(2E,4R*,6S*,7S*)]-	1.6452	C16H23NO5
1-[2-(1-HYDROXYETHYL)-1-CYCLOHEXEN-1-YL]ETHANONE	1.6452	C10H16O2
Tumerone	1.6219	C15H22O
1b,5,5,6a-Tetramethyl-octahydro-1-oxa-cyclopropa[a]inden-6-one	1.6071	C13H20O2
n-Hexadecanoic acid	1.5547	C16H32O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	1.4834	C20H24O5
1,3-METHANONAPHTHALENE, DECAHYDRO-2,2-DIMETHYL-, [1R-(1à,3à,4Aà,8Aá)]-	1.4818	C13H22
BENZENEPROPANOL, ACETATE	1.4596	C11H14O2
Phenol, 4-pentyl-	1.4265	C11H16O
Ledol	1.3924	C15H26O
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-6-[1-(HYDROXYMETHYL)ETHENYL]-4,8A-DIMETHYL-, [4AR-(4Aà,6à,8Aá)]-	1.3924	C15H22O2
2-Butanone, 4-(4-hydroxyphenyl)-	1.293	C10H12O2
37.23 Cedroxyde	1.1996	C15H24O
2-Butanone, 4-(4-hydroxyphenyl)-	1.1719	C10H12O2
3-BUTEN-2-ONE, 4-(2,5,5-TRIMETHYL-3,8-DIOXATRICYCLO[5.1.0.02,4]OCT-4-YL)-, [1à,2à,4à(E),7à]-	1.1217	C13H18O3
CYCLOHEXENE, 5,6-DIETHENYL-1-METHYL-	1.0169	C11H16

Oxacyclotetradeca-4,11-diyne	1.0169	C13H18O
27.05 Sesquisabinene	0.98961	C15H24
3,4-DIMETHYL-4-PENTEN-1-YN-3-OL	0.97889	C7H10O
1-Cyclohexyl-1-propyne	0.9519	C9H14
FUROSARDONIN A	0.95157	C15H20O2
2-PROPENYL IONONE 2	0.95157	C16H24O
2-PROPENAL, 3-(2,3-DIMETHYLTRICYCLO[2.2.1.0(2,6)]HEPT-3-YL)-, STEREOISOMER	0.93297	C12H16O
ISOPROPYL 2-METHYLACRYLATE	0.90172	C7H12O2
1-OCTENE, 3,7-DIMETHYL-	0.88886	C10H20
N,N-BIS(2-HYDROXYETHYL)DODECANAMIDE	0.88886	C16H33NO3
1,5-Decadiyne	0.83536	C10H14
EXO-3-ETHYL-10,10-DIMETHYLTRICYCLO[5.2.1.0(2,6)]DECANE	0.81833	C14H24
3,6-DIBENZOYLPYRIDAZINE-DIOXIME	0.60637	C18H14N4O2
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	0.59137	C15H22
4,4'-DIMETHYL-BICYCLOHEXYL-3,3'-DIENE-2,2'-DIONE	0.54432	C14H18O2
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.5207	C13H20O2
OLEALDEHYDE, DIMETHYL ACETAL	0.51846	C20H40O2
Bicyclo[3.1.1]heptan-2-one, 3,6,6-trimethyl-	0.51846	C10H16O
19.77 Tridecene<1->	0.51767	C13H26
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.5105	C15H24O
8-Heptadecene	0.50771	C17H34
Isoborneol	0.50322	C10H18O
18.42 Carvone oxide<cis->	0.50149	C10H14O2
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.46334	C20H24O5
23.80 Angustione<dehydro->	0.34867	C11H14O3
EXO-2-(PHENYLIMINO)-PERHYDROCYCLOPENTANO[E]1,3,2-OXAZINE	0.34147	C13H16N2O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.33887	C20H24O5
BICYCLO[3.2.0]HEPT-6-EN-2-OL, 1,4,4-TRIMETHYL-, (1à,2á,5à)-	0.33758	C10H16O
Bicyclo[2.2.1]heptan-2-ol, 2-allyl-1,7,7-trimethyl-	0.33717	C13H22O
24.84 Sesquithujene	0.33486	C15H24
(R,R)-3,8-DIMETHYLDECANE	0.32673	C12H26
SPIRO[4.4]NONA-1,6-DIENE, (S)-	0.31209	C9H12
3,3,4-TRIMETHYL-4-(4-METHYLPHENYL)CYCLOPENTANONE #	0.31209	C15H20O
HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.31158	C22H42O4
PENTADECANE	0.30291	C15H32
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, [S-(Z)]-	0.2965	C15H26O

