In the Name of Allah

Sudan University of Science and Technology

Collage of Graduate Studies

Extraction, Characterization and Antimicrobial Activity of Citrus Oil from Lemon Peels

إستخلاص ودراسة خصائص زيت قشور الليمون مع نشاطه المضاد للمايكروبات

A Thesis Submitted in Partial Fulfillment of the Requirements of the Master Degree in Chemistry

By

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الآيـــــــة

قال تعالى:

((اللَّهُ نُورُ السَّمَوَاتِ وَالْأَرْضِ مَثَلُ نُورِهِ كَمِشْكَاةٍ فِيهَا مِصْبَاحٌ الْمِصْبَاحُ فِي زُجَاجَةٍ الزُّجَاجَةُ كَأَنَّهَا كَوْكَبٌ دُرِّيٌّ يُوقَدُ مِنْ شَجَرَةٍ مُبَارَكَةٍ زَيْتُونَةٍ لَا شَرْقِيَّةٍ وَلَا غَرْبِيَّةٍ يَكَادُ زَيْتُهَا يُضِيءُ وَلَوْ لَمْ تَمْسَسْهُ نَارٌ نُورٌ عَلَى نُورٍ يَهْدِي اللَّهُ لِنُورِهِ مَنْ يَشَاءُ وَيَضْرِبُ اللَّهُ الْأَمْثَالَ لِلنَّاسِ وَاللَّهُ بِكُلِّ شَيْءٍ عَلِيمٌ))

صدق الله العظيم

سورة النور الآية (35)

Dedication

To My father and mother,

My husband,

My dear sisters and brothers,

My babies' leen and mohammed

Acknowledgement

First off all, I would like to thank Allah almighty for making this work possible. Secondly, I would like to express my gratitude to my supervisor Dr. Kamal Mohamed Saeed for his supervision, valuable advice, kind treatment and guidance during this work period and chemistry department, colleagues and all whom support me.

List of table

Abstract

The essential oil from the dry peels of *Citrus Limon* was extracted by hydro distillation. The essential oil yield was found to be 0.6% (v/w). Physical and chemical properties of the oil were studies; refractive index (1.462), density (0.918) and viscosity (1.462).

The chemical properties of the oil were measured: iodine value (97.583), acid value (2.244), saponification value (86.25), ester value (70.583), unsaponifiable matter (0.673), and ratio value (31.627). Also the extracted essential oil was analyzed by gas chromatography – mass spectrometry (GC-MS) to determine the chemical constituents. From the GC-MS analysis 53 compounds were identified. The main constituents of essential oil were: d-limonene 30.57%, β-pinene 18.96%, γ-Terpinene 8.09%.

Different concentrations of the crude product of *Citrus Limon* peels (100, 50, 25, 12.5, 6.25 mg/ml) were tested for antimicrobial activity against bacterial strains and one fungus. *Citrus Limon* peel oil showed inhibition against all the test organisms (Gram positive, Gram negative and fungus) at 100mg/ml, 50mg/ml and 25mg/ml. At 12.5mg/ml four organisms showed inhibition zone, at 6.25mg/ml just three organism's showed inhibition.

ملخص

تم إستخلاص الزيت العطري من قشرة فاكهة نبات الليمون المزروع محلياً بواسطة التقطير المائي. حيث تمت دراسة الخواص الفيزيائية والكيميائية لهذا الزيت. ووجد أن نسبة الزيت العطري في القشرة 0.6 % (حجم/وزن). الخواص الفيزيائية للزيت كانت كالاتي: معامل الانكسار الضوئي 1.462، الكثافة 0.918 واللزوجة 1.462. اما الخواص الكيميائية العدد اليودي 97.583، العدد الحمضي 2.244، عدد التصبن 86.25، عدد الاستر70.583 والمواد الغير متصبنة 0.673. تم تحليل الزيت المستخلص بواسطة كروماتوغرافيا الغاز الملحق بجهاز طيف الكتلة وذلك لتعيين المكونات الكيميائية. تم التعرف علي 53 مركب في الزيت العطري. ووجد أن المكونات الاساسية للزيت العطري هي: دي ليمونيين (30.57%) وبيتا-بينين (18.96%) وقاما تيربينين (8.09%) علي التوالي.

أُجري اختبار مضاد الميكروبات للزيت المستخلص عبر سلسله من التراكيز ضد بعض الميكروبات القياسية (أربعة أنواع من البكتيريا موجبة الصبغة وسالبة الصبغة وفطر واحد) وأعطي الزيت المستخلص فعالية عند التراكيز (100 - 50 – 25) ملغم/مل اما عند التراكيز (12.5- 6.25) ملغم/مل فقد أظهر فعاليه واعده.

List of contents

CHAPTER ONE

1 INTRODUCTION

1.1 Fundamentals

Citrus fruits are among the most popular fruits nowadays and have a very long history of production and use. However, within the past century, industrial technologies began to develop in order to convert citrus fruits into commercial products (Swisher *et al*., 1977). Each year, millions of tons of citrus fruits are delivered to factories for processing and juice production. Historically, the oldest citrus product is the oil. In ancient Sicily, where early Italian citrus industry had just been introduced, lemons were primarily grown for production of lemon oil, and juice was treated as a waste product until its later use for citric acid recovery. The early use of lemon and orange oils was mainly in perfumery and pharmaceuticals (Swisher *et al*., 1977). With rapid development of science and technology, more areas of use of citrus oils were found, for which more detailed information on chemical composition and properties were required. The modern perfume and flavor industries have benefited from further research on citrus peel oil and essence. Besides, the yield of citrus seed oil has increased since citrus seeds were discovered as a new source of edible oil. Citrus has proven to be a very good option for the oil and essence production. The genus citrus, according to Tanaka's system, has been divided into eight groups, Papeda, Limonellus, Citruphorum, Cephalocitrus, Aurantium, Osmocitrus, Acrumen, and Pseudofortunella, with a number of species within each group and a larger number of fine-quality hybrids as well (Ogawa *et al*., 2000).

The essential oils are aromatic compounds that are widely used in the perfume, pharmaceutical and food industries. Essential oils are mixtures of more than 200 different compounds. These compounds are mainly formed of monoterpene and sesquiterpene hydrocarbons and their oxygenated derivatives such as esters, alcohols and aliphatic aldehydes and ketones. Essential oils are

generally created by aromatic plants. The specific gravity of essential oils is often less than water and only a small number of essential oils have a higher specific gravity than water. Essential oils are non-miscible with water but can transfer their odors to aqueous layer. These compounds are solved in most of organic solvents such as diethyl ether, hexane and ethyl acetate. Essential oils in the presence of air and heat are evaporated, therefore they might be called volatile oils or ethereal oils (Aberoomand *et al*., 2011; Kamal *et al*., 2011). Some physical and chemical properties of essential oils are different from fixed oils. The most important is that the essential oils are condensable and can be extracted by distillation methods and they are not glycerol esters. The essential oils do not produce soap with alkaline and do not make permanent stains on paper (Jaymand, 2001). The essential oils are complex natural mixtures that can be formed from different chemical compounds with various concentrations. Constituent compounds of essential oils are in two groups with two distinct biosynthetic pathways from each other. Terpenoids derivatives created of the intermediate acetate – malonic acid and aromatic compounds made from shikimic acid and phenylpropanoids. In addition to the above classification, components of essential oils might be classified based on the functional groups present in the structure that include hydrocarbons, alcohols, aldehydes, ketones, esters, phenols, phenolic ethers, oxides and peroxides. Terpenes and their oxygenated derivatives (Terpenoids) are the most important categories of the ingredients of essential oils. Depending on the number of isoprene units in the structure of terpenes, these compounds are classified to hemiterepens (C5) monoterpenes (C10), sesquiterpenes (C15), diterpenes (C20), sesterterpenes and, (C25) triterpenes (C30), tetra-terpenes (C40) and poly-terpenes (C5) n, where n is greater than 8.

Citrus peel oils of very complex composition are contained in oval, balloon-shaped oil sacs, or vesicles, located in the outer rind, or flavedo, of the

fruit (Usai *et al*., 1992). The oil is usually extracted by mechanical separation or hydro distillation. The five main types of citrus from which peel oils are recovered are orange, grapefruit, tangerine, lemon, and lime (Shaw and Veldhuis, 1977). Mechanical separation, known as cold-pressing of peel oils, does not use heat in order to avoid loss of volatile components. Swisher and Swisher (Swisher and Swisher, 1977) described three general commercial methods that are widely used in citrus industry to extract crude oils from fruit peels:

(1) Oil recovery from peel after juice extraction

(2) Simultaneous extraction of juice and oil emulsion from whole fruit

(3) Recovery of oil from the peel flavedo after removal from the whole fruit by abrasion or shaving

Citrus peel oils for small-scale use may be obtained by hand-pressing. Fruits are sliced, and mesocarp and albedo layers are peeled from the flavedo before hand-pressing. Peel oils are collected in brine solution on ice, and oil extract is centrifuged at 4^{o}C. Afterwards, the supernatant is dehydrated with anhydrous sodium sulfate and filtered (Choi and awamura, 2000). The total final oil extract is about 1% of the flavedo by weight (Choi, 2003). Citrus peel oils other than cold-pressed oils have a lower price in the marketplace and are known as distilled oil, which is recovered from peels by steam distillation. This oil possesses an odor and flavor that is generally inferior to that of the cold-pressed oil (Swisher *et al*., 1977). The final oil extract is a liquid with its color varying depending on the species of the fruit, lemon oil is pale yellow to pale greenish-yellow (Bauer *et al*., 1990).

Lemon essential oil are complex mixtures of chemical compounds like limonene, Y-terpinene, citral, linalool and β-caryophyllene among others, which can be represented by three main classes, namely terpenes, oxygenates, and sesquiterpenes (Benvenuti, *et al*., 2001 and Van Straten *et al*., 1983). The most significant flavour compound is citral, while linalool possesses highly

distinctive organoleptic characteristics. In addition, limonene, myrcene, octanol, and Y-terpene among others contribute with high aroma flavour of lemon oil (Benvenuti, *et al*., 1983).

Lemon is an important medicinal plant of the family Rutaceae. It is cultivated mainly for its alkaloids, which are having anticancer activities and the antibacterial potential in crude extracts of different parts (viz., leaves, stem, root and flower) of Lemon against clinically significant bacterial strains has been reported (Kawaii *et al*., 2000). Citrus flavonoids have a large spectrum of biological activity including antibacterial, antifungal, antidiabetic, anticancer and antiviral activities (Burt, 2004; Ortuno *et al*., 2006). Flavonoids can function as direct antioxidants and free radical scavengers, and have the capacity to modulate enzymatic activities and inhibit cell proliferation (Duthie and Crozier, 2000). In plants, they appear to play a defensive role against invading pathogens, including bacteria, fungi and viruses (Sohn *et al*., 2004). The peel of Citrus fruits is a rich source of flavonoid glycosides, coumarins, and sitosterol, glycosides and volatile oils (Shahnah *et al*., 2007). Many polymethoxylated flavones have several important bioactivities, which are very rare in other plants (Ahmad *et al*., 2006). In addition, the fiber of citrus fruit also contains bioactive compounds, such as polyphenols, the most important being vitamin C (or ascorbic acid), and they certainly prevent and cure vitamin C deficiency-the cause of scurvy (Aronson, 2001). Antimicrobial activity of the peel extract is directly concerned with the components that they contain. The studies showed that essential oils, protopine and corydaline alkaloids, lactons, polyacetylene, acyclic sesquiterpenes, hypericin and pseudohypericin compounds are effective toward various bacteria. Nevertheless, other active terpenes, as well as alcohols, aldehydes, and esters, can contribute to the overall antimicrobial effects of the essential oils (Keles *et al*., 2001).

1.2 Objectives

- To extract and characterize the oil.
- To identify the major components of the oil.
- To test the antimicrobial activity of the oil.

CHAPTER TWO

2 LITERTURE REVIEW

2.1 Classification of *Citrus Limon*

Kingdom : Plantae

Order : Sapindales

Family : Rutaceae

Genus : Citrus

Species : C. × limon

Binomial name: C. Limon (L.) Burm.f.

Potential name: Citrus Limon

Common name: lemon

2.2 History of citrus Limon

2.2.1 Origin

The origin of the lemon is unknown, though lemons are thought to have first grown in Assam (a region in northeast India), northern Burmaor China (Morton, 1987). A study of the genetic origin of the lemon reported it to be hybrid between bitter orange (sour orange) and citron (Gulsen and Roosa, 2011).

Lemons entered Europe near southern Italy no later than the first century AD, during the time of Ancient Rome (Morton, 1987). However, they were not widely cultivated. They were later introduced to Persia and then to Iraq and Egypt around 700 AD (Morton, 1987). The lemon was first recorded in literature in a 10th-century Arabic treatise on farming, and was also used as an ornamental plant in early Islamic gardens (Morton, 1987).It was distributed widely throughout the Arab world and the Mediterranean region between 1000 and 1150 (Morton, 1987).

The first substantial cultivation of lemons in Europe began in Genoa in the middle of the 15th century. The lemon was later introduced to the Americas in

1493 when Christopher Columbus brought lemon seeds to Hispaniola on his voyages. Spanish conquest throughout the New World helped spread lemon seeds. It was mainly used as an ornamental plant and for medicine (Morton, 1987). In the 19th century, lemons were increasingly planted in Florida and California (Morton, 1987).

In 1747, James Lind's experiments on seamen suffering from scurvy involved adding lemon juice to their diets, though vitamin C was not yet known (Lind, 1757).

The origin of the word "lemon" may be Middle Eastern (Morton, 1987). The word draws from the Old French limon, then Italian limone, from the Arabic laymūn or līmūn, and from the Persian līmūn, a generic term for citrus fruit, which is a cognate of Sanskrit (nimbū, “lime”).

2.2.2 Description of the tree

The true lemon tree reaches 10 to 20 ft (3-6 m) in height and usually has sharp thorns on the twigs. The alternate leaves, reddish when young, become dark-green above, light-green below; are oblong, elliptic or long-ovate, 2 1/2 to 4 1/2 in (6.25-11.25 cm) long, finely toothed, with slender wings on the petioles. The mildly fragrant flowers may be solitary or there may be 2 or more clustered in the leaf axils. Buds are reddish; the opened flowers have 4 or 5 petals 3/4 in (2 cm) long, white on the upper surface (inside), purplish beneath (outside), and 20-40 more or less united stamens with yellow anthers. The fruit is oval with a nipple-like protuberance at the apex; 2 3/4 to 4 3/4 in (7 -12 cm) long; the peel is usually light-yellow though some lemons are variegated with longitudinal stripes of green and yellow or white; it is aromatic, dotted with oil glands; 1/4 to 3/8 in (6-10 mm) thick; pulp is pale-yellow, in 8 to 10 segments, juicy, acid. Some fruits are seedless, most have a few seeds, elliptic or ovate, pointed, smooth, 3/8 in (9.5 mm) long, white inside (Morton, 1987).

2.2.3 Distribution of citrus in Sudan

The most important citrus fruit trees grown in Sudan include sweet orange (Citrus sinensis Osbeck), grapefruit (C.paradisi Macf.) and lime (C.auranfifofia). Other citrus trees are grown but on a limited scale, like mandarin (C.reticulata Blanco), lemon (C.limon) and pummelo (Cgrandis). This is in addition to other types of citrus trees used mainly as rootstocks, of which the sour orange (C.aurantium) is the most widely used. The northern, eastern and central regions are important areas of production. Jebel Matra area inWestern Darfur State is of a special importance in citrus production as almost all the sweet navel orange fruits (seedless fruits) are produced there. Small areas of citrus fruits are found in some parts of Kordofan states. All cultivars of citrus fruits grown are introduced old varieties. The distinct old cultivars in citrus fruits are five for sweet orange, three for grapefruit, and three for lime. Some wild citrus trees are also reported to be growing in some parts of western and central Sudan. During the eighties, some new orange and grapefruit varieties were officially released.

Citrus is an important cash crop in the Sudan. In addition, it is one of the major sources of human diet due to its high nutritive value, especially vitamin C (Bedri, 1984). Its cultivation is native to tropical and subtropical regions. Nowadays, it is grown all over the world wherever there is sufficient rainfall and irrigation to sustain the trees.

Total area of citrus in Sudan is estimated as 100000 Fed (National Horticulture Administration, 2001). However, the productivity of this area may not satisfy the ever- increasing demand for citrus products for local consumption and export. Therefore, the national strategy of citrus expansion is directed towards the large national schemes, e.g. Gezira, Suki, Rahad and the Blue Nile Schemes in the Central Clay Plain (Sidahmed and Geneif, 1984). Soils of this area are characterized by high clay contents, low nitrogen level and high pH values (Blockhuis, 1993). Citrus trees grown in this area are stunted

and of low yield (Hamid, 1986). Fruit quality is also poor indicated by low total soluble solids (%TSS), low ascorbic acid (vitamin C) and high acidity (%TA). Many factors were suspected to cause the low yield and poor quality of fruits in this area. These factors may include use of local low yielding cultivars, soil problems and poor management practices such as lack of fertilizers application.

2.3 Varieties

The 'Bonnie Brae' is oblong, smooth, thin-skinned, and seedless (William, 1885); mostly grown in San Diego County (Carque and Otto, 2006).

The 'Eureka' grows year-round and abundantly. This is the common supermarket lemon, also known as 'Four Seasons' (Quatre Saisons) because of its ability to produce fruit and flowers together throughout the year. This variety is also available as a plant to domestic customers (Buchan and Ursula, 2005). There is also a pink-fleshed Eureka lemon, which's outer skin is variegated from green and yellow stripes.

The 'Femminello St. Teresa', or 'Sorrento' is native to Italy. This fruit's zest is high in lemon oils. It is the variety traditionally used in the making of limoncello.

The 'Meyer' is a cross between a lemon and possibly an orange or a mandarin, and was named after Frank N. Meyer, who first introduced it to the USA in 1908. Thin-skinned and slightly less acidic than the Lisbon and Eureka lemons, Meyer lemons require more care when shipping and are not widely grown on a commercial basis. Meyer lemons often mature to a yellow-orange color. They are slightly more frost-tolerant than other lemons.

The 'Ponderosa' is more cold-sensitive than true lemons; the fruit are thick-skinned and very large. It is likely a citron-lemon hybrid.

The 'Yen Ben' is an Australasian cultivar.

2.4 Culinary uses

Lemon juice, rind, and zest are used in a wide variety of foods and drinks. Lemon juice is used to make lemonade, soft drinks, and cocktails. It is used in marinades for fish, where its acid neutralizes amines in fish by converting them into nonvolatile ammoniumsalts, and meat, where the acid partially hydrolyzes tough collagen fibers, tenderizing the meat, but the low pH denatures the proteins, causing them to dry out when cooked. Lemon juice is frequently used in the United Kingdom to add to pancakes, especially on Shrove Tuesday.

Lemon juice is also used as a short-term preservative on certain foods that tend to oxidize and turn brown after being sliced (enzymatic browning), such as apples, bananas, and avocados, where its acid denatures the enzymes.

Lemon juice and rind are used to make marmalade, lemon curd and lemon liqueur. Lemon slices and lemon rind are used as a garnish for food and drinks. Lemon zest, the grated outer rind of the fruit, is used to add flavor to baked goods, puddings, rice, and other dishes.

The leaves of the lemon tree are used to make a tea and for preparing cooked meats and seafood's.

2.5 Other uses

2.5.1 Industrial

Lemons were the primary commercial source of citric acid before the development of fermentation-based processes (Rauf et al, 2014).

2.5.2 As a cleaning agent

The juice of the lemon may be used for cleaning. A halved lemon dipped in salt or baking powder is used to brighten copper cookware. The acid dissolves the tarnish and the abrasives assist the cleaning. As a sanitary kitchen deodorizer the juice can deodorize, remove grease, bleach stains, and disinfect; when mixed with baking soda, it removes stains from plastic food

storage containers (Penniston et al, 2008). The oil of the lemon's peel also has various uses. It is used as a wood cleaner and polish, where its solvent property is employed to dissolve old wax, fingerprints, and grime. Lemon oil and orange oil are also used as a nontoxic insecticide treatment.

A halved lemon is used as a finger moistener for those counting large amounts of bills, such as tellers and cashiers.

2.5.3 Medicinal

Lemon oil may be used in aromatherapy. Lemon oil aroma does not influence the human immune system, but may enhance mood (Hofrichter, 2010). The low pH of juice makes it antibacterial, and in India, the lemon is used in Indian traditional medicines (Siddha medicine and Ayurveda).

2.6 Other

One educational science experiment involves attaching electrodes to a lemon and using it as a battery to produce electricity. Although very low power, several lemon batteries can power a small digital watch. These experiments also work with other fruits and vegetables.

Lemon juice may be used as a simple invisible ink, developed by heat (Kiecolt-Glaser *et al*., 2008).

2.7 Alternative lemon

Many plants taste or smell similar to lemons.

- Certain cultivars of basil
- Cymbopogon (lemongrass)
- Lemon balm, a mint-like herbaceous perennial in the Lamiaceae family
- Two varieties of scented geranium: *Pelargonium crispum* (lemon geranium) and *Pelargonium x melissinum* (lemon balm)
- Lemon thyme
- Lemon verbena
- Limes, another common sour citrus fruit, used similarly to lemons

- Certain cultivars of mint
- Magnolia grandiflora trees

2.8 Production

In 2013, world production of lemons (together with limes) was 15.2 million tonnes, led by India, Mexico and China as the main producers. Argentina and Brazil also had significant production (Cooke and Emst, 2000).

2.9 Volatile Oils from citrus fruit

Volatile oils from citrus fruits contain various type of natural flavors and fragrances, which are popularly used in food industries, daily chemical products and health care field (Sheng-min *et al*., 2012). Citrus species are potential sources of variable oils which might be utilized for edible and other industrial applications (maria *et al*., 2012). Humankind used plants for healing many thousands of years, and it's from this tradition the use of aromatic plant compounds in medicine was begun. Oils were used in the embalming process, in medicine and in purification rituals. There are also over 200 references to aromatic, incense, and ointments in the old and new Testaments (Frankincense, 3 Myrrh, Galbanum, Cinnamon, Cassia, Rosemary, Hyssop and Spikenard) are noted for being used anointing rituals and healing of the sick. Research confirmed centuries of practical use of essential oils, and we now know that the fragrant pharmacy contains compounds with an extremely broad range of biochemical effect (Sheng-min *et al*.,2012).Essential oils are broadly used as pharmaceutical components, in nutritious supplements and for cosmetic industry and aromatherapy (Maria *et al*., 2012).Guenther (1955) also stated that the oil is also employed in perfumes, toilet water, beaux cologne, and in cosmetics to, which it impacts a refreshing top note. There are about three hundred essential oils in general use today by professional practitioners. With continual bombardment of viral, bacterial, parasitic and fungal contamination in our world. Essential oils are a great benefit to help protect our bodies and health

from sickness. Essential oils are products obtained from vegetable raw materials (Berger2007). They are complex mixtures their composition may include volatile terpenic compounds, which have the formula $(C5H8)_n$. where the compounds are monoterpenes if n=2, sesquiterpenes when n=3, diterpenes if n=4,etc(Smith *et al*.,2001). These are secondary metabolites in plants (Mazen, 2002) and responsible for the characteristic aroma on the fruit. Immune system needs support and essential oils give that, because of the enormous amount of raw product used to make wholly natural essential oils, lots of products on the market have been polluted with lower quality, commercial grade oils or contain other chemical substances to reduce the cost or increase the profit margin a fact that not usually revealed on the label. This 4 is why it is important to study the chemical composition of the volatile fraction once the essential oil is extracted. This fraction is characterized by the complexity in the separation of its components, which belong to various classes of compounds and which are present in wide range of concentrations. Therefore, it is complicated to establish a composition profile of essential oils. Lemon essential oils are complex mixture of chemical compounds like limonene, γ-terpinene, citral, linalool and β-caryophylene among other, which can be represented by the main classes,namely terpenes, oxygenates, and sesquiterpenes (Benvenuiti *et al*,2001).The most significant flavor compound is citral, while linalool possess highly distinctive organoliptic characteristic. In addition, limonene, octanol, and Y-terpene among other contribute with high aroma flavor of lemon oil (Benvenuiti *et al*, 2001). The quality of essential oil depends on different factors, among them are the chemo type and biotype of the plant, the climatic conditions, as well as, the extractive process. Citrus fruits have a rough, robust, and bright (green to yellow) color skin they are 5 usually 4- 30cm long and 4-20cm in diameter with peel surrounding known as (epicarp) that covered the fruit and protect it from damages. Citrus fruits are notable for their fragrance partly due to flavanoids and lemonoids contained in the rind (Manthey, 2004).

The endocarp is rich in soluble sugar and contains significant amounts of vitamin c, pectin, different organic acids and potassium salt which give the fruits its characteristic citrus flavor (Ezejiofor *et al*, 2011).

2.10 Function of the essential oils in the plants

Essential oils are extracted from oil sacs, in flowers, seeds, leaves, roots, wood and bark. They differ significantly from the well-known vegetable, nut 7 and seeds oils which are made up of various fatty acids, essential oils are used by the plants in somewhat the same way by humans,they fight infections, contain hormone-like compounds, initiate cellular regeneration, and work as chemical defense against fungal, viral, and animal foes. Despite their foliar origins however, essential oils have similar structure to some compounds found in blood and tissues, allowing them to be compatible with our physiology (GUENTHER, 1955).

2.11 Chemical constituents of essential oil

Pure essential oils are mixtures of more than 200 components, normally mixtures of terpenes or phenylpropanic derivatives, in which the chemical and structural differences can be classified into two groups;

Volatile fractions

Essential oils constituting 90-95%of the oil in weight, containing the monoterpene and sesquiterpene hydrocarbons, as well as their oxygenated derivatives along with aliphatic aldehydes, alcohols, and esters .

Nonvolatile residues

That comprises 1-10% of the oil, containing hydrocarbons, fatty acids, sterol, carotenoids, waxes, and flavonoids.

2.11.1 Hydrocarbons

Essential oils consist of chemical compounds that have hydrogen and carbon as their building blocks. Basic hydrocarbons found in plants are (Isoprene) having the following structure (CH3-CH2-C=CH-CH2)

2.11.2 Terpenes

These are generally have names ended by ”ene” eg.limonene, pinene, camphene, piperene, etc. Terpene are anti- Inflammable, antiseptic, antiviral, and bactericidal. Terpenes can be further categorized in monoterpenes, sesquiterpenes and diterpenes. Referring back to isoprene units under the hydrocarbons heading, when two of these isoprene unit join head to tail, the result is a monoterpene, when three join, it is a sesquiterpene and four linked isoprene units are diterpene.

2.11.2.1 Monoterpene ($C_{10}H_{16}$)

This terpenes are,analgestic Bactericidal, Expectorant, and Stimulant. Monoterpene are naturally occurring compounds, the majority being unsaturated hydrocarbons (C10). But some of their derivatives such as alcohols, ketones, and carboxlic acids known as monoterpene like (limonene, menthol). The branched-chain C10 hydrocarbons comprise of two isoprene units and is widely distributed in nature with more than 400 naturally occurring monoterpene identified. Moreover, besides being linear derivatives Geraniol, Citronellol, the monoterpene can be cyclic molecules (menthol-monocyclic, Camphor- bicyclic; Pinenes, pine genera as well. Thujone (a monoterpene) is toxic agent found in Artemisia absinthium(wormwood) from which the absinthe is made. Borneol and camphor are two commonmonoterpenes.

Borneol, derived from pine oil, is used as disinfectant and deodorant. Camphor is used as counterirritant, anesthetic, expectorant, and antipruritic,among many other uses.e.g Camphene and pinene in cypress oil.Camphene, pinene,andthujhene in black pepper.

2.11.2.2 Sesquiterpenes ($C_{15}H_{24}$)

They are anti-inflammatory, anti-septic, analgestic, anti-allergic. And in structure may be linear, monocyclic, or bicyclical Sesquiterpene are biogenetically derived from farensylpyrophosphate. They constitute a very large group of secondary metabolites; some have been shown to be stress compounds formed as a result of disease or injury.

2.11.2.3 Sesquiterpene lactones

Over 500 compounds of this group are known; they are particularly characteristics of the composite but do occur sporadically in other families. Not only they have proved to be of interest from chemical and chemotaxonomic points of view, but also possess many antitumor, anti-leukemia, cyto toxic and antimicrobial activities. They may be responsible for skin allergies in human and they can also act as insect detergents. Chemically the compounds can be classified according to their carboxylic skeleton, thus, from the germacranolidesguaianolides, pseudoguaianolides, eudesmanolides, eremophilanolides, xanthanolides,etc can be derived. A structural feature of all these compounds, which appears to be associated with much of the biological activity, is the alpha- betaunsaturated-Gama-lactones.e.g franesene in chamomile and lavender.betacaryophyllene in basil and black pepper.

2.11.2.4 Diterpenes ($C_{20}H_{32}$)

These are Anti-fungal, expectorant, hormonal balancers, and hypertensive. Diterpene are made up of four isoprene units. These molecules are too heavy to allow for evaporation with steam in distillation process. So they are rarely found in distilled essential oils. Diterpenes occur in all plant families and consist of compounds having a C20 Skeleton. There are about 2500 known diterpenes that belong to 20 major structural types. Plants hormones Gibberellins and phytol occurring as aside chain on cholorophyll are diterpenic derivatives. The biosynthesis occurs in plastid and interestingly mixtures of monoterpenes and diterpenes are amajor constituents of plant resins. In asimilar manner to

monoterpenes, diterpenes arise from metabolism of gernalygernalypyrophpsphate GGPP Diterpenes have limited therapeutical importance and are used in certain sedatives (coughs) as well as in antispasmodics and antoxiolytics.e.g.sclareol in clary sage is an example of a diterpene alcohol.

2.11.3 Alcohols

These are Anti-septic, anti-viral, bactericidal and germicidal. Alcohols exist naturally, either as free compounds, or combined with terpene or ester. When terpenes are attached to an oxygen atom, and hydrogen atom, the result is an alcohol. When the terpene is amonoterpene, the resulting alcohol is called monoterpenol. Alcohols have very low or totally absent toxic reaction in the body or on the skintherefore, they are considered safe to use.e,g. linalool found in ylang-ylang and lavender,geraniol in geranium and rose. nerol in neroli.

2.11.4 Aldehydes

These are Anti-fungal, anti-inflammatory, anti-septic, antiviral, bactericidal, disinfectant, sedative,medicinally, essential oils containing aldehydes are effective in treating candida and other fungal infections.e.g.citral in lemon, lemongrass and lemon balm,citronellal in lemongrass, lemon balm and citrus eucalyptus.

2.11.5 Acids

Anti-infalmmatory, Organic acids in their free state are generally founds in very small quantities within essential oils. Plant acids act as components or buffer system to control acidity.e.g.cinnamic and benzoic acids in benzoin.citric and lactic in essential oil lemongrass and lemon balm,citronellal in lemongrass, lemon balm, and citrus eucalyptus.

2.11.6 Esters

Essential oil containing esters are used for their thooting, balancing effects. Because of the presence of alcohol, they are effective antimicrobial agents. Medicinally, esters are characterized as antifungal and

Sedative, with a balancing action on the nervous system, they are generally free from precautions with the exception of methyl slicylate found in birch and wintergreen which is toxic within the ayatem.e.g., linyl acetate in bergamot and lavender, geranylformate in geranium.

2.11.7 Ketones

Anti-catarrhal, cell proliferant, expectorant, vulnery.Ketones often are found in plants that are used for upper respiratory complaints, they assist the flow of mucus and ease congestion, essential oils containing ketones are beneficial for promoting wound healing and encouraging the formation of scar tissue .ketones are usually very toxic, the most toxic ketone is thujone founds in mugwort, stage, tansy, thuja and wormwood oils, other toxic ketones found in essential oils are pulegone in pennyroyal, and pincocamphone in hyssop, some non-toxic ketones are jasmine in jasmine oil,fenchone in fennel oil, carvone in spearment and oil and menthone in peppermint oil.e.g.fenchone in fennel, carvone in speariment and dill, menthone in peppermint.

2.11.8 Lactones

These are Anti-inflammatory, antiphlogistic,expectorant, febrifugethey are found to be particularly effective for their anti-inflammatory actions and they are have an even stronger expectorant action then ketones.

2.12 Extraction of Essential Oils Using Steam Distillation Method:

Essential oils can be extracted using a variety of methods, although some are not commonly used today. Nowadays, a reputable distiller will try to preserve the original qualities of the plant, but the final therapeutic result is often not formed until after the extraction process. During extraction, the

qualities of the oil change to give it more value - for example, chamazulene (characteristic of the pure blue colour of German Chamomile) is formed during the steam distillation process. Currently, the most popular method for extraction is steam distillation. Many old-time distillers favor this method for most oils, and say that none of the newer methods produces better quality oils. Steam distillation is a special type of distillation or a separation process for temperature sensitive materials like oils, resins, hydrocarbons, etc. which are insoluble in water and may decompose at their boiling point. The fundamental nature of steam distillation is that it enables a compound or mixture of compounds to be distilled at a temperature substantially below that of the boiling point(s) of the individual constituent(s). Essential oils contain substances with boiling points up to 200°C or higher temperatures. In the presence of steam or boiling water, however, these substances are volatilized at a temperature close to 100°C at atmospheric pressure. Fresh, or sometimes dried, botanical material is placed in the plant chamber of the still and the steam is allowing to pass through the herb material under pressure which softens the cells and allows the essential oil to escape in vapor form. The temperature of the steam must be high enough to vaporize the oil present, yet not so high that it destroys the plants or burns the essential oils. As they are released, the tiny droplets of essential oil evaporate and, together with the steam molecules, travel through a tube into the still's condensation chamber. As the steam cools, it condenses into water. The essential oil forms a film on the surface of the water. To separate the essential oil from the water, the film is then decanted or skimmed off the top. The remaining water, a byproduct of distillation, is called floral water, distillate, or hydrosol. It retains many of the therapeutic properties of the plant, making it valuable in skin care for facial mists and toners. In certain situations, floral water may be preferable to be pure essential oil, such as when treating a sensitive individual or a child, or when a more diluted treatment

is required. Rose hydrosol, for example, is commonly used for its mild antiseptic and soothing properties, as well as its pleasing floral aroma.

Essential oil isolated by steam distillation are different in composition to those naturally occurring in the oil bearing glands of plants, since the steam distillation conditions cause chemical reactions to occur which result in the formation of certain artificial chemicals, called artifacts. Some of these are considered beneficial e.g. the formation of chamazulene during the steam distillation of Chamomile oil; whilst others may not be e.g. the hydrolysis of linalyl acetate during the distillation of clary sage. Few, if any, essential oils are unscathed by the thermal conditions of steam distillation, but some distillation techniques can, in certain instances, be a measure less damaging than others (e.g. hydro diffusion – a sort of inverted steam distillation where steam is introduced at the top of the vegetable material-packed container, and oil and condensate issue from the bottom – can produce oils with higher ester contents i.e. less thermally induced hydrolysis).

A number of factors determine the final quality of a steam distilled essential oil. Aside from the plant material itself, most important are time, temperature and pressure, and the quality of the distillation equipment. Essential oils are very complex products. Each is made up of many, sometimes hundreds, of distinct molecules which come together to form the oil's aroma and therapeutic properties. Some of these molecules are fairly delicate structures which can be altered or destroyed by adverse environmental conditions. So, much like a fine meal is more flavorful when made with patience, most oils benefit from a long, slow 'cooking' process. It is possible that longer distillation times may give more complete oil. It is also possible however, that longer distillation time may lead to the accumulation of more artifacts than normal. This may have a curious effect of appearing to improving the odour, as sometimes when materials that have a larger number of components are sniffed, the perception is often of

slightly increased sophistication, added fullness and character, and possibly, and extra pleasantness.

Advantage of steam distillation is that it is a relatively cheap process to operate at a basic level, and the properties of oils produced by this method are well known. Newer methodology, such as sub critical water extraction, may well eventually replace steam distillation the, but so far even contenders such as carbon dioxide extraction - although establishing a firm market niche - have not really threatened to take over as the major preparative technique.

2.13 Uses of Essential Oils

Essential oils are products of the secondary metabolism of plants, and generally are fragrant volatile materials consisting of complex mixtures of mono- and sesqui-terpene hydrocarbons, and oxygenated materials biogenically derived from them hence essential oils are used in flavourings, perfumes, in Aromatherapy, as insect & animal repellents, in pharmaceutical preparations, as anti-microbial agents and in many other ways

2.14 Peel oil

The quality and quantity of citrus peel essential oils depend on many factors, such as the nature of the fruit itself, provenance, genotype, soil type and climate but also on the extraction process (Dugo *et al*., 2000). The oil content of citrus peels ranges between 0.5 and 5.0 % (w/v). Essential oils extracted from citrus peel are very complex matrices containing numerous compounds of different chemical classes. These compounds are generally divided in two fractions: the volatile fraction, which is the most representative and ranges between 85 and 99% in the different cold-pressed citrus oils, and the non-volatile residue, containing fatty acids, sterols, carotenoids, waxes, coumarins, and polymethoxylated flavonoids (2-6% of the oil), which ranges between 1 and 15% (Dugo *et al*.,2000). The volatile constituents are a mixture of monoterpene (limonene) and sesquiterpene hydrocarbons and their oxygenated derivatives

including aldehydes (citral), ketones, acids, alcohols (linalool) and esters (Borgmann *et al*., 2004; Flamini *et al*., 2007).

2.15 Properties of oil

2.15.1 Physical properties

2.15.1.1 Density

A part from determining whether or not an oil will float, its density can often give a general indication of other properties of the oil. Oils with low densities tend to have low viscosities and contain a high proportion of volatile components. (Catherine, 1934) The density of crude oils is often expressed as API gravity

Where:

API = (141.5 / s.g) – 131.5

Where s.g = specific gravity, density relative to pure water.

API = American institute petroleum.

API values range from below 10 to over 40 but it should be appreciated that high API values relate to low density oils and vice versa.

2.15.1.2 Viscosity

The viscosity of oil is its resistance to flow through a capillary tube.

Since viscosity involves the size and the shape of the macro molecular, it was considered as the one of the most important analytical and commercial parameter. The viscosity of a solution may have a complicated variation with composition due to possibility of hydrogen bonding among the solute and solvent molecules more hydrogen groups make high viscosity, because a network of hydrogen.

Bonds are formed between the molecules. High viscosity oils flow difficulty while oils with low viscosity are highly mobile and spread quickly. Viscosity decreases as temperature increase (Beancraff, 1932).

2.15.1.3 Refractive index

The refractive index (n) of a substance with reference to air is the ratio of the sine of the angle of incidence to the sine of the angle of refraction of a beam of light passing from air into the substance. It varies with the wavelength of the light used in its measurement. Refractive indices (nD20), are stated in terms of the wavelength of the sodium D-line (589.3 nm) at a temperature of 19.5C^{o} to 20.5C^{o} unless otherwise specified.

The index of refraction is related to the unsaturation of fatty acids, being altered besides, by the presence of abnormal or unusual acids, in which the presence of the hydroxyl group raises the refractive index.

2.15.2 Chemical properties: (Backette and Stenlke, 2002)

2.15.2.1 Acid value

Acid value is defined as the number of mgs of potassium hydroxide required to neutralize the free acid in one gram of substance. The acid value is used to eliminate low grade and rancid oils which tend to have higher acid value.

2.15.2.2 Saponification value

The average length of the chain of the fatty acids incorporated into a fat or an oil is expressed by the saponification number, which is defined as the number of mg of potassium hydrolysis required to neutralize the fatty acids resulting from the complete hydrolysis of one gram of substance. The saponification value is a measure of both free and combined acids. All edible oils have saponification value lying between 188 –196. The saponification value is a measure of the equivalent weight of the acids presents, and is therefore useful as an indication of purity. Adulteration with mineral oils would be shown by low saponification values whereas rancidity which leads to the formation of low molecular weight acids would be indicated by an abnormally high

saponification values. The acid value of most edible oil is small relative to the saponification value.

2.15.2.3 Aster value

Ester value is defined as the number of mg potassium hydroxide required to neutralize the acids resulting from the complete hydrolysis of one gram of materials. Ester value is a measure of the combined acids present in the substance.

2.15.2.4 Iodine value

The degree of unsaturation of a fat is described by the iodine number, which is defined as the weight of iodine absorbed by 100 parts by weight of the substance. It is a measure of the unsaturated compounds present in the substance, and is based upon the addition of halogen cross a carbon –carbon double bond. Most edible oils have iodine values in the range 87 – 62.

A quantitative measurement of the unsaturation present is obtained, provided that, certain experimental conditions are complied with, since there is a tendency with both reagents for substitution reaction as well as addition to take place.

2.16 Previous Studies on essential oil of Citrus Limon peel

Yassen (2015) in Sudan Studied some properties of lemon peel oil in comparative study between three types of citrus. He reported that refractive index (1.48), density (0.86), acid value (1.79), saponification value (13.5) and peroxide value (13.67). He identified 12 compounds in lemon peel oil obtained by gas chromatography-mass spectrometry, also the major components were found D-limonene (64%), 2-cyclohexen-1-ol (6.21%) and β-pinene (3.82%) respectively.

In deferent region of the world number of studies from C. Limon were reported; Marie-Laure et al (2002) identified 55 compounds in lemon peel oil obtained by gas chromatography (GC), GC/mass spectrometry (GC-MS) and ^{13}C NMR with

accounted (96.1-99.9%) of the total amount of the oil. Peels oil consisted almost exclusively of hydrocarbons, the olefin fraction being much higher than oxygenated one (84.4-99.2 vs 0.4-13.3%). Limonene was always the main constituent (38.1-95.8%) of all oils. β-Pinene (0.1-15.8%), γ-terpinnene (trace-18.0%) and Linalool/linalyl acetate (up to 23.3 and 31.2%, respectively) were present in appreciable amounts. Among other monoterpenes, α-pinene, sabinene, myrecene, β-phellandrene, p-cymene, neral, genial and neryl and geranyl acetate ere present in almost all sample at appreciable levels.Afew olefinic sesquiterpenes were also present in low amounts, namely, trans-α-bergamotene. (E)-caryophyllene, germacrene D and β-bisabolene.

L.Kamaliroosta *et al* (2015) identified 55 compounds in lemon peel oil obtained by Clevenger apparatus and characterization them by gas chromatography-mass spectrometry. The results of this study were similar and in agreement to the result obtained by other researchers.

Shalu *et al* (2015) studied the antimicrobial activity of citrus Limon (lemon) peel oil on selected food borne pathogens, Nada and Zainab (2013) showed the antimicrobial activity of different aqueous lemon extracts, Marti *et al* (2011) studied antimicrobial activity of lemon (citrus lemon L.) peel extract.

2.17 Storage condition of peel oil

One of the most important reactions involved in chemical changes in citrus peel oils is certainly the oxidation reaction, due to the high content of terpenes (Usai *et al*., 1992). Usually, quality deterioration in oils may occur under autoxidation, photo-oxidation, lipoxygenase-assisted oxidation, or thermal oxidation, all of which should be controlled in order to protect the oils from deterioration and off-flavor development (Shadi and Nahrung 2000). To maintain the original quality of citrus oils, undue exposure to air and contact with metals such as iron and copper, which act as pro-oxidants, should be avoided during processing and subsequent storage (Swishre *et al*., 1977). In some cases, citrus peel oils are stored refrigerated (0 – 5 ^{0}C) under an inert gas

(Njoroge *et al*., 2003). Meanwhile, the addition of antioxidants may help retard or control oxidation of citrus oils. Citrus peel oils are themselves very good antioxidants capable of inhibiting free radical-mediated reactions (Choi *et al*., 2000). As reported by Song et al. (Song *et al*.,2001), abundant tocopherols were found in citrus peel oils, yet there was little correlation between tocopherol content and antioxidative activity in the oils, suggesting that the composition of terpenes present might be a major determinant of the antioxidative status of citrus peel oils. The compounds b-pinene, myrcene, a-terpinene, and g-terpinene were identified to have higher or similar antioxidative activities compared with that of d-tocopherol. Encapsulation is a technique frequently used in the storage of citrus peel oils, which isolates the oils from the atmospheric oxygen, moisture, temperature, and light, and hence minimizes the oxidation of oil and reduces the release of volatile flavor compounds (Edris *et al*., 2001).