12-Oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl-, [1R-(1R*,3E,7E,11R*)]-	0.29512	C15H24O
2-Methoxymethylene-bicyclo[2.2.1]heptane	0.29512	C9H14O
Butyl 6,9,12,15-octadecatetraenoate	0.29512	C22H36O2
3-Methyl-2-butenic acid, 3-phenylpropyl ester	0.29224	C14H18O2
trans,trans-3,5-Heptadien-2-one	0.28984	C7H10O
1-PROPANAMINE, 2-METHYL-	0.27838	C4H11N
Octanal, 7-methoxy-3,7-dimethyl-	0.27838	C11H22O2
1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(E,E)]-	0.27075	C15H24
CYCLOPROPANE, ETHYL(1,2,2-TRIMETHYLPROPYLIDENE)-, (E)-	0.24416	C11H20
7,7-DIBROMONORCARANE	0.23865	C7H10Br2
3-TETRADECENE, (Z)-	0.23865	C14H28
2-[2-(METHOXY)ETHYL]-4(5)-METHYLIMIDAZOLE	0.22449	C7H12N2O
N-((S)-à-METHOXY-à-(TRIFLUOROMETHYL)PHENYLACETYL)-1-(3',5'-DIDEUTERO-4'-METHOXYPHENYL)-2-AMINOPROPANE	0.21521	C20H18D2F3NO3
2-CYCLOHEXYL-2-ISOBUTYLMALONONITRILE	0.20208	C13H20N2
Doconexent	0.20208	C22H32O2
(2,3,3-TRIMETHYL-4-PENTENYL)BENZENE	0.19895	C14H20
HEPTADECANE	0.19778	C17H36
2-PROPANONE, 1-(2-ACETYLCYCLOPENTYL)-	0.17881	C10H16O2
27.84 Allyl decanoate	0.17276	C13H24O2
4-Methyl-2-octyn-4-ol	0.17276	C9H16O
Tumerone	0.1648	C15H22O
6Z-2,5,5,10-Tetramethyl-undeca-2,6,9-trien-8-one	0.1648	C15H24O
Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-, (1à,2à,5à)-	0.1476	C10H16O
3-Buten-2-one, 4-(4-hydroxy-3-methoxyphenyl)-	0.14203	C11H12O3
(6E,9Z)-6-(DIMETHYLPHENYLSILYL)HEPTADEC-6,9-DIENE	0.1408	C25H42Si
METHYLENECYCLOOCTANE	0.13887	C9H16
1-Ethyl-1(1-cyclobutylidenethyl)cyclobutane	0.13705	C12H20
(1RS,8ARS)-1-(3-FURYL)-4A-HYDROXY-5,5,8A-TRIMETHYLOCTAHYDRO-2-BENZOPYRAN-3-ONE	0.13612	C16H22O4
1-(4-METHYLPHENYL)ETHANAMINE	0.1354	C9H13N
BENZENE, (8-BROMOOCTYL)-	0.13196	C14H21Br
36.98 Atlantone<(E)-gamma->	0.13067	C15H22O
4-Methyl-2-octyn-4-ol	0.12614	C9H16O
2-Methyl-4-octenal	0.11829	C9H16O
3,7-DIMETHYL-7-OCTEN-1-OL	0.11054	C10H20O
Pentadec-7-ene, 7-bromomethyl-	0.11054	C16H31Br
PENTADECANE	0.10174	C15H32
9-OCTADECENOIC ACID (Z)-	0.1012	C18H34O2
36.98 Atlantone<(E)-gamma->	0.096847	C15H22O
Acetaminophen	0.090757	C8H9NO2

3-Cyclohexen-1-one, 3,5,5-trimethyl-	0.084063	C9H14O
3-Methylbut-2-enoic acid, 4-cyanophenyl ester	0.083386	C12H11NO2
2-(1H-IMIDAZOL-4-YL)ETHANAMINE DIHYDROCHLORIDE	0.079276	C5H11Cl2N3
4-BROMO-N-[(6-METHYL-2-PYRIDYL)AMINOMETHYL]PHTHALIMIDE	0.079276	C15H12BrN3O2
2-PENTYL-3-METHYL-2-CYCLOPENTEN-1-ONE	0.077688	C11H18O
HIRSUTENE	0.076133	C15H24
1-Methoxybicyclo[2,2,2]oct-5-en-2-yl methyl ketone	0.074771	C11H16O2
6,10-DIMETHYLUDECA-5,9-DIEN-2-OL	0.07096	C13H24O
29.48 Himachalene<alpha-dehydro-ar->	0.070583	C15H20
4H-PYRAZOLO[3,4-D]PYRIMIDIN-4-ONE, 1,5-DIHYDRO-	0.070316	C5H4N4O
1-Naphthalenol, decahydro-4a-methyl-	0.070316	C11H20O
Methane, bromo-	0.067244	CH3Br
1,2,4-TRIAZOLIDINE-3,5-DIONE, 4-METHYL-2-(1-METHYL-1-PHENYLETHYL)-	0.065883	C12H15N3O2
BENZENE, METHYL(1-METHYLETHYL)-	0.065883	C10H14
BENZALDEHYDE, 4-HYDROXY-3-METHOXY-	0.065564	C8H8O3
2,7-Nonadienoic acid, 3,8-dimethyl-, methyl ester, (Z)-	0.065358	C12H20O2
SPIRO[4.4]NONA-1,6-DIENE, (S)-	0.062188	C9H12
1-Methoxy-5-trimethylsilyloxyhexane	0.05626	C10H24O2Si
HEPTANOIC ACID, METHYL ESTER	0.055938	C8H16O2
Benzene, 1,3-bis(1,1-dimethylethyl)-2-methoxy-5-methyl-	0.054626	C16H26O
1,3-Cyclopentadiene, 2-(4-bromobutyl)-5,5-dimethyl-	0.053102	C11H17Br
PYRIDINE, 2-METHYL-3-(1H-TETRAZOL-5-YL)-	0.051206	C7H7N5
(RAC)-1,3,6,8-TETRAMETHYLCYCLODODECA-1,2,6,7-TETRAENE	0.048556	C16H24
2-Propanone, 1-bromo-	0.048491	C3H5BrO
METHANE, DICHLORO-	0.048464	CH2Cl2
4-HEXEN-1-OL, 3-ETHENYL-5-METHYL-2-METHYLENE-, (S)-	0.048385	C10H16O
2,4-DINITRO-6-(2-BUTYL)-PHENYL-à,à-DIMETHYLACRYLSAEUREESTER	0.047406	C15H18N2O6
4H-Cyclopentacycloocten-4-one, decahydro-	0.044003	C11H18O
2-CYCLOHEXEN-1-ONE, 3-METHYL-6-(1-METHYLETHYL)-	0.043106	C10H16O
4,5-HEPTADIEN-2-ONE, 3,3,6-TRIMETHYL-	0.043014	C10H16O
9-OCTADECENE, (E)-	0.042974	C18H36
38.52 Bisabolone <6S,7R->	0.042512	C15H24O
36.98 Atlantone<(E)-gamma->	0.038136	C15H22O
1-(DIMETHYLPHENYLSILYL)-PROP-2-YNE	0.036874	C11H14Si
2-Methylbenzoic acid, 2,3-dichlorophenyl ester	0.035959	C14H10Cl2O2
1-Docosene	0.034317	C22H44
1-[2-METHYL-2-(4-METHYL-3-PENTENYL)CYCLOPROPYL]ETHANOL	0.034243	C12H22O
6-Octen-1-yn-3-ol, 3,7-dimethyl-	0.034226	C10H16O
5-Methyl-1-heptanol	0.034084	C8H18O