2.18 Applications of citrus peel oil

The applications of citrus oils are versatile and in many domains. As a result of their freshness, lightness, and fine fruity aroma, citrus peel oils and essences are widely used in the food and beverage industries as well as in some nonfood applications (Swisher *et al*., 1977). The applications of cold-pressed peel oils in food and beverage are mainly in the soft drinks, sherbet, confectionery, bakery, and household extracts (Swisher *et al*., 1977). In addition, they can act as reducing agents of peroxidase activity in leafy vegetables and antioxidants for edible oils, such as olive oil, to improve their sensory properties (Charai *et al*., 1999; Ponce *et al*.,2004). Moreover, they are effective inhibitors for the formation of N-nitrosodimethylamine (NDMA), a known carcinogen that may occur during production and storage of food (Sawamura *et al*., 2002). Citrus peel oils are also added as flavoring agents to pharmaceutical and drugs as well as herbal medicines in order to mask their unpleasant tastes (Lota *et al*., 2002). Distilled peel oils, different from cold-

pressed oils, have found their place in the perfumery and cosmetic industries as well as in the manufacturing of soap and paper (Swisher *et al*., 1977).

Citrus peel oils may also be used for their antioxidative, antitumor, and radicalscavenging activities. The radical-scavenging ability of citrus peel oil may help prevent free radical-induced and various chronic diseases (Choi *et al*., 2000; Calabrese *et al*., 1999; Clabrese *et al*., 1999). Monoterpenes from volatile components and polymethoxylated flavones from nonvolatile residues have been reported to be effective inhibitors of tumor cell growth, implicating that citrus peel oils may be good cancer preventive food additives (Chen *et al*., 1997; Takahashi et al., 1999). Furthermore, citrus peel oils are useful to alleviate pain from burnt skin (Brown *et al*., 1999). Demonstrating anxiolytic and sedative effect, they could also be used in primary medical care against insomnia, anxiety, and epilepsy (Carvalho-Freitas *et al*., (2002). The insecticidal property and antimicrobial activity of citrus peel oils have been reported. The oil can repel moth, mosquito, cockroach, domestica, and housefly (Su *et al*., 1972; Ezeonu *et al*., 2001). It also inhibits the growth of microbes such as fungi and salmonellae, with monoterpenes being the major compounds that account for pathogen fungi inhibition (Vargas *et al*., 2000; Coccioni *et al*., 1998;Parish *et al*., 2003).

CHAPTER THREE

3 MATERIALS AND METHODS

3.1 Materials

3.1.1 Plant Materials

Citrus Limon fruits were purchased from the local market, the fruits collected in rainy season in August in the year 2016. The fruits were identified by the botanist Babeker siddig, University of Medical Sciences and Technology, where a voucher specimen No. (85439) was deposited.

3.1.2 Chemicals

Acetic acid, glacial acetic acid, carbon tetrachloride, diethyl ether and hydrochloric acid were obtained from LOBA Chemi, India. Potassium hydroxide, potassium iodide and sodium thiosulphate all (GPR) were obtained from BDH, England. Ethanol, chloroform and sodium carbonate anhydrous all (GPR) were obtained from Scharulu, Spania. Iodine (GPR) was obtained from Egyption Company for chemical, Egypt

3.1.3 Preparation of chemical reagents

i- Potassium hydroxide 0.1 N: prepared by dissolving KOH 5.61g in 1000 ml distilled water.

ii- Potassium hydroxide 0.5 N: prepared by dissolving 14.02 g KOH in 500 ml distilled water.

iii- Ethanolic potassium hydroxide 0.5 N: prepared by dissolving 7.01 g KOH in 250 ml 95% ethanol.

vi- Sodium thiosulphate 0.1 N: prepared by dissolving 7.9 g $Na_2S_2O_3$ in 1000 ml distilled water.

v- Wijs Solution:

Wije solution was prepared by dissolving 12.6 g iodine in 100 ml acetic acid. Dry chlorine was pass through it until the colour of iodine disappeared.

iv- Starch prepared by dissolving 2 g of starch powder in distilled water, few drops of chloroform was added for protection.

iiv- Phenolphthalein indicator (0.1%) prepared by dissolving 1g of phenolphthalein poder in 100 ml ethanol 95%.

3.2 Methods

3.2.1 Preparation of plant material

Lemon peels were obtained by riding the fruits of Limon were dried at room temperature for 7 days after that it was cut into small pieces to enhance the extraction.

3.2.2 Extraction procedure of essential oil

The dried fruit Peels (3000 g) of *Citrus Limon* were extracted by hydro distillation using Clevenger apparatus. The peels are fully submerged in around-bottomed flask, equipped with a condenser and boiled, using a heater, to produce vapors which condensed yielding a two phase of oil and water, the water returned to the round-bottomed flask and the oil was separated. Extraction was carried out at the boiling temperature of the water about 4 hours. The separated volatile oil was dried over anhydrous sodium sulphate, the volume was measured, and the % yield was calculated. The volatile oil was kept in a well closed vial at 5^{o}C for further analysis.

3.3 Determination of Refractive index

The refractive index of the oil was determined using refractometer.

The sample chamber containing the lens was opened and cleaned with acetone then plugged to source of light.

The equipment was calibrated with a drop of water, after which a drop of the oil sample was added into the sample chamber and closed. The adjustment

knob was turned crossed the cross bar then reading were taken. The reading was taken at 40^{o}C.

Temperature correction R = R' + K (T' - T)

Where:

R = the reading of the refractometer reduced to specified temperature, T ^{O}C

R' = the reading at T' ^{o}C

K = constant, 0·000 385 for oils

T' = the temperature at which the reading R' is taken;

T = the specified temperature (.generally 40'0°0).

3.4 Determination of the color

Color was measured with Lovibond Tintometer Type D, (The Tintometer Ltd) Salisbury, England.

The glass cell was cleaned and allowed to dry. The dry cell was filled with the oil sample, then the cell was placed in position in the tintometer. The color was matched with sliding red and yellow colors. The color of the oil reported in terms of lovibond unit as follows:

Colour reading in cell $= (a\,Y + 5bR)$

Where

a = the sum total of the various yellow (Y) slides used, and

b = the sum total of the various red (R) slides used.

3.5 Determination of viscosity

Capillary Tube Viscometer Test Method

The method of determination viscosity (kinematic viscosity) utilized the capillary tube viscometer.

The oil was placed into a glass capillary U-tube and the sample was drawn through the tube using suction it reached the start position indicated on the tube side. The suction was then released, allowing the sample to flow back through the tube under gravity. The narrow capillary section of the tube controls the oils flow rate.

Once the oil meniscus touched the highest line time was started and continued until the oil meniscus touched the lower line.

Time of distilled water was reported under the same condition

$$\text{Viscosity} = \frac{\text{time of oil}}{\text{time of distilled water}}$$``

3.6 Determination of density

The density of oil was determined using pycnometer and sensitive balance. The pycnometer was cleaned with ethanol and dried in an oven. The dry pycnometer was filled with water and water level was adjusted to proper point on pycnometer; the pycnometer was wiped dry with towel and weighted. After that the pycnometer was emptied and dried in an oven, and then the dry pycnometer was filled with the oil sample in such amanner to prevent entrapment of air bubbles. Carefully any oil has come out of the capillary was wiped off, after that it was weighted. Both weights were carried out in the same temperature.

$$\text{Density} = \frac{\text{Mass}}{\text{Volume}}$$

$$\text{Density of water} = \frac{\text{weight of water}}{\text{Volume of wate}}$$

$$\text{Density of Oil} = \frac{\text{weight of oil}}{\text{weight of water}} \times \text{density of water}$$

3.7 Determination of acid value

One gram of the oil was weighted accurately in 250 ml conical flask. 25 ml diethyl ether was mixed with 25 ml 95% ethanol and 1 ml of phenolphthalein solution (1.0% in 95% ethanol) the mixture was neutralized by titration with a few drops of 0.1 N aqueous potassium hydroxide. This solution introduced in to the flask which contained the sample and shaken well to dissolve the fatty acid, which are present in the oil the mixture was cooled to room temperature and titrated with 0.1 N aqueous potassium hydroxide. The flask was continuously shaken during the titration until the pink color of the indicator persist for 15 seconds. The above process was repeated three times.

$$RCOOH + KOH \rightarrow RCOOK + H_2O$$

5.61 g KOH = 0.1 N

56.1 g KOH =1.0 N

$$\text{Acid value} = \frac{\text{Burette reading} \times \text{factor of alkali} \times 5.61}{\text{Weight of the sample in g}}$$

3.8 Determination of saponification value

One gram of lemon peels oil was weighted accurately in small glass sample tube. The tube and the sample were introduced in to 250 ml conical

flask. 25 ml of ethanolic potassium hydroxide 0.5 N was pipetted into the flask. A reflux condenser was fitted, and the flask was immersed in a boiled water-- bath for one hour. The water—bath was then removed and the condenser was washed-- down with 5 ml 97% ethanol. 1 ml of phenolphthalein solution was added to the flask. The condenser was removed, and a beaker placed over the neck of the flask and cooled under a tap. When it was quite cool, the excess of potassium hydroxide was titrated with 0.5 N hydrochloric acid until the pink color of the phenolphthalein disappeared. A blank determination was carried out simultaneously. The process was repeated three times.

$$\text{The saponification value} = \frac{(b-a)\times \text{factor} \times 28.05}{\text{sample weight in g}}$$

Where:

b = burette reading for blank

a = burette reading for the sample

The remain solution after the titration of the saponification value was transferred and added 10ml of hydrochloric acid into separator funnel, washed by hydrochloric acid and shaken. The solution extracted three time with 50 ml quantities of diethyl ether. Each ether extract poured into weighed flask ($W_{1)}$, the solvent evaporated off, and the flask weight again (W_2).

unsaponifiable matter = $W_2 - W_1$

3.9 Determination of ester value

One gram of lemon peels oil sample weighted accurately in a glass sample tube. The tube with the sample was transferred to 250 ml conical flask, and 5 ml 95% ethanol (previously boiled, coded and neutralized to phenolphthalein) was added. The free acid in the solution were neutralized by titration with 0.1N

ethanolic potassium hydroxide until just pink color of phenolphthalein appear. To the solution, 20ml off ethanolic potassium hydroxide 0.5N was added, and the flask was immersed in a boiling water–bath for an hour with refluxing. After cooling, 20ml of water was added, and then solution was back titrated for the excess alkali with 0.5N hydrochloric acid, added 0.2ml of phenolphthalein solution further. A blank determination was carried out under the same condition. The process was repeated three times.

$$\text{Ester value} = \frac{\text{m} \times \text{factor of acid} \times 28.05}{\text{W}}$$

Where:

W=weight of the sample in g

M=different in burette reading for sample and blank determination

3.10 Determination of iodine value

One gram of lemon peels oil was weighted accurately in 250 ml conical flask. 20 ml carbon tetrachloride was added to the flask with the sample to dissolve the oil. 25 ml Wijs solution was pipette and inserted into the flask which contain the mixture of the sample and carbon tetrachloride. The flask with content was stored in the dark for 30 minutes at a temperature bellow 20 C. After 30 minutes 20 ml of aqueous potassium iodide (10%) was added to the mixture in the flask. The mixture was titrated with 0.1 N sodium thiosulphate with shaking vigorously during the titration until the yellow colour has almost disappeared. 2ml of starch mucilage as indicator was added, and back titration with sodium thiosulphate until the blue colour has just disappeared. Blank determination wae carried out in the same conditions.

$$\text{Iodine value} = \frac{(B-S) \times N \times 12.69}{Sample\ weight\ in\ g}$$

Where:

B = burette reading for blank determination

S = burette reading for the sample

N = normality of the sodium thiosulphate

3.11 Gas chromatography-mass spectrometry of the *citrus Limon* peels oil

GC-MS was carried out on sample of oil used GC.MS QP2010 Ultra instrument, operating with following parameter:

Column: Rtx-5MS Diameter 0.25mm, Thickness 0.25µ, length 30m, Carrier gas: Helium, column oven temp: 50.0^{o}C, injection temp: 300.00 ^{o}C, injection mode: -split, flow control mode: pressure, pressure:100.0kpa, total flow: 50.0ml/min, column flow: 1.69ml/min.

Oven temperature program: from 50^{o}C to 180^{o}C; rate: 7 c/m and from 180C^{o} to 300 C^{o} by rate 10 c/m.

[GC Program]

Ion Source Temp: 200.00^{o}C.

Interface Temp: 250.00^{o}C.

[MS Table]

Start m/z: 40.00

End m/z: 500.00

Preparation of the sample: 10µ of the essential oil was diluted by 1 ml of ethyl alcohol.

Injected sample: (1 µl) of oil solution in ethyl alcohol was injected.

The compounds were identified by the GC-MS intensity of retention time (RT) and by comparison with those present in NIST11S.LIB. The results were expressed as the relative percentage of each individual compound present in sample given by the corresponding RT.

3.12 Antimicrobial activity

3.12.1 Preparation of crude

Series decreasing concentration of the crude (100, 50, 25, 12.5, 6.25 mg/ml) were employed.

3.12.2 Preparation of standard test organism

One ml aliquot of 24 hours broth culture of test organisms (Echerichia coli, Staphylocous aureus, Bacillus subtile , Pseudomonas aeruginosa ,Candidealbacans) were aseptically distributed onto nutrient agar slopes and incubated at 37^{o}C for 24 hours. The organism growth was harvested and washed off with sterile normal saline to produce a suspension containing about $10^{8} – 10^{6}$ colony formimg units per ml. The suspension was stored in the refrigerator at 4 ^{O}C till used.

3.12.3 Testing for antimicrobial activity

To determine the activity of *Citrus Limon* peels oil against the five standard organism; Echerichia coli, Staphylocous aureus, Bacillus subtile, Pseudomonas aeruginosa, Candide albancans, the cup-plate agar diffusion method was adopted with some minor modifications. (2ml) of standard bacteria and funglal stock suspension were mixed with 200ml of sterile molten nutrient agar which was maintained at 45^{o}C.

(20 ml) Aliquots of incubated agar were distribution into sterile petri-dishes. The agar was left to settle and each plate was cut using a sterile corkborer (No.4) and agar disc removed. Alternated cups were filled with 0.1ml sample of the crude extract using adjustable pipette, and allowed to diffuse at room temperature. The plates were then incubated in the upright position at 37^{o}C for 18 hours. These tests were carried out for each of the tested organisms. After incubation, the diameter of the resultant growth inhibition zones were measured, and averaged.

CHAPTER FOUR

RESULTS AND DISCUSSITON

Extraction of essential oil

The essential oil of the peels of *citrus Limon*, a medicinal plant which is widely used in the traditional medicine of the Sudan, was extracted by the method described in section (2.2.2). The method used for extraction is hydrodistillation, so the resulted oil is free of solvent residue and can be safely used in medicine and as a food additive. The quantity of the plant used in this experiment is 3000g of the dry peels and 18 ml of the neat oil was obtained after drying on anhydrous sodium sulphate. The yield % was calculated as follows:

$$\text{Yield } \% = \frac{18 \times 100}{3000} = 0.6\%$$

The yield is 0.6% on volume to weighted basis.

The oil which was extracted from *Citrus Limon* peels was subjected to different physical and chemical test in order to evaluate some of its properties.

Physicochemical properties of *citrus Limon* peels oil

Table 4.1 Physicochemical properties of *citrus Limon* peels oil

Determination	**peel oil**
Color	Y= 22±0.3 R=0.367±0.03
State	Liquid
Density (30^{o}C) (g/cm^{3})	0.918±0.001
Viscosity (mpa.s)	1.462±0.001
Refractive index	1.462±0.001
Acid value (mg of KOH/goil)	2.244±0.1
Ester value (mg/g)	70.583±0.1
Iodine value (g of I/100g of oil)	97.583±0.1
Peroxide value (mgO_2/g oil)	1.493±0.2
Saponification value (mg of KOH/g oil)	86.25±0.2
Unsaponifiable matter	0.673±0.2
Ratio value	31.627

Table 1-3, Shows the results of the physicochemical analysis of the oil of *Citrus Limon* peel was visually pale yellow in colour, liquid at room temperature (30 ^{0}C) and has density of (0.918±0.001) g/cm^{3} which is higher than the value (0.86) found by Yaseen (2015), the Refractive index (1.462±0.001) while approximately similar than the value (1.48) found by Yaseen (2015) and Viscosity (1.462±0.001) mpa.s.

The acid value of *Citrus Limon* peels oil is found to be about (2.244±0.1) mgKOH/g which is higher than the value (1.79) reported by Yaseen (2015), in

spite of that this value it is not high that mines the oil have low rancidity. Since the acid value is used to determine the ability of any oil for resisting the rancidity or not (Johnson and lusus, 1983) , all studies reported before showed that, the acid value of any oil is proportional directly to the rancidity (increase of acid value make the rancidity increase and vice versa). But on the other hand (Backette and Stenlk 2002) reported that; some oils have high rancidity in spite of its low grade of acid value.

The saponification value was used to measure both free and combined acid as an indication of purity, and the low saponification value show that the oils are adulterated with mineral oils. Whereas rancidity which leads to formation of low molecular weight would be indicated by an abnormally high saponification values (Watterson and Butler. 1983). Some of studies showed that the relationship between saponification value and acid value of most edible oils is that, the latter is small relative to the former. The saponification value of *Citrus Limon* peels oil is (86.25). While higher than the value (13.5) found by Yaseen (2015). The unsaponifiable matter equal (0.673) this value indicates to same martial present in oil after saponification of oil me be hydrocarbons, higher alcohols and sterols.

The iodine value was used to study the saturation and unsaturation of compounds (Herout, 1971), which are present in the substance. The iodine value *Citrus Limon* peels was determined and its value (97.583). This value when compared with others results, especially with iodine value of not edible oil, this value is an indication that *Citrus Limon* peels oil is edible oil.

GC-MS Analysis of *citrus Limon* peels oil

GC-MS is a technique widely used for analysis of the essential oils. In this study the essential oil extracted from the dry peels of *citrus Limon* was analyzed by shimadzu, QP2010 Gas Chromatography-Mass Spectrometer with an ultra-detector under condition described in section 2.3. The resulted total ion chromatogram was shown in figure (3.1) by this technique 53 compounds were

identified. The identification of these compounds was obtained by comparing the MS fragmentation pattern of these unknown compounds with those of standard compounds from the library of the machine (see Appendix 2 and 3). The identified compounds were shown in Table 3.2 with their retention time (R_T) and % area calculated from the area under peak.

The total number of identified compounds is fifty three.

Lemon peel oil as well as most citrus fruits consists almost exclusively in the form of monoterpenes, sesquiterpenes, and other aliphatic hydrocarbons. Among these, monoterpenes were dominant. Limonene, a monoterpene often used as a functional index of ripeness, was the major component (30.57%), followed by b-pinene (18.96%), g-terpenene (8.09%), α-pinene (2.67%) and β-Myrecene. The compounds α-Thujene, β-Cimene, β-Trans-Ocimene, Sabinene and α-Fellandrene were present at lower levels. A few sesquiterpenes were also found in very small amounts but made appreciable contributions to flavor and odor; these included trans-α-bergamotene(2.83%), α-Caryophyllene (2.47%), α and β Bisabolene and Farnesene also (E)-β-Famesene. Although terpene hydrocarbons, especially monoterpenes, are the most abundant constituents of citrus peels oil, they serve only as a flavor carrier and contribute little to flavor on their own (Shen *et al*., 2002). These terpenoid hydrocarbons are usually removed by deterpenation in order to increase the concentration of flavor and fragrance compounds. Furthermore, unsaturated hydrocarbons (terpenes) are unsatable to heat and light, and may oxidize rapidly to produce undesirable off-flavor compounds that adversely affect the desirable aroma of products (Sato *et al*., 1995). Therefore, concentrated and deterpenated oils have become popular in the citrus oil market. Oxygenated compounds, mainly oxygenated terpenes, rather than terpene hydrocarbons, have been found to be responsible for the characteristic odor and flavor of citrus fruits, although they occur in relatively small amounts. When the hydrocarbon fraction is removed from the oil, the oxygenated fraction becomes more odorous due to a higher concentration (Tu *et*

al., 2002). Oxygenated fraction includes many simple aliphatic aldehydes, such as trans-citral(2.69%), beta-citral(1.69%), decanal(0.2%), and octenal(0.17%), also we found trace of perilla aldehyde and 3-cyclohexene-1-carboxaldehyde,2,4,6-trimethyl. Among alcohols, monoterpene alcohols such as linalool (4.5%), followed by L-terpinen-4-ol (2.33%) and a–terpeneol(2.02%), are most predominant.Lemonol and Nerol are also found in low levels. Among these, linalool is regarded as the most odor-active compounds in such citrus. Ketones, esters, oxides, and acids are less represented, but make appreciable contributions to flavor.

While 12 compounds in lemon peel oil obtained by gas chromatography-mass spectrometry identified by Yaseen (2015), also the major components were found D-limonene (64%), 2-cyclohexen-1-ol (6.21%) and β-pinene (3.82%) respectively.

Table 4.2 Retention time (R_T) and % area of the compounds identified in the essential oil of *Citrus Limon* peels. By GC-MS.

peak#	R. Time	Area	Area%	Name
1	4.733	698270	0.36	Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-
2	4.874	5118450	2.67	.alpha.Pinene
3	5.160	374795	0.20	Camphene
4	5.610	7232872	3.77	Bicyclo[3.1.1]hexane, 4-methtlene-1-(1-methylethyl)-
5	5.696	36410528	18.96	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-,(IS)-
6	5.899	2727693	1.42	.beta.-Myrcene
7	6.145	61513	0.03	Octanal
8	6.208	342359	0.18	.alpha.-Phellandrene
9	6.450	1604730	0.84	(+)-4-Carene
10	6.619	681311	0.35	P-Cymene
11	6.721	58696682	30.57	D-Limonene
12	6.782	661087	0.34	Eucalyptol
13	6.838	402630	0.21	Trans-.beta.-Ocimene
14	7.058	1524303	0.79	1,3,6-Octatriene, 3,7-dimethyl-, (Z)-
15	7.323	15531520	8.09	.gamma.-Terpinene
16	7.527	135790	0.07	Bicyclo[3.1.0]hexane-2-ol, 2-methyl-5-(1-methyiethyl)- ,(1.alpha.,2.beta.,5.alpha.)-
17	7.952	1741454	0.91	4-Carene(+)-
18	8.165	7772305	4.05	1,6-Octadien-3-0l, 3,7-dimethy-l
19	9.222	128111	0.07	Bicyclo[2.2.1]heptan-2-one,1,7,7,-

				trimethyl-, (IS)
20	9.295	332436	0.17	6-Octenal, 3,7-dımethyl-,(R)-
21	9.538	217359	0.11	3-Cyclohexene-1-carboxaldehyde, 2,4,6-trimethyl-
22	9.675	269823	0.14	Endo-borneol
23	9.896	4463938	2.33	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-
24	10.176	3882250	2.02	.alpha.-Terpıneol
25	10.319	174590	0.09	Estragole
26	10.394	415756	0.22	Decanal
27	10.911	511526	0.27	2,6-Octadıen-1-ol, 3,7-dımethyl-, (Z)-
28	11.188	3708006	1.93	2,6-Octadıenal, 3,7-dımethyl-, (Z)-
29	11.440	1685735	0.88	Geranıol
30	11.793	5158545	2.69	2,6-Octadienal, 3,7-dımethy-, (E)-
31	11.955	190404	0.10	1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)-
32	12.151	249732	0.13	Bornyl acetate
33	12.565	282228	0.15	2-Propenoıc acıd, 3-phenyl-, methyl ester
34	13.192	969514	0.50	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethyl)-, (3R-trans)-
35	13.631	647896	0.34	2,6-Octadıen-1-ol, 3,7-dımethyl-, acetate, (Z)-
36	14.006	1279823	0.67	Geranyl acetate
37	14.133	2530578	1.32	Cınnamaldehyde, (E)-
38	14.292	1010050	0.53	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(i-methylethenyl)-,[IS-(1.alpha.,2.beta.,4.beta.)]-
39	14.481	1461346	.076	Methyleugenol

40	14.718	214881	0.11	Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4methyl-3-pentyl)-
41	14.896	4737996	2.47	Caryophyllene
42	15.106	5427423	2.83	Trans-.alpha.-Bergamotene
43	15.422	250678	0.13	.beta.-Famesene-(E)-
44	15.552	592177	0.31	Humulene
45	16.062	786099	0.41	Bicyclo[2.2.1]heptanes, 2-cyclopropylidene-1,7,7-trimethyl-
46	16.331	46259	0.24	Cis-.alpha.-Bisabolene
47	16.386	1628324	0.85	.alpha.-Farnesene
48	16.458	3912194	2.04	.beta.-Bisabolene
49	16.653	732438	0.38	.gamma.-Muurolene
50	17.978	231117	0.12	Caryophyllene oxide
51	18.493	133834	0.07	Cubenol
52	18.918	1192294	0.62	.tau.-Cadinol
53	19.582	402236	0.21	Trans-Sesquisabinene hydrate
		191992158	100.00	

Peak# No as shown in figure 3.1

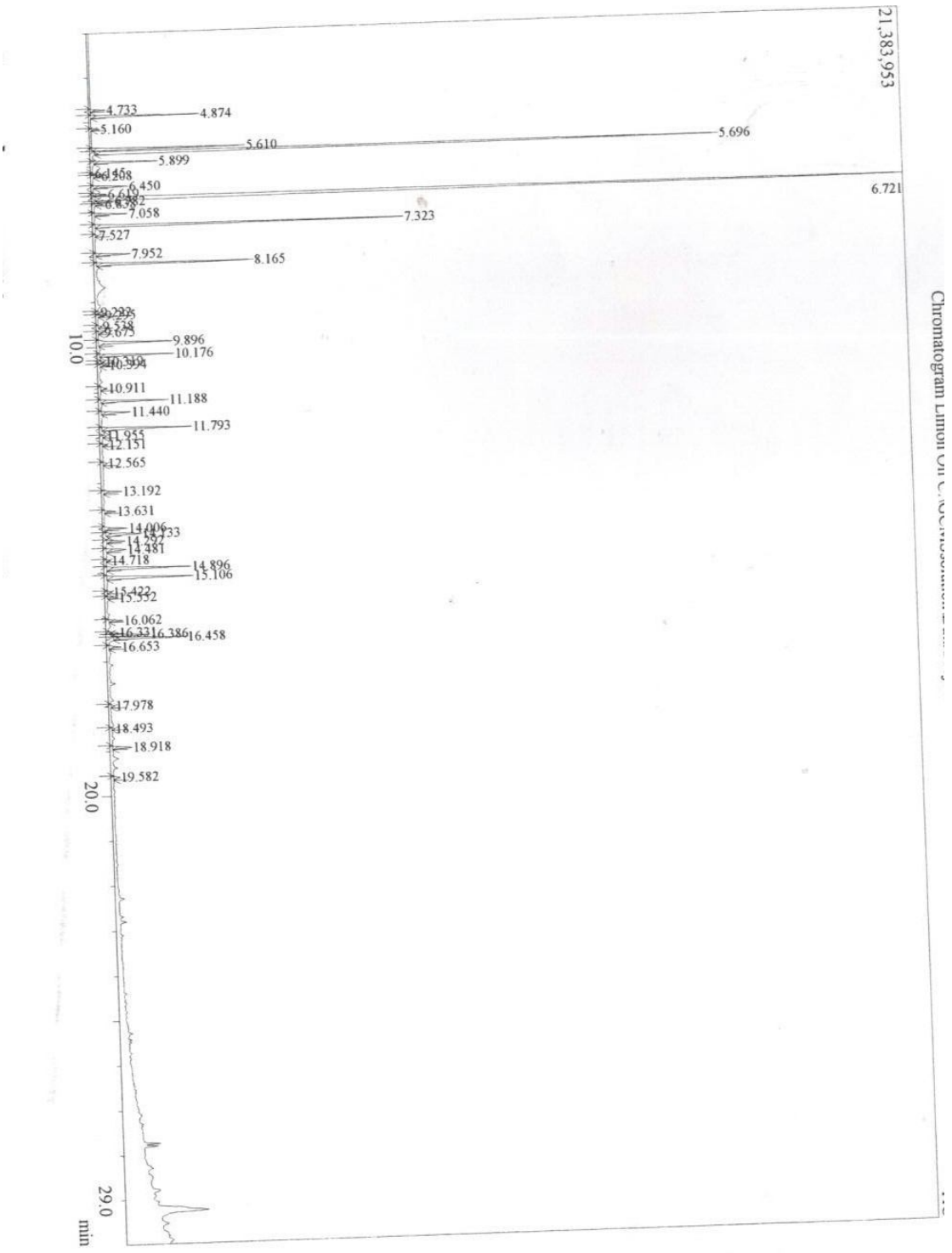

Figure 4.1 GC.MS total ion chromatogram of the essential oil of *Citrus Limon* peel

Antimicrobial activity

The crude product of *Citrus Limon* peels was tested for antimicrobial activity against fore bacterial strains and one fungi by method described in section (2.5). After the incubation the diameter of the resulted growth inhibition zones were measured, averaged and the results were summarized in table (3.3).

Table 4.3 Antimicrobial activity of *Citrus Limon* peels oil

organisms / Concentration (mg/ml)	Mean diameter Of Inhibitory Zone (mm)				
	E.coli	P.s	S.a	B.s	C.a
100	12	18	20	20	20
50	12	17	19	18	18
25	11	14	18	16	14
12.50	-	13	15	7	14
6.25	-	9	14	-	-

E coli: Escherichia coli (gram -ve bacterial).

P s: Pseudomonas aeruginosa (gram –ve bacterial).

S a: Staphylococcus aureus (gram +ve bacterial).

B s: Bacillus subtilis (gram +ve bacterial).

C a: Candida albicans (fungus)

- = No inhibition zone * = Average of two replicates

- 9mm = inactive

9 – 12mm = partially active

13 – 18mm = active

19mm – very active

The oil of the peels of *citrus Limon* was subjected to antimicrobial activity. The oil was effective against Pseudomonas aeruginosa, Staphyocous aureus, Bacillus subtilis, Escherichia coli and Candida albiacans (see Appendix 4). In

highest concentration it was particularly effective toward gram +ve bacterial Staphylococcus aureus (inhabitation zone 20mm), Bacillus subtilis (inhibition zone 20mm) and Candida albacans fungi (inhabitation zone 20mm). And it was effective against Pseudomonas aeruginosa (inhibition zone 18mm), but it was partially active against Escherichia coli (inhibition zone 12mm).

Lemon peel oil showed inhibition against all the test organisms (Gram positive, Gram negative and fungus) at 100mg/ml, 50mg/ml and 25mg/ml with a maximum zone of inhibition against Candida albicans and minimum zone of inhibition against Escherichia coli. In 12.5mg/ml Escherichia coli don't show inhibiting zone, also at 6.25mg/ml beside two other organisms (Bacillus subtilis and Candida albicans) don't showed any inhibiting zone.

Lemon peel oil thus showed abroad activity against all the Gram positive, Gram negative and fungi used in the present study

The inhibitory activity of the essential oil may be a cumulative effect of D-limonene and some other unidentified components or flavonoids and phenolic compound present. Unal et al. also demonstrated the antifungal and inhibitory effect of D-limonene on a variety of yeast strains. For instance, flavonoids are known as antimicrobial agents and some phenolic compounds have been shown to inhibit the growth of Staphylococcus aureus (Cushnie and Lamb, 2005).

The reason for the different sensitivity of the Gram-negative bacteria compared to that of Gram-positive bacteria could be due to differences in their cell wall composition. Gram-positive bacteria contain an outer peptidoglycan layer, which acts as a permeability barrier, whereas Gram-negative bacteria have an outer phospholipid membrane (Samarakoon et al., 2012).

Conclusion and recommendation

The following points can be concluded and/or recommended according to the results of this work:

- The essential oil extracted from the dry peels of *citrus Limon*. Was pale yellow in color and possesses the characteristic of the citral. The yield 0.6% (v/w) is low when compared with other essential oil of other citrus.
- Physical and chemical properties of the extracted oil of the peels of *citrus Limon* prove the oil is edible for human consumption. Studies were recommended to evaluate the properties of this oil.
- The qualitative and quantitative determination of major and minor constituents of peel oil are done by GC-MS which are the techniques widely applied for analysis of oil and fat. We are able to identify 53 compounds, the main components are monoterpenes.
- After performing the antimicrobial activity by using cup-plate agar diffusion methods we found that *Citrus Limon* peel oil have activity against gram +ve and gram –ve bacteria also fungi. And can be further studied for developing herbal antibiotic.

Suggestion for further work

- Other methods of extraction, which can be effectively applied on wide area of industry.
- Further research to evaluate effect of *Citrus Limon* treatments on the anti-oxidant principle of extracted oil is recommended to explore their potential uses for pharmaceutical applications.
- To encourage the research of other possible part of lemon that contains appreciated percentage of oil, such as pulp, seed and juice.
- Isolation of nonvolatile residues in the oil.
- By- product at factory peel can be used as animal feed.

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APPENDICES

Appendix1

Lemon fruits

Lemon peels sample

Oil gland in lemon peels

Lemon peel oil

Appendix 2

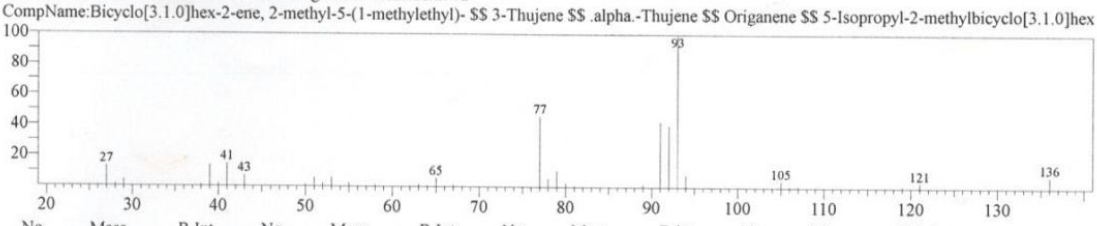
Compounds mass spectral information

Compound Information

Entry:9791 Library:NIST11.LIB

Formula:C10H16 CAS:2867-05-2 MolWeight:136 RetIndex:902

CompName:Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)- $$ 3-Thujene $$ .alpha.-Thujene $$ Origanene $$ 5-Isopropyl-2-methylbicyclo[3.1.0]hex



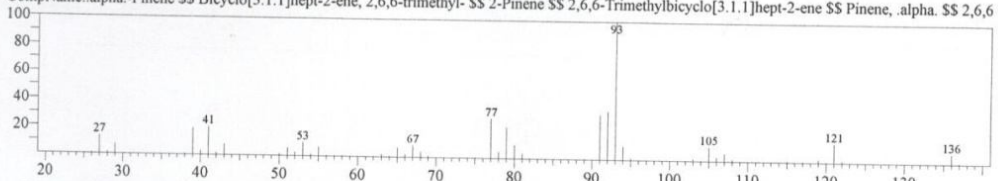
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.53	15	53.00	5.74	29	75.00	0.52	43	103.00	0.44
2	27.00	12.94	16	54.00	0.28	30	76.00	0.21	44	104.00	0.45
3	28.00	1.61	17	55.00	2.47	31	77.00	46.15	45	105.00	4.13
4	29.00	4.39	18	57.00	0.18	32	78.00	5.48	46	106.00	1.06
5	38.00	1.15	19	58.00	1.19	33	79.00	10.61	47	107.00	1.18
6	39.00	13.82	20	62.00	0.58	34	80.00	2.50	48	115.00	0.37
7	40.00	2.01	21	63.00	1.70	35	81.00	1.02	49	117.00	0.44
8	41.00	14.85	22	64.00	0.78	36	87.00	0.29	50	119.00	1.46
9	42.00	0.48	23	65.00	5.68	37	89.00	1.84	51	121.00	3.31
10	43.00	7.17	24	66.00	0.52	38	91.00	42.87	52	122.00	0.26
11	44.00	0.11	25	67.00	1.70	39	92.00	40.30	53	130.00	0.37
12	50.00	1.46	26	68.00	0.62	40	93.00	100.00	54	136.00	7.64
13	51.00	5.80	27	69.00	0.29	41	94.00	7.91	55	137.00	0.70
14	52.00	2.39	28	73.00	0.14	42	95.00	0.37			

Compound Information

Entry:6669 Library:NIST11S.LIB

Formula:C10H16 CAS:80-56-8 MolWeight:136 RetIndex:948

CompName:.alpha.-Pinene $$ Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- $$ 2-Pinene $$ 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene $$ Pinene, .alpha. $$ 2,6,6



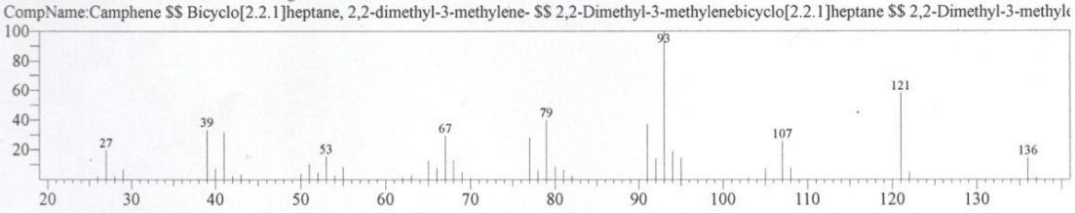
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.78	19	55.00	6.64	37	77.00	28.50	55	104.00	0.69
2	27.00	13.09	20	56.00	0.60	38	78.00	4.79	56	105.00	10.23
3	28.00	1.55	21	57.00	0.52	39	79.00	22.77	57	106.00	2.96
4	29.00	7.03	22	58.00	0.82	40	80.00	9.86	58	107.00	5.75
5	30.00	0.27	23	59.00	0.40	41	81.00	3.85	59	108.00	1.50
6	37.00	0.18	24	60.00	0.08	42	82.00	0.53	60	109.00	0.49
7	38.00	0.95	25	62.00	0.53	43	83.00	0.13	61	115.00	0.74
8	39.00	18.97	26	63.00	2.06	44	87.00	0.06	62	116.00	0.21
9	40.00	3.10	27	64.00	0.76	45	89.00	0.60	63	117.00	0.60
10	41.00	20.06	28	65.00	6.74	46	90.00	0.18	64	119.00	2.02
11	42.00	1.51	29	66.00	1.94	47	91.00	32.34	65	120.00	0.51
12	43.00	7.59	30	67.00	8.44	48	92.00	34.92	66	121.00	13.60
13	44.00	0.25	31	68.00	4.18	49	93.00	100.00	67	122.00	1.39
14	50.00	1.56	32	69.00	1.20	50	94.00	10.09	68	123.00	0.07
15	51.00	5.67	33	70.00	0.13	51	95.00	1.64	69	135.00	0.19
16	52.00	2.86	34	74.00	0.33	52	96.00	0.11	70	136.00	7.20
17	53.00	9.61	35	75.00	0.36	53	102.00	0.31	71	137.00	0.87
18	54.00	1.32	36	76.00	0.28	54	103.00	1.81			

Compound Information

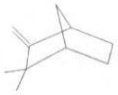
Entry:9817 Library:NIST11.LIB

Formula:C10H16 CAS:79-92-5 MolWeight:136 RetIndex:943

CompName:Camphene $$ Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- $$ 2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane $$ 2,2-Dimethyl-3-methyl



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	2.35	12	51.00	10.52	23	69.00	5.58	34	94.00	18.82
2	27.00	19.71	13	52.00	4.58	24	70.00	1.58	35	95.00	14.65
3	28.00	2.40	14	53.00	15.47	25	77.00	28.07	36	103.00	1.36
4	29.00	6.86	15	54.00	2.76	26	78.00	6.67	37	105.00	8.04
5	39.00	33.50	16	55.00	8.71	27	79.00	39.97	38	107.00	25.95
6	40.00	7.89	17	62.00	1.55	28	80.00	8.90	39	108.00	7.89
7	41.00	31.73	18	63.00	3.14	29	81.00	6.67	40	121.00	58.30
8	42.00	2.54	19	65.00	12.95	30	82.00	2.76	41	122.00	5.43
9	43.00	3.90	20	66.00	8.25	31	91.00	37.34	42	136.00	14.73
10	44.00	0.38	21	67.00	29.48	32	92.00	14.25	43	137.00	1.69
11	50.00	3.99	22	68.00	13.06	33	93.00	100.00	44	138.00	0.08

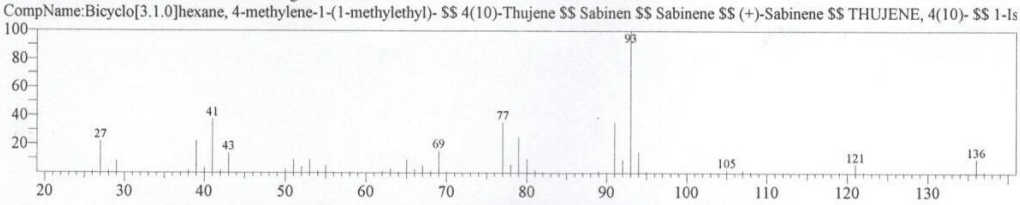


Compound Information

Entry:9781 Library:NIST11.LIB

Formula:C10H16 CAS:3387-41-5 MolWeight:136 RetIndex:897

CompName:Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- $$ 4(10)-Thujene $$ Sabinen $$ Sabinene $$ (+)-Sabinene $$ THUJENE, 4(10)- $$ 1-Is



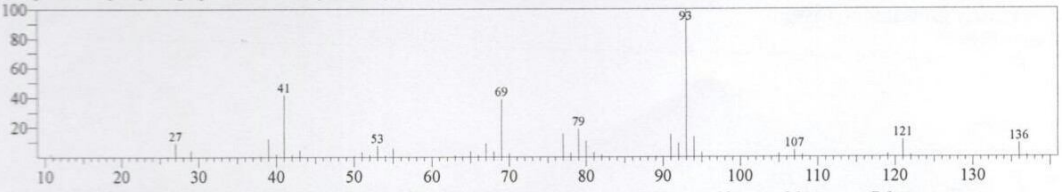
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	1.27	20	52.00	4.57	39	75.00	0.70	58	104.00	0.35
2	27.00	22.09	21	53.00	9.36	40	76.00	0.18	59	105.00	2.48
3	28.00	1.63	22	54.00	1.48	41	77.00	35.49	60	106.00	0.48
4	29.00	8.58	23	55.00	5.49	42	78.00	6.05	61	107.00	2.26
5	30.00	0.10	24	56.00	0.52	43	79.00	25.35	62	108.00	0.90
6	32.00	0.14	25	57.00	0.50	44	80.00	10.12	63	115.00	0.38
7	37.00	0.58	26	58.00	0.43	45	81.00	2.25	64	116.00	0.20
8	38.00	1.98	27	59.00	0.15	46	82.00	0.65	65	117.00	0.25
9	39.00	22.74	28	61.00	0.19	47	86.00	0.16	66	119.00	0.82
10	40.00	3.79	29	62.00	1.12	48	87.00	0.24	67	120.00	0.25
11	41.00	37.67	30	63.00	3.12	49	89.00	1.49	68	121.00	6.39
12	42.00	1.97	31	64.00	0.94	50	90.00	0.87	69	122.00	0.54
13	43.00	14.06	32	65.00	9.47	51	91.00	35.53	70	134.00	0.12
14	44.00	0.12	33	66.00	2.86	52	92.00	9.48	71	135.00	0.20
15	45.00	0.10	34	67.00	5.48	53	93.00	100.00	72	136.00	10.10
16	47.00	0.12	35	68.00	1.47	54	94.00	15.19	73	137.00	1.03
17	49.00	0.18	36	69.00	15.66	55	95.00	1.04			
18	50.00	2.67	37	70.00	0.84	56	102.00	0.19			
19	51.00	9.55	38	74.00	0.57	57	103.00	0.87			