EXO-5,5-DIMETHYL-6-(2'-METHYL-1'-PROPENYL)-BICYCLO[2.2.2]OCT-2-ENE	0.033237	C14H22
4-METHYLTHIOBENZYL CHLORIDE	0.031312	C8H9ClS
Dodecyl acrylate	0.030679	C15H28O2
cis-4-Hydroxy-2-methyl-5-(1-hydroxy-1-isopropyl)-2-cyclohexen-1-one	0.029953	C10H16O3
TRANS-7-PENTADECENE	0.029667	C15H30
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	0.02839	C12H18
4,4-BIS(CHLOROMETHYL)-3,5-DIOXATRICYCLO[5.2.2]UNDECANE	0.027509	C11H16Cl2O2
Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)-	0.026615	C15H24
Bicyclo[4.1.0]heptane, 7-pentyl-	0.02627	C12H22
TRANS-2-BROMOPHENYLCYCLOPROPANE-CIS-1,3-D2	0.025341	C9H7D2Br
2-OXO-2-PHENYLETHYL 4-TERT-BUTYLBENZOATE	0.025053	C19H20O3
TRICYCLO[4.1.0.0(2,7)]HEPT-3-ENE	0.022071	C7H8
2H-Inden-2-one, 1,4,5,6,7,7a-hexahydro-7a-methyl-, (S)-	0.021855	C10H14O
1,2,2-TRIMETHYLCYCLOPROPYLAMINE	0.021253	C6H13N
5-ISOPROPYLIDENE-4,6-DIMETHYL-NONA-3,6,8-TRIEN-2-OL	0.020812	C14H22O
1-INDANONE, 5-METHYL-	0.020696	C10H12O
5-PHENYL-3-(TRIMETHYLSILYLMETHYL)PENT-1-EN-3-OL	0.020696	C15H24OSi
Tungsten, tris(ã-allyl)(ã-crotyl)-	0.020356	C13H22W
4(5H)-BENZOXAZOLONE, 6,7-DIHYDRO-6,6-DIMETHYL-	0.020225	C9H11NO2
Dibutyl phthalate	0.019524	C16H22O4
tris(hydroxymethyl)aminomethane	0.019137	C4H11NO3
9.88 Artemisia ketone	0.019137	C10H16O
(Z,Z)-HEPTADEC-8,11-DIEN-1-YL BROMIDE	0.01873	C17H31Br
Oxalic acid, cyclohexyl tetradecyl ester	0.018274	C22H40O4
Hexadecane	0.018124	C16H34
Methylene Chloride	0.015909	CH2Cl2
Benzene, [(3,3,5,5-tetramethylcyclohex-1-en-1-yl)thio]-	0.015046	C16H22S
CYCLOHEXANE, OCTYL-	0.014899	C14H28
DOCOSANE	0.014876	C22H46
Pyridine, 2-methyl-, 1-oxide	0.014824	C6H7NO
1,3,5-TRIAZINE, 1,3,5-TRICYCLOHEXYLHEXAHYDRO-	0.012866	C21H39N3
1-BROMO-2-CHLORO-1,1,2,2-TETRAFLUOROETHANE	0.012208	C2BrClF4
à-D-1-PHENYLPROPAN-2-OL	0.012193	C9H11DO
2-Cyclohexen-1-one, 3,4,4-trimethyl-	0.011805	C9H14O
23.65 Allyl nonanoate	0.011488	C12H22O2
CARBAMIC ACID, METHYLNITROSO-, 3,5,?-TRIMETHYLPHENYL ESTER	0.010253	C11H14N2O3
Anthranilic acid	0.010079	C7H7NO2
OXIRANE, 3-ETHYNYL-2,2-DIMETHYL-	0.010065	C6H8O
4-ENDO-AZIDO-2-OXABICYCLO[3.3.0]OCT-7-EN-3-ONE	0.010006	C7H7N3O2
BENZENE, [(3-BROMOPROPOXY)METHYL]-	0.0097587	C10H13BrO

Sodium chlorate	0.0090212	CINaO3
TRANS-ACRYLIC ACID, 3[(3-(2,2-DIMETHYLCYCLOPROPYL)-2,2-DIMETHYLCYCLOPROPYL)]-, METHYLESTER	0.0089502	C14H22O2
44.84 Carissone	0.0079038	C15H24O2
4H-INDEN-4-ONE, OCTAHYDRO-2-METHYLENE-, CIS-	0.0077209	C10H14O
3-PENTENOIC ACID, 2,4-DIMETHYL-, 3-PHENYLPROPYL ESTER, (S)-	0.0073465	C16H22O2
BICYCLO[3.2.0]HEPT-2,6-DIENE-1,2,3,4,4,5,6-D(7)	0.0073076	C7HD7
1-BUTANONE, 3-CHLORO-1-(2-HYDROXYPHENYL)-	0.0068934	C10H11ClO2
Sodium chlorate	0.0067369	CINaO3
CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL-	0.0066259	C5H5Br2ClO
2-BUTYN-1-ONE, 1-(1-METHYLCYCLOPENTYL)-	0.0060957	C10H14O
Methylene Chloride	0.0059189	CH2Cl2
6-OXA-1-AZABICYCLO[3.1.0]HEXANE, 5-METHOXY-	0.0055917	C5H9NO2
CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL-	0.0054676	C5H5Br2ClO
DOCOSANE	0.0054116	C22H46
7-INDOLIZINOL, 5,6,7,8-TETRAHYDRO-	0.0047157	C8H11NO
9-OXATRICYCLO[5.2.1.0(1.6)] DECAN-5-ONE	0.0047088	C9H12O2
6-OXA-1-AZABICYCLO[3.1.0]HEXANE, 5-METHOXY-	0.0046521	C5H9NO2
Dicumyl peroxide	0.004415	C18H22O2
1H-IMIDAZOLE-1-PROPANOIC ACID, 2-METHYL-4-NITRO-	0.0041342	C7H9N3O4
(Z)-3-PHENYL-2-BUTENAL	0.0039348	C10H10O
10-EXO,11-EXO-DIMETHYL-ANTI-TRICYCLO[4.3.1.1(2,5)]UNDECANE-10-ENDO,11-ENDO-DIOL	0.0039245	C13H22O2
2-TRIDECANONE	0.0038073	C13H26O
Spiro(1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-4a-methyl-5-hydroxy-7,7-di(allyl)-phenanthren-8-one)-2,2'-(1',3'-dioxolane)	0.0037814	C23H32O4
7-INDOLIZINOL, 5,6,7,8-TETRAHYDRO-	0.0032215	C8H11NO
1-HEXADECANOL	0.0030473	C16H34O
1,2,2-TRIMETHYLCYCLOPROPYLAMINE	0.0030057	C6H13N
METHANE, DICHLORO-	0.0030041	CH2Cl2
TRICYCLO[4.1.0.0(2,7)]HEPT-3-ENE	0.0024581	C7H8
CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL-	0.0023333	C5H5Br2ClO
Picolinyl 4-tetradecenoate	0.0022511	C20H31NO2
Sodium chlorate	0.0020836	CINaO3
CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL-	0.0020762	C5H5Br2ClO
3-Ethyl-3-methylheptane	0.0020588	C10H22
TERT-BUTYL N-[(1R,2R,4R)-4-BROMO-2-(6-CHLORO-3-PYRIDYLCYCLOHEXYL)CARBAMATE	0.0020222	C16H22BrClN2O2
METHANE, DICHLORO-	0.0019222	CH2Cl2
2,2-DIFLUORO-2-(3-PHENYLPHENYL)ACETONITRILE	0.001839	C14H9F2N
3-TRIMETHYLSILYLOXY-4-METHOXYPHENETHYL-N,N-BIS(TRIMETHYLSILYL)AMINE	0.0018082	C18H37NO2Si3
2(3H)-FURANONE, 4-(ACETYLOXY)DIHYDRO-3-METHYL-, TRANS-	0.0016608	C7H10O4

3-ETHOXY-4-METHYL-3-CYCLOBUTENE-1,2-DIONE	0.0016484	C7H8O3
2'-Deoxyguanosine	0.0016452	C10H13N5O4
(E)-2-METHYL-2,5-NONADIENE-4-ONE	0.0016346	C10H16O
Cyclohexene, 3,5-dimethyl-	0.0016263	C8H14
HEXADECANOIC ACID, 2,3-DIHYDROXYPROPYL ESTER	0.0012764	C19H38O4
1,4:5,8-DIMETHANOPHTHALAZINE, 1,4,4A,5,8,8A-HEXAHYDRO-10,10-DIMETHYL-, (1à,4à,4Aà,5á,8á,8Aà)-	0.0010828	C12H16N2
[1,1'-BIBICYCLO[2.2.2]OCTANE]-4-CARBOXYLIC ACID	0.0010578	C17H26O2
1,5-HEPTADIEN-4-ON, 3,3,6-TRIMETHYL- (ARTEMISIAKETON)	0.00079	C10H16O
METHANE, DICHLORO-	0.00069687	CH2Cl2
CYCLOHEXANONE-2-SPIRO-2'-(3',6'-DIHYDRO-4',5'-DIMETHYL-2'H-THIAPYRAN) 1'-OXIDE	0.00052257	C12H18O2S
trans-2,3-Dimethoxycinnamic acid	0.00048208	C11H12O4
7-INDOLIZINOL, 5,6,7,8-TETRAHYDRO-	0.00042328	C8H11NO
Benzoic acid, 4-ethoxy-, ethyl ester	0.00027708	C11H14O3
7-INDOLIZINOL, 5,6,7,8-TETRAHYDRO-	0.00024636	C8H11NO
BENZENEETHANAMINE, 3,4-DIMETHOXY-	0.00019996	C10H15NO2
UNDECANE, 3,5-DIMETHYL-	0.0001415	C13H28
2á,8á-DICYANO-4,6-DIMETHYL-3,5,7-TRIOXATETRACYCLO[7.2.1.0(4,11).0(6,10)]DODECANE	0.000084724	C13H14N2O3
BENZENE, 1-[[1-ETHENYL-5-ETHOXY-2-METHOXY-4-PENTYNYL)OXY]METHYL]-4-METHOXY-, [S-(R*,S*)]-	0.000070502	C18H24O4
1-PROPANAMINE, 2-METHYL-	4.1581E-06	C4H11N
CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL-	1.8956E-06	C5H5Br2ClO
METHANE, DICHLORO-	0	CH2Cl2
BENZENE, (8-BROMOOCTYL)-	0	C14H21Br
5-Amino-2-methoxyphenol	0	C7H9NO2
CYCLOHEXANEETHANOL	0	C8H16O
PHOSPHINIC AMIDE, N-METHOXY-P,P-BIS(1-METHYLETHYL)-	0	C7H18NO2P
2,4-LUTIDINE, 6-PROPYL-	0	C10H15N
Total	100	