Compound Information

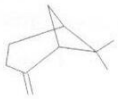
Entry:9776 Library:NIST11.LIB

Formula:C10H16 CAS:18172-67-3 MolWeight:136 RetIndex:943

CompName:Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)- $$ 2(10)-Pinene, (1S,5S)-(-)- $$ (-)-.beta.-Pinene $$ (-)-2(10)-Pinene $$ L-.beta.-Pinen



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.50	19	54.00	1.09	37	75.00	0.20	55	103.00	0.50
2	26.00	0.50	20	55.00	5.99	38	76.00	0.10	56	104.00	0.20
3	27.00	9.19	21	56.00	0.50	39	77.00	15.89	57	105.00	2.39
4	28.00	0.50	22	57.00	0.30	40	78.00	2.89	58	106.00	0.60
5	29.00	4.59	23	58.00	0.30	41	79.00	19.09	59	107.00	4.59
6	30.00	0.10	24	59.00	0.10	42	80.00	10.79	60	108.00	1.69
7	37.00	0.20	25	61.00	0.10	43	81.00	3.29	61	109.00	0.30
8	38.00	0.80	26	62.00	0.40	44	82.00	1.69	62	115.00	0.30
9	39.00	12.39	27	63.00	1.19	45	83.00	0.20	63	116.00	0.10
10	40.00	2.19	28	64.00	0.40	46	89.00	0.40	64	117.00	0.20
11	41.00	41.79	29	65.00	4.09	47	90.00	0.20	65	119.00	2.09
12	42.00	1.89	30	66.00	1.49	48	91.00	14.99	66	120.00	0.30
13	43.00	4.79	31	67.00	9.09	49	92.00	9.19	67	121.00	11.69
14	44.00	0.20	32	68.00	3.59	50	93.00	100.00	68	122.00	1.19
15	50.00	1.09	33	69.00	38.99	51	94.00	13.69	69	134.00	0.10
16	51.00	3.39	34	70.00	2.39	52	95.00	3.09	70	135.00	0.20
17	52.00	1.79	35	71.00	0.10	53	96.00	0.30	71	136.00	8.99
18	53.00	7.69	36	74.00	0.20	54	102.00	0.10	72	137.00	1.09

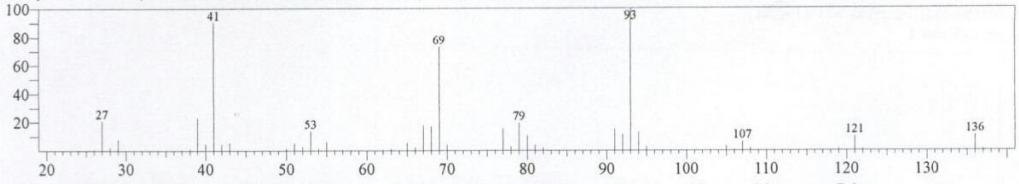


Compound Information

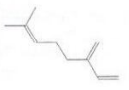
Entry:6636 Library:NIST11S.LIB

Formula:C10H16 CAS:123-35-3 MolWeight:136 RetIndex:958

CompName:.beta.-Myrcene $$ 1,6-Octadiene, 7-methyl-3-methylene- $$ Myrcene $$ 7-Methyl-3-methylene-1,6-octadiene $$ 7-Methyl-3-methyleneoctadie



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.91	21	54.00	1.69	41	76.00	0.13	61	105.00	3.25
2	27.00	20.89	22	55.00	6.46	42	77.00	15.40	62	106.00	0.82
3	28.00	2.30	23	56.00	0.55	43	78.00	2.73	63	107.00	6.43
4	29.00	7.91	24	57.00	0.14	44	79.00	19.41	64	108.00	1.74
5	30.00	0.14	25	58.00	0.31	45	80.00	10.55	65	109.00	0.35
6	32.00	0.32	26	59.00	0.13	46	81.00	4.22	66	110.00	0.07
7	37.00	0.24	27	61.00	0.11	47	82.00	2.16	67	115.00	0.34
8	38.00	1.17	28	62.00	0.39	48	83.00	0.24	68	116.00	0.09
9	39.00	22.96	29	63.00	1.44	49	84.00	0.07	69	117.00	0.37
10	40.00	4.72	30	64.00	0.33	50	89.00	0.44	70	119.00	1.27
11	41.00	90.62	31	65.00	5.38	51	90.00	0.20	71	120.00	0.29
12	42.00	4.64	32	66.00	2.40	52	91.00	15.22	72	121.00	10.08
13	43.00	5.36	33	67.00	17.73	53	92.00	11.54	73	122.00	1.12
14	44.00	0.11	34	68.00	17.04	54	93.00	100.00	74	123.00	0.17
15	47.00	0.06	35	69.00	73.22	55	94.00	12.95	75	133.00	0.14
16	49.00	0.05	36	70.00	4.50	56	95.00	2.95	76	134.00	0.21
17	50.00	1.70	37	71.00	0.20	57	96.00	0.31	77	135.00	0.26
18	51.00	5.14	38	73.00	0.04	58	102.00	0.10	78	136.00	10.88
19	52.00	2.69	39	74.00	0.13	59	103.00	0.64	79	137.00	1.27
20	53.00	13.72	40	75.00	0.31	60	104.00	0.23	80	138.00	0.16

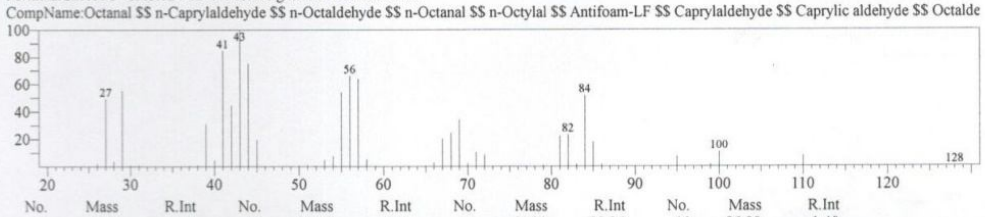


Compound Information

Entry:5153 Library:NIST11S.LIB

Formula:C8H16O CAS:124-13-0 MolWeight:128 RetIndex:1005

CompName:Octanal $$ n-Caprylaldehyde $$ n-Octaldehyde $$ n-Octanal $$ n-Octylal $$ Antifoam-LF $$ Caprylaldehyde $$ Caprylic aldehyde $$ Octalde



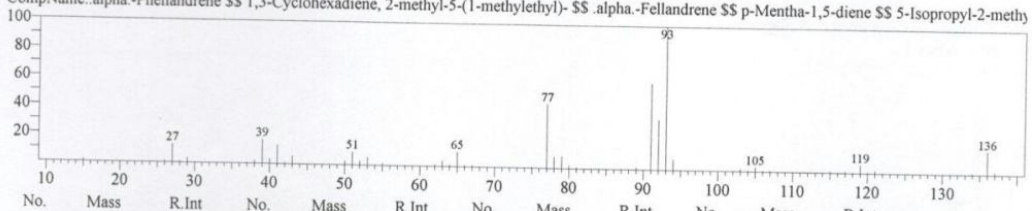
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	2.17	16	46.00	0.34	31	67.00	20.25	46	86.00	1.40
2	27.00	49.17	17	50.00	0.58	32	68.00	24.35	47	87.00	0.09
3	28.00	3.81	18	51.00	1.12	33	69.00	34.05	48	93.00	0.11
4	29.00	55.37	19	52.00	0.45	34	70.00	2.11	49	95.00	7.35
5	30.00	1.07	20	53.00	4.85	35	71.00	10.17	50	96.00	0.32
6	31.00	1.28	21	54.00	7.37	36	72.00	8.53	51	97.00	0.24
7	37.00	0.39	22	55.00	53.96	37	73.00	0.38	52	99.00	1.61
8	38.00	0.92	23	56.00	66.14	38	77.00	0.29	53	100.00	10.66
9	39.00	31.13	24	57.00	63.81	39	79.00	0.93	54	101.00	0.39
10	40.00	4.33	25	58.00	5.30	40	80.00	0.46	55	109.00	0.45
11	41.00	84.48	26	59.00	0.42	41	81.00	22.11	56	110.00	7.85
12	42.00	44.44	27	62.00	0.12	42	82.00	23.03	57	111.00	0.50
13	43.00	100.00	28	63.00	0.21	43	83.00	1.65	58	128.00	0.30
14	44.00	75.05	29	65.00	0.62	44	84.00	51.71			
15	45.00	19.44	30	66.00	2.62	45	85.00	17.91			

Compound Information

Entry:6660 Library:NIST11S.LIB

Formula:C10H16 CAS:99-83-2 MolWeight:136 RetIndex:969

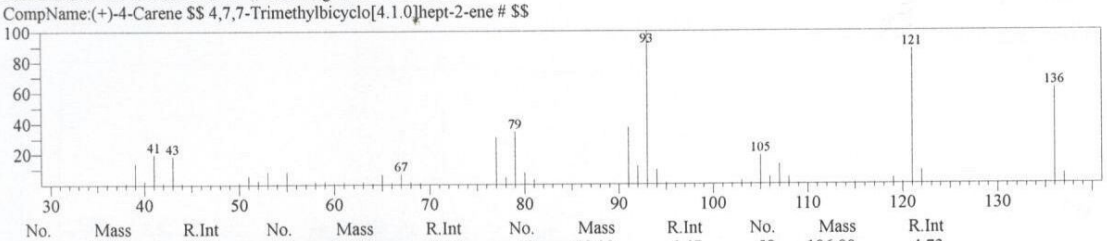
CompName:.alpha.-Phellandrene $$ 1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- $$ .alpha.-Fellandrene $$ p-Mentha-1,5-diene $$ 5-Isopropyl-2-methy



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	1.81	17	51.00	9.23	33	75.00	0.67	49	105.00	3.09
2	16.00	0.23	18	52.00	2.97	34	77.00	44.48	50	106.00	0.61
3	18.00	0.37	19	53.00	5.41	35	78.00	7.85	51	107.00	0.78
4	26.00	1.32	20	54.00	0.51	36	79.00	8.35	52	115.00	1.26
5	27.00	12.82	21	55.00	1.61	37	80.00	2.27	53	116.00	0.37
6	28.00	1.10	22	58.00	0.70	38	81.00	0.72	54	117.00	1.23
7	29.00	3.18	23	59.00	0.25	39	87.00	0.34	55	118.00	0.37
8	37.00	0.55	24	61.00	0.31	40	89.00	1.35	56	119.00	5.53
9	38.00	2.41	25	62.00	1.33	41	91.00	59.94	57	120.00	0.73
10	39.00	16.91	26	63.00	4.00	42	92.00	34.95	58	121.00	1.99
11	40.00	3.17	27	64.00	1.31	43	93.00	100.00	59	122.00	0.31
12	41.00	13.32	28	65.00	10.35	44	94.00	7.64	60	134.00	1.03
13	42.00	1.15	29	66.00	1.21	45	95.00	0.47	61	136.00	16.02
14	43.00	5.62	30	67.00	1.13	46	102.00	0.46	62	137.00	1.76
15	44.00	0.29	31	68.00	0.35	47	103.00	1.83			
16	50.00	2.73	32	74.00	0.44	48	104.00	0.89			

Compound Information

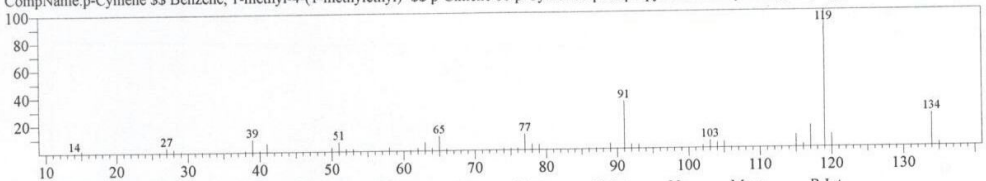
Entry:9827 Library:NIST11.LIB
Formula:C10H16 CAS:29050-33-7 MolWeight:136 RetIndex:919
CompName:(+)-4-Carene $$ 4,7,7-Trimethylbicyclo[4.1.0]hept-2-ene # $$



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	36.00	0.63	20	56.00	0.36	39	78.00	4.47	58	106.00	4.73
2	37.00	0.18	21	57.00	0.67	40	79.00	34.29	59	107.00	12.77
3	38.00	1.22	22	58.00	1.82	41	80.00	7.71	60	108.00	4.44
4	39.00	14.06	23	59.00	1.95	42	81.00	3.10	61	109.00	0.33
5	40.00	2.37	24	60.00	0.89	43	82.00	0.23	62	115.00	0.62
6	41.00	19.62	25	61.00	1.36	44	86.00	0.11	63	116.00	0.10
7	42.00	1.20	26	62.00	0.51	45	87.00	0.02	64	117.00	0.69
8	43.00	18.52	27	63.00	1.49	46	88.00	0.08	65	118.00	0.02
9	44.00	0.93	28	64.00	0.79	47	89.00	0.46	66	119.00	3.87
10	45.00	0.35	29	65.00	6.35	48	90.00	0.14	67	120.00	0.73
11	46.00	0.10	30	66.00	1.25	49	91.00	37.14	68	121.00	87.98
12	47.00	0.01	31	67.00	6.61	50	92.00	11.60	69	122.00	8.54
13	49.00	0.13	32	68.00	1.87	51	93.00	100.00	70	123.00	0.37
14	50.00	1.28	33	69.00	0.97	52	94.00	9.50	71	134.00	0.02
15	51.00	5.70	34	70.00	0.06	53	95.00	1.19	72	135.00	0.69
16	52.00	2.68	35	74.00	0.22	54	102.00	0.19	73	136.00	62.26
17	53.00	8.30	36	75.00	0.20	55	103.00	2.46	74	137.00	6.43
18	54.00	0.73	37	76.00	0.07	56	104.00	0.55	75	138.00	0.21
19	55.00	8.20	38	77.00	30.66	57	105.00	18.70			

Compound Information

Entry:6204 Library:NIST11S.LIB
Formula:C10H14 CAS:99-87-6 MolWeight:134 RetIndex:1042
CompName:p-Cymene $$ Benzene, 1-methyl-4-(1-methylethyl)- $$ p-Cimene $$ p-Cymol $$ p-Isopropyltoluene $$ p-Methylisopropylbenzene $$ Campho



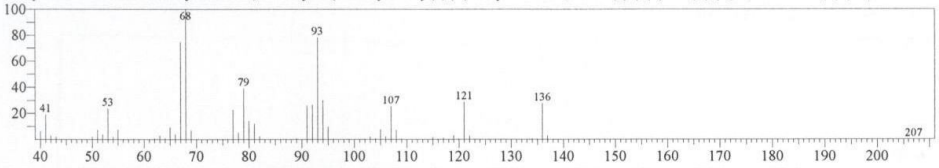
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	0.59	14	52.00	1.97	27	78.00	4.24	40	105.00	4.57
2	15.00	2.06	15	53.00	1.78	28	79.00	3.96	41	106.00	0.37
3	26.00	0.59	16	58.00	2.58	29	86.00	0.54	42	115.00	8.91
4	27.00	3.62	17	61.00	0.45	30	87.00	0.67	43	116.00	2.47
5	28.00	2.59	18	62.00	2.20	31	88.00	0.42	44	117.00	16.09
6	29.00	0.56	19	63.00	6.15	32	89.00	3.97	45	118.00	0.37
7	32.00	0.65	20	64.00	2.03	33	90.00	0.42	46	119.00	100.00
8	38.00	1.17	21	65.00	10.45	34	91.00	34.76	47	120.00	9.25
9	39.00	9.22	22	66.00	1.37	35	92.00	3.37	48	121.00	0.45
10	40.00	1.23	23	74.00	1.16	36	93.00	3.16	49	128.00	0.38
11	41.00	6.37	24	75.00	1.36	37	102.00	2.07	50	134.00	23.85
12	50.00	2.92	25	76.00	1.41	38	103.00	5.52	51	135.00	2.62
13	51.00	6.79	26	77.00	11.37	39	104.00	3.83			

Compound Information

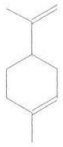
Entry:6621 Library:NIST11S.LIB

Formula:C10H16 CAS:5989-27-5 MolWeight:136 RetIndex:1018

CompName:D-Limonene $$ Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- $$ p-Mentha-1,8-diene, (R)-(+)- $$ (+)-(R)-Limonene $$ (+)-(4R)-Limonene



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	40.00	6.33	24	66.00	3.79	47	90.00	0.23	70	116.00	0.37
2	41.00	19.01	25	67.00	74.68	48	91.00	25.95	71	117.00	1.23
3	42.00	2.99	26	68.00	100.00	49	92.00	26.43	72	118.00	0.21
4	43.00	2.23	27	69.00	7.08	50	93.00	78.39	73	119.00	3.24
5	44.00	0.10	28	70.00	0.24	51	94.00	30.06	74	120.00	0.60
6	45.00	0.08	29	71.00	0.00	52	95.00	9.68	75	121.00	28.62
7	46.00	0.02	30	73.00	0.04	53	96.00	0.67	76	122.00	2.81
8	49.00	0.07	31	74.00	0.43	54	97.00	0.03	77	123.00	0.15
9	50.00	2.24	32	75.00	0.42	55	98.00	0.05	78	126.00	0.02
10	51.00	7.41	33	76.00	0.36	56	99.00	0.02	79	127.00	0.06
11	52.00	3.76	34	77.00	22.89	57	101.00	0.07	80	128.00	0.13
12	53.00	23.72	35	78.00	5.50	58	102.00	0.42	81	129.00	0.06
13	54.00	1.98	36	79.00	39.12	59	103.00	1.99	82	130.00	0.01
14	55.00	7.47	37	80.00	14.10	60	104.00	0.74	83	131.00	0.07
15	56.00	0.43	38	81.00	11.77	61	105.00	7.55	84	132.00	0.19
16	58.00	0.69	39	82.00	2.33	62	106.00	2.11	85	133.00	0.09
17	59.00	0.13	40	83.00	0.14	63	107.00	25.28	86	134.00	0.64
18	60.00	0.00	41	84.00	0.01	64	108.00	7.19	87	135.00	0.38
19	61.00	0.19	42	85.00	0.04	65	109.00	0.63	88	136.00	27.67
20	62.00	0.85	43	86.00	0.14	66	110.00	0.04	89	137.00	3.04
21	63.00	2.98	44	87.00	0.18	67	113.00	0.02	90	138.00	0.18
22	64.00	0.75	45	88.00	0.05	68	114.00	0.02	91	139.00	0.00
23	65.00	9.23	46	89.00	0.88	69	115.00	1.55	92	207.00	0.00

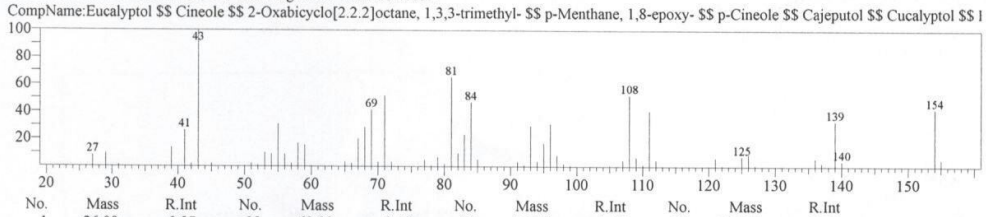


Compound Information

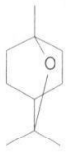
Entry:9939 Library:NIST11S.LIB

Formula:C10H18O CAS:470-82-6 MolWeight:154 RetIndex:1059

CompName:Eucalyptol $$ Cineole $$ 2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- $$ p-Menthane, 1,8-epoxy- $$ p-Cineole $$ Cajeputol $$ Cucalyptol $$ I

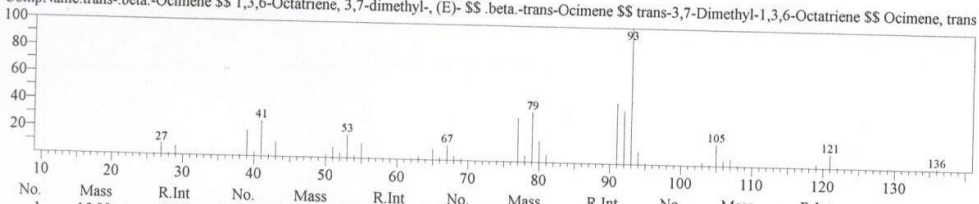


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.37	32	62.00	0.19	63	94.00	3.88	94	125.00	7.21
2	27.00	8.11	33	63.00	0.55	64	95.00	16.88	95	126.00	8.85
3	29.00	9.59	34	64.00	0.21	65	96.00	31.14	96	127.00	0.92
4	30.00	0.13	35	65.00	3.37	66	97.00	8.19	97	128.00	0.13
5	31.00	1.32	36	66.00	2.44	67	98.00	2.18	98	129.00	0.04
6	33.00	0.03	37	67.00	20.57	68	99.00	0.96	99	130.00	0.13
7	34.00	0.03	38	68.00	28.44	69	100.00	0.08	100	131.00	0.12
8	35.00	0.03	39	69.00	41.55	70	101.00	0.09	101	132.00	0.10
9	36.00	0.03	40	70.00	3.18	71	102.00	0.14	102	133.00	0.09
10	37.00	0.27	41	71.00	51.73	72	103.00	0.14	103	134.00	0.02
11	38.00	0.26	42	72.00	3.40	73	104.00	0.04	104	135.00	0.05
12	39.00	13.68	43	73.00	0.36	74	105.00	0.63	105	136.00	6.06
13	41.00	26.31	44	74.00	0.11	75	106.00	0.37	106	137.00	2.63
14	42.00	2.04	45	75.00	0.09	76	107.00	4.67	107	138.00	0.31
15	43.00	100.00	46	77.00	4.98	77	108.00	52.14	108	139.00	33.11
16	45.00	2.13	47	78.00	0.83	78	109.00	6.55	109	140.00	3.84
17	46.00	0.08	48	79.00	7.04	79	110.00	1.44	110	141.00	0.18
18	47.00	0.16	49	80.00	1.78	80	111.00	40.49	111	142.00	0.07
19	48.00	0.06	50	81.00	65.41	81	112.00	4.62	112	143.00	0.10
20	50.00	0.36	51	82.00	9.67	82	113.00	0.27	113	145.00	0.13
21	51.00	2.29	52	83.00	23.11	83	114.00	0.11	114	146.00	0.02
22	52.00	1.24	53	84.00	47.04	84	115.00	0.19	115	147.00	0.04
23	53.00	10.08	54	85.00	4.93	85	116.00	0.13	116	148.00	0.05
24	54.00	9.09	55	86.00	0.29	86	117.00	0.14	117	149.00	0.09
25	55.00	31.06	56	87.00	0.08	87	118.00	0.06	118	150.00	0.05
26	56.00	8.93	57	88.00	0.03	88	119.00	0.14	119	151.00	0.05
27	57.00	2.13	58	89.00	0.04	89	120.00	0.27	120	152.00	0.09
28	58.00	16.96	59	90.00	0.09	90	121.00	6.39	121	153.00	0.13
29	59.00	15.49	60	91.00	3.65	91	122.00	0.60	122	154.00	42.13
30	60.00	0.63	61	92.00	1.29	92	123.00	0.42	123	155.00	5.24
31	61.00	0.09	62	93.00	29.50	93	124.00	0.08			



Compound Information

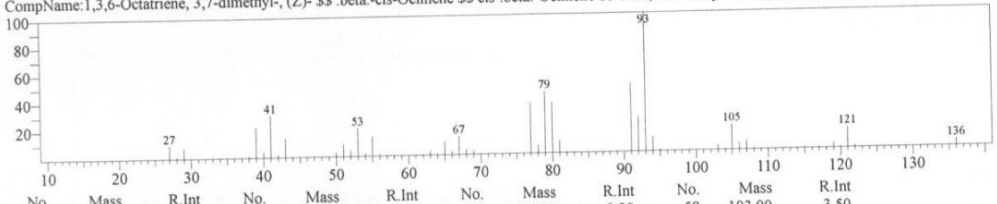
Entry:6664 Library:NIST11S.LIB
Formula:C10H16 CAS:3779-61-1 MolWeight:136 RetIndex:976
CompName:trans-.beta.-Ocimene $$ 1,3,6-Octatriene, 3,7-dimethyl-, (E)- $$ .beta.-trans-Ocimene $$ trans-3,7-Dimethyl-1,3,6-Octatriene $$ Ocimene, trans



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.20	18	54.00	1.80	35	76.00	0.30	52	106.00	4.10
2	26.00	0.40	19	55.00	11.30	36	77.00	32.10	53	107.00	5.20
3	27.00	8.00	20	56.00	0.90	37	78.00	5.10	54	108.00	0.70
4	28.00	1.00	21	57.00	0.40	38	79.00	37.00	55	109.00	0.30
5	29.00	6.30	22	58.00	0.50	39	80.00	15.80	56	115.00	0.90
6	37.00	0.20	23	59.00	0.10	40	81.00	5.70	57	116.00	0.20
7	38.00	1.10	24	61.00	0.20	41	82.00	0.60	58	117.00	0.70
8	39.00	19.10	25	62.00	0.80	42	89.00	0.50	59	118.00	0.20
9	40.00	3.30	26	63.00	2.70	43	91.00	44.90	60	119.00	3.10
10	41.00	26.40	27	64.00	0.60	44	92.00	39.50	61	120.00	0.70
11	42.00	1.70	28	65.00	8.30	45	93.00	100.00	62	121.00	10.20
12	43.00	10.70	29	66.00	2.20	46	94.00	9.50	63	122.00	1.10
13	44.00	0.40	30	67.00	11.00	47	95.00	1.00	64	135.00	0.10
14	50.00	2.50	31	68.00	3.20	48	102.00	0.30	65	136.00	1.30
15	51.00	7.80	32	69.00	1.70	49	103.00	2.90	66	137.00	0.10
16	52.00	3.70	33	74.00	0.40	50	104.00	0.80			
17	53.00	17.10	34	75.00	0.30	51	105.00	15.90			

Compound Information

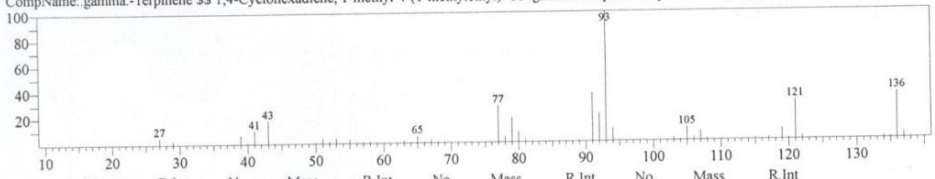
Entry:6662 Library:NIST11S.LIB
Formula:C10H16 CAS:3338-55-4 MolWeight:136 RetIndex:976
CompName:1,3,6-Octatriene, 3,7-dimethyl-, (Z)- $$ .beta.-cis-Ocimene $$ cis-.beta.-Ocimene $$ cis-3,7-Dimethyl-1,3,6-octatriene $$ Ocimene, cis-.beta.- $



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.20	20	53.00	20.10	39	76.00	0.30	58	103.00	3.50
2	26.00	0.50	21	54.00	2.20	40	77.00	36.10	59	104.00	0.90
3	27.00	9.40	22	55.00	14.00	41	78.00	5.60	60	105.00	18.10
4	28.00	1.20	23	56.00	1.20	42	79.00	44.10	61	106.00	4.60
5	29.00	7.20	24	57.00	0.70	43	80.00	36.50	62	107.00	5.80
6	30.00	0.20	25	58.00	0.60	44	81.00	8.50	63	108.00	0.90
7	37.00	0.30	26	59.00	0.10	45	82.00	0.90	64	109.00	0.50
8	38.00	1.20	27	61.00	0.20	46	83.00	0.20	65	115.00	1.00
9	39.00	21.80	28	62.00	0.90	47	85.00	0.30	66	116.00	0.20
10	40.00	3.80	29	63.00	3.10	48	86.00	0.10	67	117.00	0.70
11	41.00	30.20	30	64.00	0.80	49	87.00	0.10	68	118.00	0.10
12	42.00	2.00	31	65.00	9.60	50	89.00	0.70	69	119.00	3.70
13	43.00	13.50	32	66.00	2.70	51	91.00	49.10	70	120.00	0.80
14	44.00	0.50	33	67.00	13.10	52	92.00	25.00	71	121.00	14.80
15	45.00	0.20	34	68.00	3.60	53	93.00	100.00	72	122.00	1.50
16	49.00	0.10	35	69.00	2.40	54	94.00	10.70	73	135.00	0.20
17	50.00	2.90	36	70.00	0.30	55	95.00	1.30	74	136.00	4.80
18	51.00	8.70	37	74.00	0.50	56	96.00	0.20	75	137.00	0.60
19	52.00	4.40	38	75.00	0.40	57	102.00	0.30	76	139.00	0.30

Compound Information

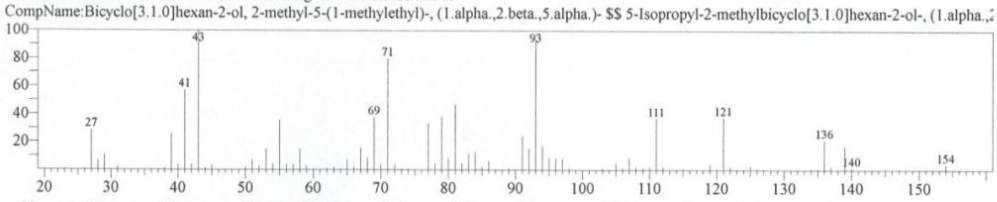
Entry:9811 Library:NIST11.LIB
Formula:C10H16 CAS:99-85-4 MolWeight:136 RetIndex:998
CompName:.gamma.-Terpinene $$ 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- $$ .gamma.-Terpinen $$ p-Mentha-1,4-diene $$ Crithmene $$ Moslene



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.10	19	56.00	0.20	37	79.00	18.59	55	108.00	1.29
2	26.00	0.10	20	57.00	0.80	38	80.00	7.79	56	109.00	0.10
3	27.00	5.19	21	58.00	1.09	39	81.00	2.09	57	115.00	1.49
4	28.00	0.40	22	59.00	0.50	40	82.00	0.20	58	116.00	0.40
5	29.00	2.59	23	60.00	0.20	41	87.00	0.10	59	117.00	1.69
6	38.00	0.30	24	62.00	0.40	42	89.00	0.80	60	118.00	0.30
7	39.00	6.89	25	63.00	1.59	43	90.00	0.30	61	119.00	8.69
8	40.00	0.99	26	64.00	0.50	44	91.00	37.29	62	120.00	1.09
9	41.00	9.99	27	65.00	5.19	45	92.00	21.49	63	121.00	30.39
10	42.00	0.50	28	66.00	0.80	46	93.00	100.00	64	122.00	2.99
11	43.00	17.59	29	67.00	2.59	47	94.00	9.59	65	123.00	0.10
12	44.00	0.60	30	68.00	0.90	48	95.00	0.70	66	133.00	0.10
13	50.00	0.90	31	69.00	0.50	49	102.00	0.40	67	134.00	1.89
14	51.00	4.09	32	74.00	0.20	50	103.00	2.19	68	135.00	0.80
15	52.00	1.69	33	75.00	0.30	51	104.00	0.90	69	136.00	35.89
16	53.00	4.09	34	76.00	0.20	52	105.00	9.79	70	137.00	4.19
17	54.00	0.30	35	77.00	28.19	53	106.00	2.29	71	138.00	0.20
18	55.00	2.79	36	78.00	4.29	54	107.00	7.29			

Compound Information

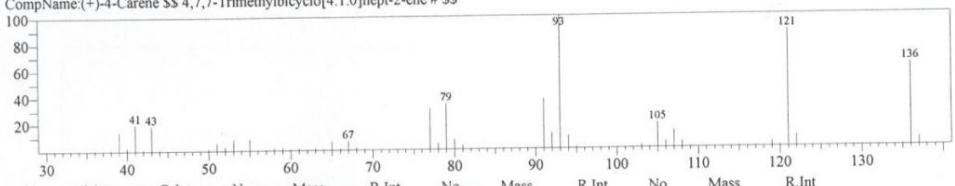
Entry:17480 Library:NIST11.LIB
Formula:C10H18O CAS:15537-55-0 MolWeight:154 RetIndex:1041
CompName:Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1.alpha.,2.beta.,5.alpha.)- $$ 5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol-, (1.alpha.,2



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	23.00	0.68	24	56.00	3.83	47	81.00	46.78	70	108.00	2.13
2	26.00	1.01	25	57.00	4.10	48	82.00	4.96	71	109.00	1.19
3	27.00	28.60	26	58.00	14.90	49	83.00	11.58	72	110.00	1.76
4	28.00	6.79	27	59.00	2.95	50	84.00	13.16	73	111.00	36.96
5	29.00	10.91	28	60.00	0.33	51	85.00	2.42	74	112.00	2.23
6	30.00	0.28	29	62.00	1.25	52	86.00	6.24	75	115.00	0.76
7	31.00	2.34	30	63.00	2.18	53	87.00	0.21	76	117.00	0.31
8	36.00	0.38	31	64.00	0.87	54	89.00	1.15	77	119.00	3.76
9	37.00	0.29	32	65.00	7.35	55	90.00	0.44	78	120.00	0.45
10	38.00	1.40	33	66.00	2.53	56	91.00	24.22	79	121.00	37.59
11	39.00	25.85	34	67.00	15.60	57	92.00	15.50	80	122.00	2.40
12	40.00	3.89	35	68.00	8.70	58	93.00	94.01	81	123.00	0.75
13	41.00	57.32	36	69.00	37.84	59	94.00	17.21	82	125.00	2.58
14	42.00	3.79	37	70.00	3.55	60	95.00	9.04	83	126.00	1.25
15	43.00	100.00	38	71.00	79.83	61	96.00	8.63	84	134.00	0.58
16	44.00	1.87	39	72.00	3.88	62	97.00	8.49	85	135.00	0.80
17	45.00	3.65	40	73.00	0.59	63	98.00	1.48	86	136.00	21.46
18	50.00	1.96	41	74.00	0.88	64	99.00	0.20	87	137.00	2.53
19	51.00	7.37	42	75.00	0.45	65	103.00	1.04	88	139.00	17.11
20	52.00	3.09	43	77.00	33.36	66	104.00	0.32	89	140.00	1.44
21	53.00	14.77	44	78.00	4.81	67	105.00	5.00	90	147.00	0.41
22	54.00	4.31	45	79.00	37.98	68	106.00	1.37	91	154.00	4.04
23	55.00	35.45	46	80.00	8.92	69	107.00	9.07	92	155.00	0.21

Compound Information

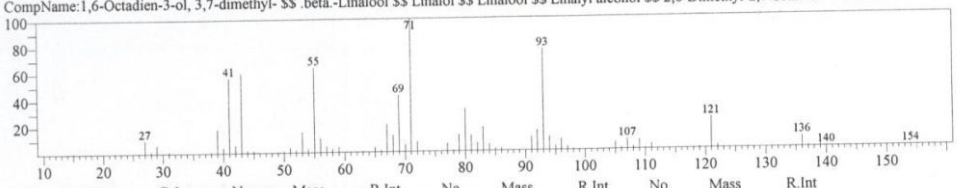
Entry:9827 Library:NIST11.LIB
Formula:C10H16 CAS:29050-33-7 MolWeight:136 RetIndex:919
CompName:(+)-4-Carene $$ 4,7,7-Trimethylbicyclo[4.1.0]hept-2-ene # $$



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	36.00	0.63	20	56.00	0.36	39	78.00	4.47	58	106.00	4.73
2	37.00	0.18	21	57.00	0.67	40	79.00	34.29	59	107.00	12.77
3	38.00	1.22	22	58.00	1.82	41	80.00	7.71	60	108.00	4.44
4	39.00	14.06	23	59.00	1.95	42	81.00	3.10	61	109.00	0.33
5	40.00	2.37	24	60.00	0.89	43	82.00	0.23	62	115.00	0.62
6	41.00	19.62	25	61.00	1.36	44	86.00	0.11	63	116.00	0.10
7	42.00	1.20	26	62.00	0.51	45	87.00	0.02	64	117.00	0.69
8	43.00	18.52	27	63.00	1.49	46	88.00	0.08	65	118.00	0.02
9	44.00	0.93	28	64.00	0.79	47	89.00	0.46	66	119.00	3.87
10	45.00	0.35	29	65.00	6.35	48	90.00	0.14	67	120.00	0.73
11	46.00	0.10	30	66.00	1.25	49	91.00	37.14	68	121.00	87.98
12	47.00	0.01	31	67.00	6.61	50	92.00	11.60	69	122.00	8.54
13	49.00	0.13	32	68.00	1.87	51	93.00	100.00	70	123.00	0.37
14	50.00	1.28	33	69.00	0.97	52	94.00	9.50	71	134.00	0.02
15	51.00	5.70	34	70.00	0.06	53	95.00	1.19	72	135.00	0.69
16	52.00	2.68	35	74.00	0.22	54	102.00	0.19	73	136.00	62.26
17	53.00	8.30	36	75.00	0.20	55	103.00	2.46	74	137.00	6.43
18	54.00	0.73	37	76.00	0.07	56	104.00	0.55	75	138.00	0.21
19	55.00	8.20	38	77.00	30.66	57	105.00	18.70			

Compound Information

Entry:17562 Library:NIST11.LIB
Formula:C10H18O CAS:78-70-6 MolWeight:154 RetIndex:1082
CompName:1,6-Octadien-3-ol, 3,7-dimethyl- $$ .beta.-Linalool $$ Linalol $$ Linalool $$ Linalyl alcohol $$ 2,6-Dimethyl-2,7-octadien-6-ol $$ allo-Ocimen



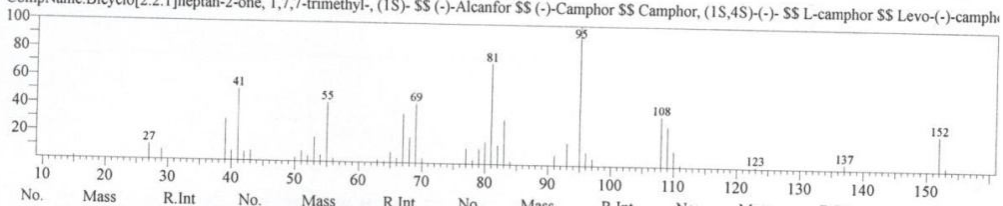
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.60	25	53.00	15.31	49	78.00	1.00	73	107.00	7.41
2	19.00	0.10	26	54.00	2.70	50	79.00	12.21	74	108.00	2.00
3	26.00	0.70	27	55.00	63.77	51	80.00	32.13	75	109.00	6.81
4	27.00	9.91	28	56.00	10.51	52	81.00	11.91	76	110.00	0.80
5	28.00	1.60	29	57.00	4.50	53	82.00	5.91	77	111.00	3.60
6	29.00	6.31	30	58.00	2.70	54	83.00	17.72	78	112.00	0.30
7	30.00	0.20	31	59.00	4.10	55	84.00	4.90	79	115.00	0.10
8	31.00	1.20	32	60.00	0.20	56	85.00	1.60	80	117.00	0.10
9	37.00	0.20	33	61.00	0.10	57	86.00	1.90	81	119.00	1.10
10	38.00	0.80	34	62.00	0.40	58	87.00	0.20	82	121.00	23.22
11	39.00	17.92	35	63.00	0.90	59	89.00	0.10	83	122.00	2.30
12	40.00	4.20	36	64.00	0.20	60	91.00	10.01	84	123.00	0.40
13	41.00	56.46	37	65.00	3.60	61	92.00	15.11	85	124.00	0.10
14	42.00	5.81	38	66.00	1.40	62	93.00	76.08	86	125.00	0.40
15	43.00	59.86	39	67.00	20.62	63	94.00	10.21	87	126.00	0.10
16	44.00	1.90	40	68.00	12.51	64	95.00	3.20	88	127.00	0.60
17	45.00	1.70	41	69.00	42.64	65	96.00	8.41	89	128.00	0.10
18	46.00	0.10	42	70.00	5.40	66	97.00	2.60	90	135.00	0.10
19	47.00	0.10	43	71.00	100.00	67	98.00	0.90	91	136.00	8.21
20	48.00	0.10	44	72.00	7.31	68	99.00	0.30	92	137.00	1.00
21	49.00	0.10	45	73.00	0.70	69	103.00	0.50	93	138.00	0.10
22	50.00	1.20	46	74.00	0.10	70	104.00	0.10	94	139.00	2.20
23	51.00	3.70	47	75.00	0.10	71	105.00	5.30	95	140.00	0.20
24	52.00	1.80	48	77.00	6.11	72	106.00	1.30	96	154.00	0.40

Compound Information

Entry:16453 Library:NIST11.LIB

Formula:C10H16O CAS:464-48-2 MolWeight:152 RetIndex:1121

CompName:Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- $$ (-)-Alcanfor $$ (-)-Camphor $$ Camphor, (1S,4S)-(-)- $$ L-camphor $$ Levo-(-)-camph



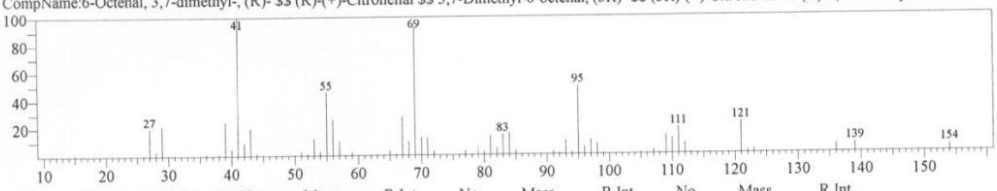
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	1.51	12	53.00	17.47	23	70.00	3.63	34	95.00	100.00
2	27.00	10.76	13	54.00	4.58	24	77.00	10.94	35	96.00	9.37
3	29.00	6.93	14	55.00	42.47	25	78.00	2.73	36	97.00	5.13
4	39.00	29.92	15	56.00	2.69	26	79.00	10.91	37	108.00	35.89
5	40.00	7.09	16	63.00	2.01	27	80.00	16.06	38	109.00	28.73
6	41.00	51.35	17	64.00	0.91	28	81.00	71.87	39	110.00	11.15
7	42.00	6.15	18	65.00	7.44	29	82.00	13.71	40	111.00	1.39
8	43.00	7.20	19	66.00	3.13	30	83.00	32.02	41	123.00	1.26
9	50.00	2.69	20	67.00	35.21	31	84.00	2.50	42	137.00	3.76
10	51.00	7.13	21	68.00	18.25	32	91.00	7.13	43	152.00	25.08
11	52.00	3.93	22	69.00	42.58	33	93.00	15.97	44	153.00	2.82

Compound Information

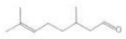
Entry:17443 Library:NIST11.LIB

Formula:C10H18O CAS:2385-77-5 MolWeight:154 RetIndex:1125

CompName:6-Octenal, 3,7-dimethyl-, (R)- $$ (R)-(+)-Citronellal $$ 3,7-Dimethyl-6-octenal, (3R)- $$ (3R)-(+)-Citronellal $$ (R)-3,7-Dimethyloct-6-enal $$