Fraction: MP 52-62

Compound Name	Area%	Formula
E-15-Heptadecenal	6.0966	C17H32O
2(1H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-4A,8A-DIMETHYL-7-(1-METHYLETHYL)-, (4Aà,7á,8Aà)-	5.3186	C15H24O
1-HEXADECENE	5.0717	C16H32
1-Docosene	4.9915	C22H44
35.51 Turmerone<ar->	3.1812	C15H20O
á TUMERONE	3.1504	C15H22O
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	2.6793	C15H24O
1-Docosene	2.6399	C22H44
trans-Z-à-Bisabolene epoxide	2.1047	C15H24O
4-(4-Dimethylaminobenzylideneamino)-4H-1,2,4-triazole	2.1047	C11H13N5
2-Pentyn-1-ol	2.0215	C5H8O
CYCLOTETRADECANE	1.988	C14H28
1-CHLOROCTADECANE	1.6889	C18H37Cl
trans-Cinnamic acid	1.6487	C9H8O2
1-TETRADECANOL	1.4695	C14H30O
10,12-Tricosadiynoic acid, methyl ester	1.4543	C24H40O2
2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-	1.4373	C10H16O
(1,3-DIMETHYL-2,4,6-CYCLOHEPTATRIEN-1-YL)METHYL METHYL ETHER	1.4338	C11H16O
4-METHYL-3-ISOPROPENYL-4-VINYL-1-CYCLOHEXENE	1.4338	C12H18
10-Heneicosene (c,t)	1.3972	C21H42
2-Propenoic acid, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, exo-	1.3614	C13H20O2
Glutaric acid	1.3096	C5H8O4
Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	1.1096	C15H22
2-Butanone, 4-(4-hydroxyphenyl)-	1.0771	C10H12O2
27.38 Thujopsadiene	1.0646	C15H22
1,5-Cyclooctadiene, 1,2-dimethyl-	1.027	C10H16
2-Butanone, 4-(4-hydroxyphenyl)-	0.98461	C10H12O2
40.01 Bisabolenol<beta->	0.96344	C15H24O
BENZALDEHYDE, 4-HYDROXY-3-METHOXY-	0.95772	C8H8O3
Curlone	0.92378	C15H22O
2-Butanone, 4-(4-hydroxyphenyl)-	0.91784	C10H12O2
1-Docosene	0.86553	C22H44
3,5A,9,9-TETRAMETHYLDECAHYDROBENZO[2,3]CYCLOHEPTA[1,2-B]OXIREN-3-OL	0.79554	C15H26O2
35.51 Turmerone<ar->	0.76818	C15H20O
c-(6-Methyl-2-methylsulfanyl-pyridin-3-yl)-methylamine	0.74395	C8H12N2S
CIS-1,4-DIMETHYL-1-CHLORO-1-SILACYCLOHEXANE	0.71975	C7H13ClSi

PENTADECANE	0.70985	C15H32
1-(4-Hydroxybenzylidene)acetone	0.7014	C10H10O2
37.23 Cedroxyde	0.70008	C15H24O
3-Buten-2-one, 4-(4-hydroxy-3-methoxyphenyl)-	0.66872	C11H12O3
2-Propen-1-ol, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	0.65982	C12H20O
27.05 Sesquisabinene	0.63383	C15H24
1B,5,5,6A-TETRAMETHYL-OCTAHYDRO-1-OXA-CYCLOPROPA[A]INDEN-6-ONE	0.61271	C13H20O2
2-BUTANONE, 4-(4-HYDROXYPHENYL)-	0.59577	C10H12O2
2-HEPTEN-4-ONE, 2-METHYL-6-(4-METHYLPHENYL)-, (S)-	0.59374	C15H20O
1-[2-(1-METHYLETHYLIDENE)CYCLOPROPYL]ETHANOL	0.59023	C8H14O
Pentadecane	0.57738	C15H32
33.39 Biotol <beta->	0.55929	C15H24O
BENZENE, (1-CYCLOPROPYL-1-METHYLETHYL)-	0.55929	C12H16
34.85 Cedr-8(15)-en-10-ol	0.54093	C15H24O
1,2-Benzenediol, o-(4-butylbenzoyl)-o'-(2-methylbenzoyl)-	0.52954	C25H24O4
(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-, [1R-(1R*,4R*,6R*,10S*)]-	0.51377	C15H24O
DODECANOIC ACID	0.50028	C12H24O2
Phenol, 2-butyl-	0.4891	C10H14O
2-METHOXY-1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTANE #	0.45557	C11H20O
1,2-DIHYDRO-3H,11H-PYRAZOLE[1',2'-1,2]PYRAZOLO[3,4-B]QUINOLIN-3-ONE	0.44744	C13H11N3O
3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (E,E)-	0.44436	C13H20O
Z-10-Pentadecen-1-ol	0.41863	C15H30O
3-(4-Hydroxyphenyl)propionitrile	0.41093	C9H9NO
Tetradecane	0.40202	C14H30
1,3-CYCLOHEXADIENE, 5-(1,5-DIMETHYL-4-HEXENYL)-2-METHYL-, [S-(R*,S*)]-	0.40053	C15H24
1,3-DIMETHYLBENZENE-4-SULPHONIC ACID	0.38931	C8H10O3S
2-(2-METHYL-PROPENYL)-CYCLOPROPANECARBOXYLIC ACID 2-ISOPROPYL-5-METHYL-CYCLOHEXYL ESTER	0.38679	C18H30O2
(R*,R*)-(1)-ALPHA,4-DIMETHYL-ALPHA-(4-METHYL-3-PENTENYL)CYCLOHEX-3-ENE-1-METHANOL	0.36909	C15H26O
Oxalic acid, 6-ethyloct-3-yl ethyl ester	0.35853	C14H26O4
2-ALLYL-1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-OL	0.35567	C13H22O
2-ALLYL-1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-OL	0.32639	C13H22O
BENZENE, 1,1'-(1,1,2,2-TETRAMETHYL-1,2-ETHANEDIYL)BIS-	0.3174	C18H22
(6E)-2,4-DIMETHYL-2,6-OCTADIENE #	0.30423	C10H18
CYCLOPROPANECARBONYL CHLORIDE, 2,2-DIBROMO-1-METHYL-	0.3042	C5H5Br2ClO
4,4'-DIMETHYL-BICYCLOHEXYL-3,3'-DIENE-2,2'-DIONE	0.30368	C14H18O2
37.23 Cedroxyde	0.29922	C15H24O
HEPTADECANE	0.28643	C17H36

5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2- METHYL-2-BUTENOATE	0.28309	C20H24O5
6-Octen-1-yn-3-ol, 3,7-dimethyl-	0.27387	C10H16O
Benzenepropanoic acid, á,á-dimethyl-, methyl ester	0.27159	C12H16O2
3-Methyl-2-butenoic acid, 2-isopropoxyphenyl ester	0.27069	C14H18O3
o-Xylene	0.26279	C8H10
n-Hexadecanoic acid	0.26071	C16H32O2
4-Chloro-3-n-hexyltetrahydropyran	0.25816	C11H21ClO
BENZENE, 1-METHYL-4-(1-METHYLETHENYL)-	0.24699	C10H12
6-PROPENYL-BICYCLO[3.1.0]HEXAN-2-ONE	0.24377	C9H12O
Bis[bicyclo[3.2.0]hept-2-en-4-yl]ether	0.23714	C14H18O
Thujopsene	0.23714	C15H24
2-Butenoic acid, 3-methyl-, phenylmethyl ester	0.23451	C12H14O2
3-METHYLENEBICYCLO[3.2.1]OCT-6-EN-8-OL	0.23359	C9H12O
36.34 Botrydiol	0.22832	C15H26O2
1,2-BENZENEDICARBOXYLIC ACID, DIBUTYL ESTER	0.22324	C16H22O4
1-PHENYLPROPAN-2-OL	0.18923	C9H12O
1-Cyclopentene-1-methanol, 2-methyl-5-(1-methylethyl)-	0.18806	C10H18O
40.01 Bisabolenol<beta->	0.18608	C15H24O
1,8-Cyclopentadecadiyne	0.18232	C15H22
3-Methylbut-2-enoic acid, 3,5-dimethylphenyl ester	0.18058	C13H16O2
HEXADECANE	0.17677	C16H34
Tridecane	0.17447	C13H28
1-Docosene	0.17356	C22H44
Isoborneol	0.16799	C10H18O
HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.16609	C22H42O4
2-PENTANONE, 4-METHYL-4-PHENYL-	0.15897	C12H16O
4-(1-HYDROXY-2-ISOPROPYL-5-METHYLCYCLOHEXYL)-3-BUTYN-2-ONE	0.15817	C14H22O2
2-CYCLOHEXEN-1-OL, 2-METHYL-5-(1-METHYLETHENYL)-, TRANS-	0.15748	C10H16O
Globulol	0.15584	C15H26O
3-BUTYN-1-OL	0.15504	C4H6O
28.04 Curcumene<gamma->	0.15332	C15H24
12-Oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl-, [1R-(1R*,3E,7E,11R*)]-	0.15124	C15H24O
BENZALDEHYDE, 4-HYDROXY-3-METHOXY-	0.14202	C8H8O3
1,1':2',1"-TERCYCLOHEXANE	0.14171	C18H32
1-HEXADECANOL	0.14139	C16H34O
1-CHLOROCTADECANE	0.13204	C18H37Cl
1-METHOXY-3,5-DIMETHYL-CYCLOHEXENE	0.13192	C9H16O
2-Butanone, 4-(4-hydroxyphenyl)-	0.13001	C10H12O2
2,6-OCTADIENAL, 3,7-DIMETHYL-	0.12482	C10H16O
37.23 Cedroxyde	0.12392	C15H24O

6-Tridecen-4-yne, (E)-	0.12295	C13H22
3,7-DIMETHYLENEBICYCLO[3.3.1]NONANE	0.12256	C11H16
2-(4'-METHYLPHENYL)-PROPANAL	0.12161	C10H12O
32.34 Thujopsan-2-alpha-ol	0.12072	C15H26O
BENZENE, 1,2-DIMETHYL-	0.11818	C8H10
Theophylline	0.11807	C7H8N4O2
3-BROMO-9-OXABICYCLO[3.3.1]NON-6-EN-2-ONE	0.11683	C8H9BrO2
Longipinene epoxide	0.11561	C15H24O
o-Xylene	0.1152	C8H10
2,5-DIMETHYLBENZYL CYCLOHEXYL KETONE	0.1139	C16H22O
5A-METHYL-3,8-DIMETHYLENE-2- OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2- METHYL-2-BUTENOATE	0.10879	C20H24O5
4-(4-METHYLPHENYL)PENTANAL	0.10664	C12H16O
Spiro[4.5]dec-6-en-8-one, 1,7-dimethyl-4-(1-methylethyl)-	0.10565	C15H24O
12-Oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl-, [1R-(1R*,3E,7E,11R*)]-	0.1039	C15H24O
3,4-Dimethylpent-2-en-1-ol	0.10001	C7H14O
1-Eicosanol	0.10001	C20H42O
35.75 Isobornyl isobutanoate<8-hydroxy->	0.099607	C14H24O3
Betaine	0.099607	C5H11NO2
5,9-Tetradecadiyne	0.096941	C14H22
DECANE, 1-CHLORO-	0.095778	C10H21Cl
1-Methylcyclohex-1-en-4-carboxylic acid	0.093422	C8H12O2
1,5-HEPTADIEN-4-ONE, 3,3,6-TRIMETHYL-	0.090063	C10H16O
Methyl diethylphosphonoacetate	0.087287	C7H15O5P
6Z-2,5,5,10-Tetramethyl-undeca-2,6,9-trien-8-one	0.085724	C15H24O
8-Heptadecene	0.085619	C17H34
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	0.082604	C15H22O2
Indole-6-carboxaldehyde	0.07866	C9H7NO
TRICYCLO[5.1.0.0(3,5)]OCTANE, 4,4,8,8-TETRACHLORO-, (1à,3á,5á,7à)-	0.078449	C8H8Cl4
4,7-METHANOAZULENE, 1,2,3,4,5,6,7,8-OCTAHYDRO-1,4,9,9-TETRAMETHYL-	0.077265	C15H24
ETHANONE, 1-(3-METHYLPHENYL)-	0.071833	C9H10O
4-BUTYLPHENOL	0.070662	C10H14O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.070063	C15H22
SPIRO[1,3-BENZOXATHIOLE-2,1'-CYCLOHEXANE], 3-OXIDE	0.069725	C12H14O2S
1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	0.069619	C15H24
9-OCTADECENOIC ACID (Z)-	0.068598	C18H34O2
3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl-	0.068112	C10H16O
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.066358	C16H18
SPIRO[4.5]DEC-8-EN-7-ONE, 1,8-DIMETHYL-4-(1-METHYLETHYL)-	0.062664	C15H24O
5-AMINO-2-METHYL-2-PHENYL-2,3-DIHYDRO[1,2,4]TRIAZOLO[1,5-A][1,3,5]TRIAZINE	0.059782	C11H12N6