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	1.21	21	51.00	2.53	41	77.00	2.98	61	107.00	2.73
2	18.00	0.06	22	52.00	1.11	42	78.00	0.47	62	108.00	0.67
3	26.00	0.82	23	53.00	11.97	43	79.00	6.19	63	109.00	13.54
4	27.00	19.78	24	54.00	2.72	44	80.00	2.39	64	110.00	10.98
5	28.00	3.28	25	55.00	45.62	45	81.00	13.74	65	111.00	18.95
6	29.00	21.66	26	56.00	25.83	46	82.00	4.84	66	112.00	7.70
7	30.00	0.41	27	57.00	9.99	47	83.00	14.37	67	113.00	0.51
8	31.00	0.74	28	58.00	0.61	48	84.00	15.62	68	119.00	0.10
9	35.00	0.29	29	59.00	2.38	49	85.00	3.08	69	121.00	22.91
10	36.00	1.38	30	62.00	0.11	50	86.00	0.37	70	122.00	1.88
11	37.00	0.28	31	63.00	0.67	51	91.00	2.30	71	123.00	2.78
12	38.00	1.45	32	65.00	3.38	52	92.00	0.73	72	124.00	0.05
13	39.00	24.37	33	66.00	1.02	53	93.00	9.68	73	125.00	0.51
14	40.00	4.53	34	67.00	27.91	54	94.00	1.56	74	126.00	0.17
15	41.00	100.00	35	68.00	9.89	55	95.00	49.37	75	136.00	6.19
16	42.00	9.11	36	69.00	92.50	56	96.00	5.15	76	137.00	0.64
17	43.00	19.58	37	70.00	12.81	57	97.00	10.15	77	139.00	6.87
18	44.00	1.91	38	71.00	12.23	58	98.00	7.44	78	140.00	0.50
19	45.00	0.39	39	72.00	2.73	59	99.00	0.72	79	154.00	5.20
20	50.00	0.77	40	73.00	0.08	60	105.00	0.75	80	155.00	0.41

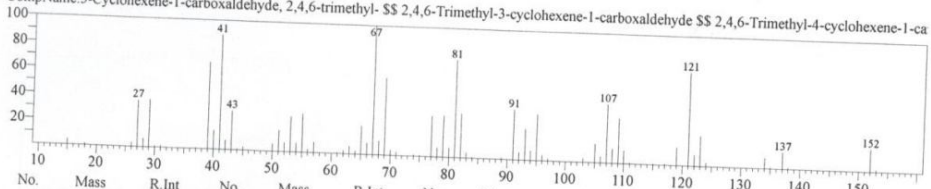


Compound Information

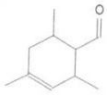
Entry:16340 Library:NIST11.LIB

Formula:C10H16O CAS:1423-46-7 MolWeight:152 RetIndex:1163

CompName:3-Cyclohexene-1-carboxaldehyde, 2,4,6-trimethyl- $$ 2,4,6-Trimethyl-3-cyclohexene-1-carboxaldehyde $$ 2,4,6-Trimethyl-4-cyclohexene-1-ca



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	4.88	20	52.00	7.01	39	77.00	31.51	58	107.00	45.44
2	18.00	1.47	21	53.00	27.59	40	78.00	7.18	59	108.00	11.16
3	26.00	3.47	22	54.00	6.80	41	79.00	32.20	60	109.00	34.93
4	27.00	36.18	23	55.00	29.76	42	80.00	7.28	61	110.00	10.26
5	28.00	6.69	24	56.00	2.39	43	81.00	75.44	62	111.00	0.84
6	29.00	36.98	25	57.00	8.03	44	82.00	34.27	63	115.00	0.82
7	30.00	1.27	26	61.00	0.87	45	83.00	4.03	64	117.00	0.96
8	31.00	1.54	27	62.00	2.31	46	84.00	0.86	65	119.00	14.14
9	32.00	0.21	28	63.00	5.95	47	89.00	1.47	66	121.00	72.03
10	37.00	0.90	29	64.00	2.67	48	91.00	38.83	67	122.00	8.64
11	39.00	67.33	30	65.00	21.90	49	92.00	5.83	68	123.00	23.38
12	40.00	14.57	31	66.00	8.83	50	93.00	24.28	69	124.00	2.73
13	41.00	88.76	32	67.00	100.00	51	94.00	7.56	70	134.00	8.23
14	42.00	7.14	33	68.00	10.83	52	95.00	35.89	71	135.00	1.14
15	43.00	30.42	34	69.00	59.76	53	96.00	4.49	72	137.00	12.86
16	44.00	1.05	35	70.00	4.14	54	97.00	1.81	73	138.00	1.45
17	45.00	2.90	36	71.00	2.66	55	103.00	2.82	74	152.00	17.53
18	50.00	5.60	37	74.00	1.15	56	105.00	14.46	75	153.00	1.88
19	51.00	16.38	38	75.00	0.91	57	106.00	4.91			

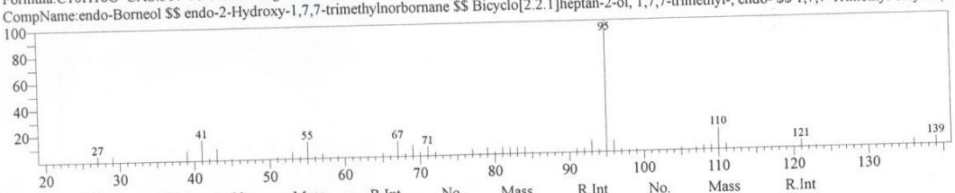


Compound Information

Entry:10018 Library:NIST11S.LIB

Formula:C10H18O CAS:507-70-0 MolWeight:154 RetIndex:1138

CompName:endo-Borneol $$ endo-2-Hydroxy-1,7,7-trimethylnorbornane $$ Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, endo- $$ 1,7,7-Trimethyl-bicyclo(2



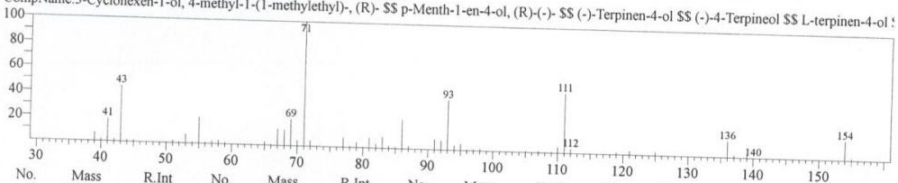
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	25.00	0.04	29	57.00	3.41	57	85.00	1.06	85	113.00	0.62
2	26.00	0.31	30	58.00	0.27	58	86.00	0.27	86	114.00	0.13
3	27.00	4.69	31	59.00	1.10	59	87.00	0.04	87	115.00	0.06
4	29.00	4.61	32	60.00	0.06	60	88.00	0.04	88	116.00	0.05
5	30.00	0.20	33	61.00	0.04	61	89.00	0.14	89	117.00	0.10
6	31.00	0.74	34	62.00	0.11	62	90.00	0.09	90	118.00	0.02
7	33.00	0.02	35	63.00	0.68	63	91.00	2.81	91	119.00	0.24
8	34.00	0.06	36	64.00	0.22	64	92.00	3.05	92	120.00	0.03
9	35.00	0.02	37	65.00	2.69	65	93.00	8.83	93	121.00	5.62
10	36.00	0.06	38	66.00	0.93	66	94.00	1.96	94	122.00	0.69
11	37.00	0.18	39	67.00	11.68	67	95.00	100.00	95	123.00	0.77
12	38.00	0.28	40	68.00	2.07	68	96.00	8.51	96	124.00	0.06
13	39.00	7.91	41	69.00	8.47	69	97.00	2.10	97	125.00	0.24
14	41.00	15.38	42	70.00	3.09	70	98.00	1.00	98	126.00	0.06
15	42.00	1.90	43	71.00	7.10	71	99.00	1.34	99	127.00	0.05
16	43.00	9.11	44	72.00	2.69	72	100.00	0.16	100	128.00	0.02
17	45.00	1.08	45	73.00	0.16	73	101.00	0.04	101	129.00	0.07
18	46.00	0.03	46	74.00	0.09	74	102.00	0.07	102	130.00	0.02
19	47.00	0.03	47	75.00	0.07	75	103.00	0.24	103	131.00	0.01
20	48.00	0.05	48	76.00	0.11	76	104.00	0.09	104	132.00	0.02
21	49.00	0.04	49	77.00	4.09	77	105.00	1.99	105	134.00	0.01
22	50.00	0.34	50	78.00	0.72	78	106.00	0.47	106	135.00	0.06
23	51.00	1.51	51	79.00	4.97	79	107.00	1.76	107	136.00	4.45
24	52.00	0.56	52	80.00	1.98	80	108.00	3.05	108	137.00	0.61
25	53.00	5.18	53	81.00	5.22	81	109.00	3.13	109	138.00	0.11
26	54.00	1.65	54	82.00	4.57	82	110.00	16.54	110	139.00	6.06
27	55.00	12.57	55	83.00	4.65	83	111.00	3.93			
28	56.00	1.83	56	84.00	4.57	84	112.00	0.38			

Compound Information

Entry:17565 Library:NIST11.LIB

Formula:C10H18O CAS:20126-76-5 MolWeight:154 RetIndex:1137

CompName:3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)- $$ p-Menth-1-en-4-ol, (R)-(-)- $$ (-)-Terpinen-4-ol $$ (-)-4-Terpineol $$ L-terpinen-4-ol $



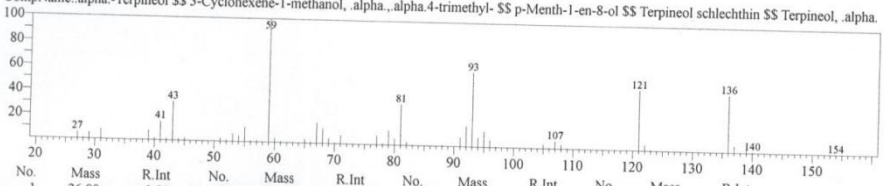
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	36.00	0.38	25	61.00	0.08	49	87.00	1.95	73	113.00	0.21
2	37.00	0.01	26	62.00	0.16	50	88.00	0.06	74	115.00	0.17
3	38.00	0.36	27	63.00	0.50	51	89.00	0.15	75	117.00	0.32
4	39.00	6.96	28	64.00	0.20	52	91.00	8.21	76	119.00	1.84
5	40.00	1.92	29	65.00	2.59	53	92.00	7.25	77	120.00	0.15
6	41.00	18.52	30	66.00	0.87	54	93.00	39.90	78	121.00	3.48
7	42.00	2.25	31	67.00	13.21	55	94.00	3.59	79	122.00	0.33
8	43.00	45.04	32	68.00	12.65	56	95.00	5.11	80	123.00	0.26
9	44.00	1.65	33	69.00	21.52	57	96.00	0.81	81	124.00	0.07
10	45.00	1.37	34	70.00	4.48	58	97.00	1.29	82	125.00	2.63
11	46.00	0.14	35	71.00	100.00	59	98.00	1.57	83	126.00	0.35
12	47.00	0.05	36	72.00	4.70	60	99.00	0.37	84	134.00	0.48
13	49.00	0.02	37	73.00	0.38	61	100.00	0.02	85	135.00	0.13
14	50.00	0.48	38	75.00	0.01	62	102.00	0.06	86	136.00	13.29
15	51.00	1.98	39	77.00	7.53	63	103.00	0.27	87	137.00	1.90
16	52.00	0.80	40	78.00	1.10	64	104.00	0.09	88	138.00	0.07
17	53.00	7.15	41	79.00	3.96	65	105.00	1.11	89	139.00	2.15
18	54.00	0.93	42	80.00	0.76	66	106.00	0.15	90	140.00	0.17
19	55.00	21.34	43	81.00	7.99	67	107.00	1.21	91	152.00	0.01
20	56.00	1.09	44	82.00	3.23	68	108.00	0.24	92	153.00	0.03
21	57.00	2.17	45	83.00	9.08	69	109.00	0.91	93	154.00	15.39
22	58.00	2.90	46	84.00	2.09	70	110.00	4.75	94	155.00	1.79
23	59.00	1.21	47	85.00	1.33	71	111.00	48.03	95	156.00	0.12
24	60.00	0.03	48	86.00	23.38	72	112.00	3.71			

Compound Information

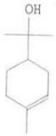
Entry:9958 Library:NIST11S.LIB

Formula:C10H18O CAS:98-55-5 MolWeight:154 RetIndex:1143

CompName:.alpha.-Terpineol $$ 3-Cyclohexene-1-methanol, .alpha.,.alpha.4-trimethyl- $$ p-Menth-1-en-8-ol $$ Terpineol schlechthin $$ Terpineol, .alpha.

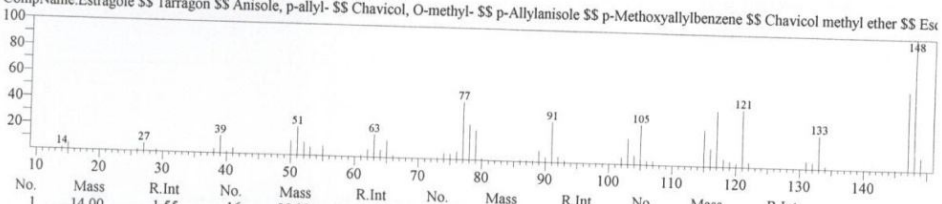


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.31	21	57.00	1.50	41	79.00	11.61	61	109.00	0.64
2	27.00	5.61	22	58.00	0.68	42	80.00	5.44	62	111.00	0.36
3	28.00	1.07	23	59.00	100.00	43	81.00	33.12	63	115.00	0.32
4	29.00	5.21	24	60.00	3.28	44	82.00	2.56	64	117.00	0.25
5	31.00	8.45	25	61.00	0.87	45	83.00	0.58	65	119.00	0.80
6	38.00	0.39	26	62.00	0.45	46	84.00	0.42	66	120.00	0.21
7	39.00	7.88	27	63.00	0.70	47	85.00	0.45	67	121.00	48.78
8	40.00	1.85	28	65.00	2.95	48	88.00	0.72	68	122.00	4.56
9	41.00	15.52	29	66.00	1.23	49	91.00	7.52	69	123.00	0.90
10	42.00	1.67	30	67.00	16.63	50	92.00	16.52	70	135.00	0.41
11	43.00	31.47	31	68.00	11.97	51	93.00	60.24	71	136.00	46.24
12	44.00	1.71	32	69.00	4.29	52	94.00	7.55	72	137.00	5.50
13	45.00	2.48	33	70.00	0.75	53	95.00	12.55	73	138.00	0.46
14	50.00	0.63	34	71.00	7.04	54	96.00	5.85	74	139.00	6.69
15	51.00	2.36	35	72.00	0.56	55	97.00	0.88	75	140.00	0.81
16	52.00	1.18	36	73.00	0.28	56	103.00	0.39	76	141.00	0.15
17	53.00	6.18	37	74.00	0.20	57	105.00	3.49	77	153.00	0.11
18	54.00	4.61	38	75.00	0.17	58	106.00	0.82	78	154.00	0.22
19	55.00	11.79	39	77.00	7.48	59	107.00	6.23			
20	56.00	0.92	40	78.00	1.28	60	108.00	3.35			



Compound Information

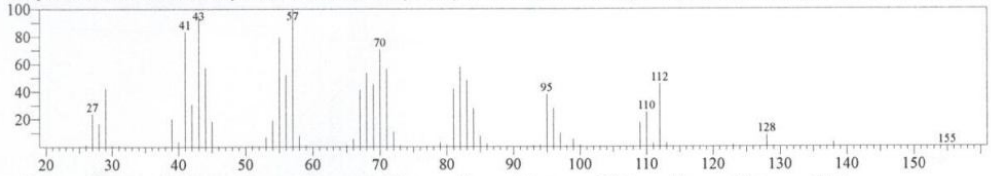
Entry:14629 Library:NIST11.LIB
Formula:C10H12O CAS:140-67-0 MolWeight:148 RetIndex:1172
CompName:Estragole $$ Tarragon $$ Anisole, p-allyl- $$ Chavicol, O-methyl- $$ p-Allylanisole $$ p-Methoxyallylbenzene $$ Chavicol methyl ether $$ Es



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	1.55	16	55.00	7.68	31	86.00	1.13	46	116.00	13.42
2	15.00	4.92	17	61.00	1.63	32	87.00	1.27	47	117.00	41.89
3	26.00	1.51	18	62.00	5.87	33	88.00	0.92	48	118.00	5.79
4	27.00	5.99	19	63.00	17.05	34	89.00	8.71	49	119.00	3.99
5	28.00	0.50	20	64.00	5.58	35	90.00	3.71	50	120.00	3.04
6	29.00	1.54	21	65.00	12.96	36	91.00	30.58	51	121.00	43.27
7	38.00	3.12	22	66.00	1.87	37	92.00	4.54	52	122.00	3.71
8	39.00	13.10	23	73.00	0.83	38	93.00	1.89	53	131.00	5.65
9	40.00	1.44	24	74.00	4.55	39	102.00	5.21	54	132.00	4.77
10	41.00	4.00	25	75.00	3.99	40	103.00	19.27	55	133.00	25.08
11	50.00	10.62	26	76.00	5.73	41	104.00	6.81	56	134.00	2.43
12	51.00	21.43	27	77.00	43.87	42	105.00	30.00	57	145.00	0.83
13	52.00	9.79	28	78.00	26.77	43	106.00	3.30	58	147.00	59.92
14	53.00	6.19	29	79.00	22.32	44	107.00	3.04	59	148.00	100.00
15	54.00	0.90	30	80.00	1.56	45	115.00	27.43	60	149.00	10.12

Compound Information

Entry:10329 Library:NIST11S.LIB
Formula:C10H20O CAS:112-31-2 MolWeight:156 RetIndex:1204
CompName:Decanal $$ n-Decaldehyde $$ n-Decanal $$ n-Decyl aldehyde $$ Aldehyde C10 $$ Capraldehyde $$ Capric aldehyde $$ Caprinaldehyde $$ Ca



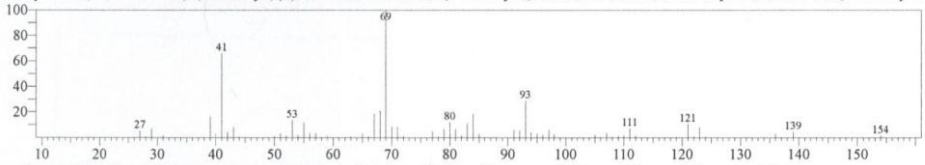
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	1.40	19	52.00	0.50	37	77.00	0.60	55	99.00	5.40
2	27.00	23.62	20	53.00	7.01	38	78.00	0.10	56	100.00	1.30
3	28.00	16.92	21	54.00	19.12	39	79.00	3.10	57	107.00	0.10
4	29.00	42.44	22	55.00	79.48	40	80.00	1.70	58	108.00	0.20
5	30.00	1.00	23	56.00	52.16	41	81.00	41.94	59	109.00	17.32
6	31.00	1.20	24	57.00	100.00	42	82.00	57.86	60	110.00	24.82
7	37.00	0.10	25	58.00	8.01	43	83.00	48.14	61	111.00	2.30
8	38.00	0.50	26	59.00	0.80	44	84.00	27.72	62	112.00	45.64
9	39.00	20.22	27	61.00	0.20	45	85.00	7.71	63	113.00	2.90
10	40.00	3.70	28	65.00	1.20	46	86.00	2.20	64	114.00	0.20
11	41.00	83.49	29	66.00	5.61	47	87.00	0.10	65	123.00	1.20
12	42.00	30.63	30	67.00	41.14	48	91.00	0.20	66	127.00	0.50
13	43.00	95.30	31	68.00	53.36	49	93.00	0.80	67	128.00	8.41
14	44.00	57.36	32	69.00	45.34	50	94.00	1.20	68	129.00	0.60
15	45.00	18.52	33	70.00	70.67	51	95.00	38.03	69	138.00	3.20
16	46.00	0.40	34	71.00	56.56	52	96.00	27.62	70	139.00	0.20
17	50.00	0.20	35	72.00	11.01	53	97.00	9.81	71	155.00	0.10
18	51.00	0.90	36	73.00	1.10	54	98.00	0.90	72	156.00	0.10

Compound Information

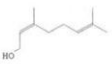
Entry:17537 Library:NIST11.LIB

Formula:C10H18O CAS:106-25-2 MolWeight:154 RetIndex:1228

CompName:2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- $$ cis-Geraniol $$ cis-3,7-Dimethyl-2,6-octadien-1-ol $$ Nerol $$ Neryl alcohol $$ 2-cis-3,7-Dimethyl-2



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.20	25	57.00	3.70	49	82.00	1.60	73	110.00	1.90
2	19.00	0.10	26	58.00	0.30	50	83.00	11.01	74	111.00	7.31
3	26.00	0.30	27	59.00	1.90	51	84.00	18.42	75	112.00	1.90
4	27.00	5.50	28	60.00	0.10	52	85.00	2.90	76	113.00	0.10
5	28.00	0.90	29	61.00	0.10	53	86.00	0.40	77	115.00	0.20
6	29.00	6.81	30	62.00	0.30	54	87.00	0.10	78	117.00	0.10
7	30.00	0.20	31	63.00	0.90	55	89.00	0.10	79	119.00	0.60
8	31.00	1.90	32	64.00	0.20	56	91.00	6.01	80	120.00	0.20
9	37.00	0.10	33	65.00	3.40	57	92.00	5.71	81	121.00	10.71
10	38.00	0.60	34	66.00	1.30	58	93.00	28.93	82	122.00	1.20
11	39.00	16.21	35	67.00	18.52	59	94.00	4.30	83	123.00	8.21
12	40.00	3.40	36	68.00	21.12	60	95.00	3.40	84	124.00	0.80
13	41.00	66.07	37	69.00	100.00	61	96.00	2.40	85	125.00	0.20
14	42.00	4.40	38	70.00	8.71	62	97.00	6.31	86	126.00	0.20
15	43.00	8.01	39	71.00	8.21	63	98.00	2.60	87	135.00	0.10
16	44.00	0.90	40	72.00	1.40	64	99.00	0.30	88	136.00	3.20
17	45.00	0.60	41	73.00	0.10	65	102.00	0.10	89	137.00	0.50
18	50.00	1.10	42	74.00	0.10	66	103.00	0.40	90	139.00	4.70
19	51.00	3.50	43	75.00	0.10	67	104.00	0.10	91	140.00	0.50
20	52.00	1.70	44	77.00	5.10	68	105.00	2.40	92	153.00	0.10
21	53.00	13.61	45	78.00	1.00	69	106.00	0.50	93	154.00	1.60
22	54.00	2.00	46	79.00	6.61	70	107.00	3.70	94	155.00	0.20
23	55.00	11.61	47	80.00	12.01	71	108.00	0.90			
24	56.00	3.60	48	81.00	6.61	72	109.00	1.50			