21.45 Patchenol<E->	0.058017	C11H18O
38.24 Bisabolone<6R,7R->	0.0574	C15H24O
2-Naphthalenamine, 1,2,4a,5,6,7,8,8a-octahydro-4a-methyl-	0.0574	C11H19N
UNDECANE, 3-METHYL-	0.057192	C12H26
CYCLOBUTANE, 2-ETHYL-1-METHYL-3-PROPYL-	0.057192	C10H20
4-ALLYLPHENOL	0.057142	C9H10O
Benzene, 1-(1,5-dimethylhexyl)-4-methyl-	0.056695	C15H24
1,2-Dimethoxy-4-(3-methoxypropyl)benzene	0.055199	C12H18O3
2-Cyclohexen-1-one, 4-hydroxy-3-methyl-6-(1-methylethyl)-, trans-	0.054468	C10H16O2
Camphenol, 6-	0.0543	C10H16O
1(4H)-NAPHTHALENONE, 4A,5,6,7,8,8A-HEXAHYDRO-3,4A,8,8-TETRAMETHYL-4-METHYLENE-, (4AS-TRANS)-	0.051524	C15H22O
2-PHENYL-2-HYDROXY-N-ISOPROPYLETHYLAMINE	0.050941	C11H17NO
OCTADECANE	0.050191	C18H38
40.01 Bisabolenol<beta->	0.048249	C15H24O
HEXADECANOIC ACID, METHYL ESTER	0.048102	C17H34O2
3-Methyl-but-2-enoic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	0.048102	C15H24O2
Sodium chlorate	0.046288	ClNaO3
TETRADECANOIC ACID, ETHYL ESTER	0.039915	C16H32O2
DODECANE	0.038614	C12H26
DODECANE	0.037334	C12H26
9-HYDROXYBICYCLO[3.3.1]NONAN-2-ONE	0.037248	C9H14O2
1,8-Cyclopentadecadiyne	0.035852	C15H22
1,3-DIOXOLANE, 2,2,4-TRIMETHYL-5-TRIDECYL-	0.035767	C19H38O2
CYCLOPROPANEMETHANOL, 2-(2-METHYL-1-PROPENYLIDENE)-3-(1-PROPENYL)-, [1à,3á(E)]-	0.035132	C11H16O
UNDECANE	0.034731	C11H24
3-ETHOXY-4-METHYL-3-CYCLOBUTENE-1,2-DIONE	0.033969	C7H8O3
1,2,3,4-TETRAKIS(1-METHYLETHYLIDENE)CYCLOBUTANE	0.033744	C16H24
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.032813	C16H18
1,2-Benzenediol, O-dichloroacetyl-O'-(3-methylbut-2-enoyl)-	0.031106	C13H12Cl2O4
NAPHTHALENE, 1-METHYL-	0.029617	C11H10
Dodecyl acrylate	0.024112	C15H28O2
2-CYCLOHEXEN-1-ONE, 3-HYDROXY-2-(1-METHYL-2-BUTENYL)-, (E)-	0.024094	C11H16O2
Benzene, 1,3-bis(1-formylethyl)-	0.023481	C12H14O2
METHYL 3,3,8,8-TETRAMETHYLTRICYCLO[5.1.0.0~2,4~]OCTANE-5-CARBOXYLATE	0.023283	C14H22O2
6-Propenylbicyclo[3.1.0]hexan-2-one	0.022212	C9H12O
2-Cyclohexen-1-one, 4,4,5-trimethyl-	0.021576	C9H14O
4,8,8-TRIMETHYLBICYCLO[4.2.0]OCT-4-ENE-7,7-DICARBONITRILE	0.02132	C13H16N2
20.12 Carquejol acetate	0.019338	C12H16O2
2-Methyl-3-pentyn-2-ol	0.019289	C6H10O

BUTANE, 1,1-DIBUTOXY-	0.019281	C12H26O2
3-Methyl-6-hepten-1-yn-3-ol	0.017843	C8H12O
5A-METHYL-3,8-DIMETHYLENE-2-OXODODECAHYDROOXIRENO[2',3':6,7]NAPHTHO[1,2-B]FURAN-6-YL 2-METHYL-2-BUTENOATE	0.017493	C20H24O5
BENZALDEHYDE-3-D	0.016703	C7H5DO
1-NEOPENTYL-1,2,3,4-TETRAHYDROISOQUINOLINE	0.016397	C14H21N
Pyrazine, isopropenyl-	0.016306	C7H8N2
N-BUTYL-2-DEUTERIOALLYLAMINE	0.01558	C7H14DN
6-DODECANONE	0.015058	C12H18O
4-VINYL-2-METHOXY-PHENOL	0.014374	C9H10O2
CYCLOHEXANOL, 2-METHYLENE-5-(1-METHYLETHENYL)-, (1S-TRANS)-	0.014172	C10H16O
ISOLONGIFOLEN, 4,5,9,10-DEHYDRO-	0.014107	C15H20
Phenol, 3,5-bis(1,1-dimethylethyl)-	0.01396	C14H22O
Pyrimidine, 2-ethoxy-4,6-dimethyl-	0.013692	C8H12N2O
2-PROPENYL IONONE 2	0.012972	C16H24O
36.51 Atlantone<(Z)-gamma->	0.012924	C15H22O
2-(BROMOMETHYL)-1,3,5-TRIMETHYLBENZENE	0.012609	C10H13Br
(4-Acetylphenyl)phenylmethane	0.012609	C15H14O
BENZENE, 1,1'-[OXYBIS(1-METHYLETHYLIDENE)]BIS-	0.012267	C18H22O
2,4-Diphenyl-4-methyl-2(E)-pentene	0.01194	C18H20
2-BUTENOIC ACID, 3-METHYL-, METHYL ESTER	0.011703	C6H10O2
BICYCLO[3.1.0]HEXAN-2-ONE, 4-METHYL-1-(1-METHYLETHYL)-, (1à,4á,5à)-	0.011605	C10H16O
Octane, 2,6-dimethyl-	0.011327	C10H22
Chloromethanesulfonyl-dichloromethanesulfonyl chloride	0.010768	C2H2Cl4O4S2
4H-PYRAZOLO[3,4-D]PYRIMIDIN-4-ONE, 1,5-DIHYDRO-	0.009169	C5H4N4O
3-(ENDO-SELENOCYANATO)CAMPHOR	0.0089467	C11H15NOSe
(+)-2-CAREN, 4-ALPHA-ISOPROPENYL-	0.0085169	C13H20
1,4-BUTANEDIAMINE	0.0083452	C4H12N2
1-[à-(1-Adamantyl)benzylidene]thiosemicarbazide	0.0083452	C18H23N3S
BENZENE, 1-METHOXY-4-(4-PROPYLCYCLOHEXYL)-, TRANS-	0.0077728	C16H24O
BENZENE, 1-(1-ETHENYL-1-METHYL-2-PROPENYL)-4-METHYL-	0.0075206	C13H16
35.60 Bulnesol	0.0072916	C15H26O
BENZENE, 1-(1,5-DIMETHYL-4-HEXENYL)-4-METHYL-	0.0066611	C15H22
BENZENE, 1,2,3,4-TETRAMETHYL-	0.0064874	C10H14
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl-	0.0057587	C18H20
6.84 Hexanoic acid	0.0056797	C6H12O2
2-(CYANAMINO)-6-METHYLPYRIDINE	0.0056513	C7H7N3
p-Toluic acid, tridec-2-ynyl ester	0.0054566	C21H30O2
4-Hexen-3-one, 5-methyl-	0.0049369	C7H12O
2,3-BUTANEDIOL, 2,3-DIMETHYL-	0.0048424	C6H14O2
1-ETHYL-3-METHYL-1H-PYRAZOLE-4-CARBALDEHYDE	0.0041628	C7H10N2O

Methanesulfonanilide, 4'-(1-hydroxy-2-(isopropylamino)ethyl)-	0.0039686	C12H20N2O3 S
BENZENE, 4-FLUORO-1,2-DIMETHYL-	0.0035892	C8H9F
BIS(OCT-3-YL) PHTHALATE	0.0032933	C24H38O4
BICYCLO[2.2.1]HEPTANE-ENDO-2,ENDO-3-DIMETHANOL. DIACETATE	0.003146	C13H20O4
d,1-trans-4-Methyl-5-methoxy-1-(1-methoxy-1-isopropyl)cyclohex-3-ene	0.0031436	C12H22O2
2-PENTANOL, 3-ETHYL-	0.0028341	C7H16O
METHYL ESTER OF 3-(3,5-DI-TERT-BUTYL-4-HYDROXYPHENYL)- PROPIONIC ACID	0.0025006	C18H28O3
NAPHTHALENE, 1-METHYL-	0.0020519	C11H10
1,1'-Biphenyl, 2,2'-diethyl-	0.0015716	C16H18
34.28 Gossonorol	0.0009025	C15H22O
Benzenemethanol, 4-methyl-à-(1-methyl-2-propenyl)-, (R*,R*)-	0.00085316	C12H16O
1,2-BIS(3-METHYL-1,2-BUTADIENYL)BENZENE	0.00071774	C16H18
BENZENE, 1,2,3,4-TETRAMETHYL-	0.00046734	C10H14
3-DODECYLOXYPHENYL BENZOATE	0.00039282	C25H34O3
Benzene, 1,2,3,5-tetramethyl-	0.00036924	C10H14
ETHANONE, 1-(1,3-DIMETHYL-1H-PYRAZOL-4-YL)-	0.00029236	C7H10N2O
BENZENE, (1-METHYL-1-PROPENYL)-, (Z)-	0.00028179	C10H12
3-Methylbut-2-enoic acid, 3-fluorophenyl ester	0.000090341	C11H11FO2
Silane, 1,8-octanediybis[trimethyl-	0	C14H34Si2
Total	100	



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