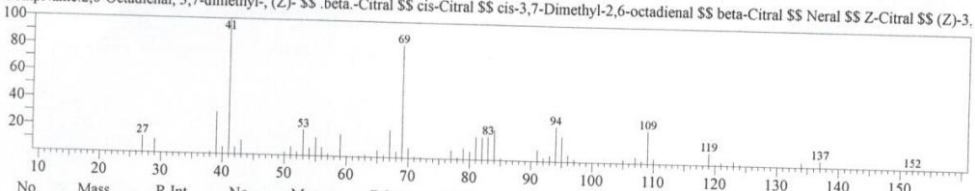


Compound Information

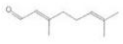
Entry:9466 Library:NIST11S.LIB

Formula:C10H16O CAS:106-26-3 MolWeight:152 RetIndex:1174

CompName:2,6-Octadienal, 3,7-dimethyl-, (Z)- $$ .beta.-Citral $$ cis-Citral $$ cis-3,7-Dimethyl-2,6-octadienal $$ beta-Citral $$ Neral $$ Z-Citral $$ (Z)-3,

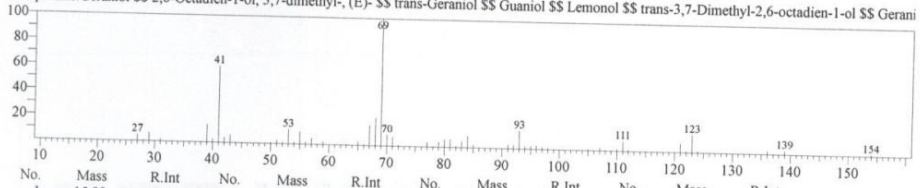


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.30	25	56.00	6.40	49	80.00	5.80	73	109.00	23.70
2	26.00	0.60	26	57.00	1.80	50	81.00	16.70	74	110.00	3.70
3	27.00	11.80	27	58.00	0.20	51	82.00	16.20	75	111.00	0.30
4	28.00	0.70	28	59.00	16.20	52	83.00	16.80	76	115.00	0.50
5	29.00	9.90	29	60.00	0.70	53	84.00	22.00	77	116.00	0.10
6	30.00	0.20	30	61.00	0.50	54	85.00	1.40	78	117.00	0.60
7	31.00	0.50	31	62.00	0.70	55	86.00	0.10	79	118.00	0.20
8	37.00	0.40	32	63.00	1.70	56	89.00	0.30	80	119.00	8.80
9	38.00	1.70	33	64.00	0.30	57	90.00	0.10	81	120.00	1.00
10	39.00	30.90	34	65.00	5.10	58	91.00	8.00	82	121.00	2.30
11	40.00	5.20	35	66.00	1.80	59	92.00	2.50	83	122.00	0.60
12	41.00	100.00	36	67.00	20.10	60	93.00	4.20	84	123.00	3.20
13	42.00	5.30	37	68.00	4.40	61	94.00	25.30	85	124.00	1.20
14	43.00	10.40	38	69.00	83.00	62	95.00	18.40	86	125.00	0.10
15	44.00	0.60	39	70.00	7.30	63	96.00	5.10	87	133.00	0.20
16	45.00	0.60	40	71.00	1.40	64	97.00	2.00	88	134.00	3.40
17	46.00	0.10	41	72.00	1.10	65	98.00	0.20	89	135.00	0.50
18	49.00	0.10	42	73.00	0.10	66	102.00	0.10	90	136.00	0.10
19	50.00	2.50	43	74.00	0.30	67	103.00	0.70	91	137.00	4.90
20	51.00	6.50	44	75.00	0.20	68	104.00	0.30	92	138.00	0.50
21	52.00	2.80	45	76.00	0.10	69	105.00	2.60	93	151.00	0.10
22	53.00	18.80	46	77.00	6.20	70	106.00	0.70	94	152.00	0.80
23	54.00	5.70	47	78.00	1.40	71	107.00	4.70	95	153.00	0.10
24	55.00	13.50	48	79.00	8.10	72	108.00	2.20			

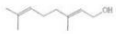


Compound Information

Entry:17535 Library:NIST11.LIB
Formula:C10H18O CAS:106-24-1 MolWeight:154 RetIndex:1228
CompName:Geraniol $$ 2,6-Octadien-1-ol, 3,7-dimethyl-, (E)- $$ trans-Geraniol $$ Guaniol $$ Lemonol $$ trans-3,7-Dimethyl-2,6-octadien-1-ol $$ Gerani

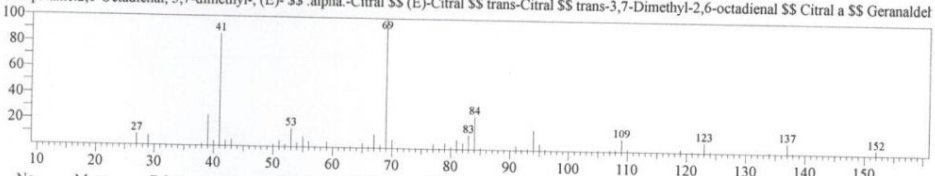


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.20	24	56.00	2.10	47	80.00	5.81	70	109.00	1.10
2	19.00	0.10	25	57.00	4.70	48	81.00	6.21	71	110.00	1.60
3	26.00	0.20	26	58.00	0.30	49	82.00	1.20	72	111.00	7.81
4	27.00	5.00	27	59.00	2.70	50	83.00	5.00	73	112.00	1.50
5	28.00	0.70	28	60.00	0.10	51	84.00	9.01	74	113.00	0.10
6	29.00	6.61	29	61.00	0.10	52	85.00	2.40	75	115.00	0.10
7	30.00	0.20	30	62.00	0.30	53	86.00	0.40	76	117.00	0.10
8	31.00	1.80	31	63.00	0.80	54	89.00	0.10	77	119.00	0.30
9	37.00	0.10	32	64.00	0.20	55	91.00	3.50	78	120.00	0.20
10	38.00	0.60	33	65.00	3.00	56	92.00	3.30	79	121.00	7.01
11	39.00	13.91	34	66.00	1.10	57	93.00	14.31	80	122.00	0.80
12	40.00	2.90	35	67.00	15.61	58	94.00	2.60	81	123.00	13.81
13	41.00	60.06	36	68.00	21.42	59	95.00	2.70	82	124.00	1.40
14	42.00	3.80	37	69.00	100.00	60	96.00	3.20	83	125.00	0.20
15	43.00	6.01	38	70.00	8.61	61	97.00	2.20	84	126.00	0.10
16	44.00	0.70	39	71.00	7.01	62	98.00	1.50	85	135.00	0.10
17	45.00	0.50	40	72.00	1.00	63	99.00	0.20	86	136.00	2.80
18	50.00	1.00	41	74.00	0.10	64	103.00	0.30	87	137.00	0.40
19	51.00	3.00	42	75.00	0.10	65	104.00	0.10	88	139.00	3.10
20	52.00	1.40	43	76.00	0.10	66	105.00	1.10	89	140.00	0.30
21	53.00	11.21	44	77.00	3.60	67	106.00	0.30	90	154.00	1.20
22	54.00	1.60	45	78.00	0.70	68	107.00	2.40	91	155.00	0.10
23	55.00	9.61	46	79.00	4.00	69	108.00	0.80			

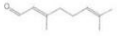


Compound Information

Entry:9502 Library:NIST11S.LIB
Formula:C10H16O CAS:141-27-5 MolWeight:152 RetIndex:1174
CompName:2,6-Octadienal, 3,7-dimethyl-, (E)- $$ .alpha.-Citral $$ (E)-Citral $$ trans-Citral $$ trans-3,7-Dimethyl-2,6-octadienal $$ Citral a $$ Geranaldeh



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.20	25	57.00	0.80	49	82.00	4.90	73	111.00	0.20
2	26.00	0.40	26	58.00	0.10	50	83.00	11.00	74	115.00	0.20
3	27.00	8.60	27	59.00	4.30	51	84.00	25.40	75	116.00	0.10
4	28.00	0.50	28	60.00	0.20	52	85.00	1.50	76	117.00	0.20
5	29.00	7.80	29	61.00	0.20	53	86.00	0.10	77	118.00	0.10
6	30.00	0.20	30	62.00	0.50	54	89.00	0.20	78	119.00	2.60
7	31.00	0.20	31	63.00	1.20	55	90.00	0.10	79	120.00	0.30
8	37.00	0.30	32	64.00	0.30	56	91.00	3.70	80	121.00	0.90
9	38.00	1.20	33	65.00	3.50	57	92.00	0.90	81	122.00	0.20
10	39.00	23.60	34	66.00	1.20	58	93.00	1.70	82	123.00	7.90
11	40.00	3.80	35	67.00	10.40	59	94.00	15.70	83	124.00	1.30
12	41.00	86.50	36	68.00	2.50	60	95.00	5.10	84	125.00	0.10
13	42.00	4.30	37	69.00	100.00	61	96.00	1.30	85	133.00	0.10
14	43.00	5.00	38	70.00	6.50	62	97.00	0.50	86	134.00	1.20
15	44.00	0.40	39	71.00	0.40	63	98.00	0.10	87	135.00	0.20
16	45.00	0.20	40	72.00	0.30	64	102.00	0.10	88	136.00	0.10
17	49.00	0.10	41	74.00	0.20	65	103.00	0.40	89	137.00	8.30
18	50.00	1.80	42	75.00	0.10	66	104.00	0.10	90	138.00	0.80
19	51.00	4.70	43	76.00	0.10	67	105.00	1.00	91	151.00	0.10
20	52.00	2.00	44	77.00	3.80	68	106.00	0.30	92	152.00	3.90
21	53.00	14.20	45	78.00	0.90	69	107.00	1.30	93	153.00	0.50
22	54.00	3.30	46	79.00	4.40	70	108.00	1.40			
23	55.00	7.90	47	80.00	1.90	71	109.00	9.60			
24	56.00	4.50	48	81.00	7.30	72	110.00	2.00			

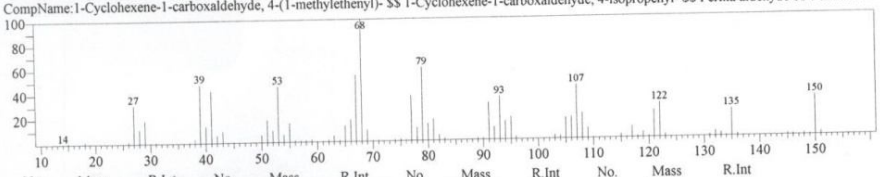


Compound Information

Entry:15335 Library:NIST11.LIB

Formula:C10H14O CAS:2111-75-3 MolWeight:150 RetIndex:1207

CompName:1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)- $$ 1-Cyclohexene-1-carboxaldehyde, 4-isopropenyl- $$ Perilla aldehyde $$ Perillal $$ l



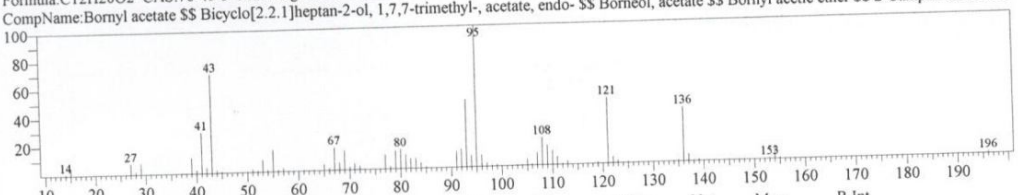
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	0.50	23	54.00	6.11	45	78.00	10.71	67	110.00	0.70
2	15.00	1.10	24	55.00	15.31	46	79.00	60.06	68	115.00	3.00
3	16.00	0.50	25	56.00	1.50	47	80.00	13.71	69	116.00	0.70
4	18.00	1.90	26	57.00	1.30	48	81.00	17.22	70	117.00	9.21
5	26.00	1.60	27	58.00	1.50	49	82.00	4.40	71	118.00	1.30
6	27.00	31.13	28	59.00	1.90	50	83.00	1.90	72	119.00	4.70
7	28.00	11.51	29	60.00	0.60	51	89.00	1.50	73	120.00	1.30
8	29.00	18.42	30	61.00	0.70	52	90.00	1.40	74	121.00	22.22
9	31.00	1.10	31	62.00	1.60	53	91.00	30.23	75	122.00	28.33
10	37.00	0.70	32	63.00	4.90	54	92.00	10.31	76	123.00	2.90
11	38.00	3.10	33	64.00	1.20	55	93.00	35.13	77	131.00	1.50
12	39.00	47.64	34	65.00	12.81	56	94.00	15.11	78	132.00	4.50
13	40.00	13.51	35	66.00	17.62	57	95.00	18.32	79	133.00	3.10
14	41.00	42.24	36	67.00	54.26	58	96.00	2.30	80	134.00	0.80
15	42.00	6.11	37	68.00	100.00	59	102.00	0.50	81	135.00	22.52
16	43.00	9.31	38	69.00	9.41	60	103.00	3.10	82	136.00	1.90
17	44.00	0.60	39	70.00	1.00	61	104.00	2.40	83	145.00	1.70
18	45.00	0.60	40	71.00	0.70	62	105.00	17.22	84	146.00	1.30
19	50.00	6.11	41	74.00	1.20	63	106.00	17.92	85	148.00	1.70
20	51.00	18.02	42	75.00	1.70	64	107.00	43.84	86	149.00	1.10
21	52.00	9.61	43	76.00	1.30	65	108.00	20.62	87	150.00	32.83
22	53.00	45.64	44	77.00	36.73	66	109.00	8.41	88	151.00	2.90

Compound Information

Entry:41489 Library:NIST11.LIB

Formula:C12H20O2 CAS:76-49-3 MolWeight:196 RetIndex:1277

CompName:Bornyl acetate $$ Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, endo- $$ Borneol, acetate $$ Bornyl acetic ether $$ 2-Camphanol acetate



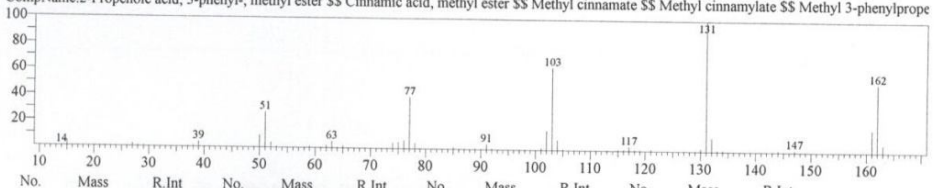
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	0.90	28	58.00	0.30	55	87.00	0.10	82	117.00	0.30
2	15.00	5.30	29	59.00	0.40	56	89.00	0.20	83	119.00	1.30
3	16.00	0.10	30	60.00	0.20	57	90.00	0.10	84	121.00	46.64
4	17.00	0.10	31	61.00	0.60	58	91.00	11.41	85	122.00	4.60
5	26.00	0.40	32	62.00	0.20	59	92.00	12.61	86	123.00	2.00
6	27.00	7.61	33	63.00	0.60	60	93.00	47.74	87	124.00	0.20
7	28.00	2.00	34	64.00	0.10	61	94.00	8.01	88	125.00	1.00
8	29.00	7.81	35	65.00	4.30	62	95.00	100.00	89	126.00	0.30
9	30.00	0.20	36	66.00	1.40	63	96.00	8.41	90	127.00	0.20
10	31.00	0.40	37	67.00	16.11	64	97.00	2.40	91	128.00	0.10
11	37.00	0.10	38	68.00	5.00	65	98.00	1.00	92	134.00	0.20
12	38.00	0.30	39	69.00	13.61	66	99.00	1.20	93	135.00	1.10
13	39.00	11.11	40	70.00	2.20	67	100.00	0.20	94	136.00	38.63
14	40.00	2.30	41	71.00	4.40	68	102.00	0.10	95	137.00	5.20
15	41.00	28.63	42	72.00	2.60	69	103.00	0.60	96	138.00	0.40
16	42.00	4.00	43	73.00	0.20	70	104.00	0.20	97	139.00	1.20
17	43.00	69.77	44	75.00	0.10	71	105.00	4.30	98	140.00	0.10
18	44.00	2.10	45	77.00	10.11	72	106.00	0.90	99	141.00	0.10
19	45.00	1.00	46	78.00	1.90	73	107.00	8.61	100	151.00	0.10
20	50.00	0.50	47	79.00	12.61	74	108.00	19.52	101	152.00	0.30
21	51.00	2.10	48	80.00	13.41	75	109.00	13.81	102	153.00	0.80
22	52.00	1.10	49	81.00	9.81	76	110.00	10.31	103	154.00	9.01
23	53.00	8.51	50	82.00	6.81	77	111.00	5.61	104	155.00	1.10
24	54.00	1.50	51	83.00	7.01	78	112.00	0.90	105	156.00	0.10
25	55.00	15.41	52	84.00	3.90	79	113.00	2.40	106	163.00	0.10
26	56.00	1.30	53	85.00	1.20	80	114.00	0.30	107	196.00	1.50
27	57.00	2.40	54	86.00	0.40	81	115.00	0.20	108	197.00	0.20

Compound Information

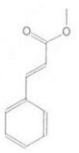
Entry:21207 Library:NIST11.LIB

Formula:C10H10O2 CAS:103-26-4 MolWeight:162 RetIndex:1267

CompName:2-Propenoic acid, 3-phenyl-, methyl ester $$ Cinnamic acid, methyl ester $$ Methyl cinnamate $$ Methyl cinnamylate $$ Methyl 3-phenylprope



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	0.10	23	54.00	0.10	45	86.00	0.30	67	118.00	0.99
2	15.00	4.19	24	55.00	0.10	46	87.00	0.50	68	119.00	0.90
3	18.00	0.20	25	59.00	1.19	47	88.00	0.10	69	120.00	0.10
4	26.00	0.50	26	60.00	0.10	48	89.00	0.80	70	121.00	1.59
5	27.00	2.19	27	61.00	0.70	49	90.00	0.70	71	122.00	0.10
6	28.00	0.99	28	62.00	1.99	50	91.00	4.09	72	129.00	0.50
7	29.00	1.09	29	63.00	5.09	51	92.00	0.90	73	130.00	2.29
8	30.00	0.40	30	64.00	0.70	52	93.00	0.10	74	131.00	100.00
9	31.00	0.30	31	65.00	1.79	53	97.00	0.10	75	132.00	10.29
10	37.00	0.60	32	66.00	0.20	54	98.00	0.60	76	133.00	0.99
11	38.00	1.49	33	67.00	0.20	55	99.00	0.20	77	134.00	0.99
12	39.00	4.09	34	69.00	0.60	56	101.00	1.59	78	135.00	0.10
13	40.00	0.20	35	73.00	0.50	57	102.00	14.89	79	144.00	1.29
14	41.00	0.20	36	74.00	4.39	58	103.00	63.20	80	145.00	0.30
15	43.00	0.10	37	75.00	4.89	59	104.00	7.89	81	146.00	0.20
16	44.00	0.10	38	76.00	6.29	60	105.00	1.09	82	147.00	1.69
17	45.00	0.20	39	77.00	39.49	61	106.00	0.10	83	148.00	0.20
18	49.00	0.60	40	78.00	4.39	62	107.00	0.40	84	160.00	0.20
19	50.00	9.29	41	79.00	0.30	63	108.00	0.10	85	161.00	17.09
20	51.00	27.09	42	81.00	0.10	64	115.00	0.99	86	162.00	52.00
21	52.00	3.89	43	84.00	0.10	65	116.00	1.09	87	163.00	5.89
22	53.00	1.09	44	85.00	1.49	66	117.00	3.19	88	164.00	0.50

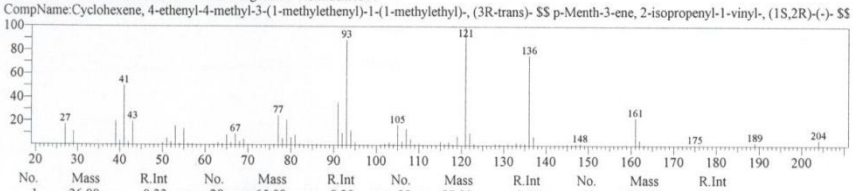


Compound Information

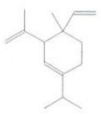
Entry:46695 Library:NIST11.LIB

Formula:C15H24 CAS:20307-84-0 MolWeight:204 RetIndex:1377

CompName:Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R-trans)- $$ p-Menth-3-ene, 2-isopropenyl-1-vinyl-, (1S,2R)-(-)- $$



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.33	28	65.00	8.29	55	97.00	0.45	82	132.00	0.48
2	27.00	17.33	29	66.00	2.04	56	98.00	0.57	83	133.00	2.31
3	28.00	0.38	30	67.00	9.26	57	101.00	0.64	84	134.00	1.69
4	29.00	11.15	31	68.00	3.08	58	102.00	1.11	85	135.00	1.80
5	32.00	0.35	32	69.00	4.79	59	103.00	2.31	86	136.00	75.68
6	37.00	0.64	33	70.00	0.61	60	104.00	1.01	87	137.00	7.26
7	38.00	0.48	34	71.00	0.52	61	105.00	16.77	88	138.00	0.29
8	39.00	19.78	35	74.00	0.37	62	106.00	3.49	89	141.00	0.21
9	40.00	3.70	36	75.00	0.57	63	107.00	13.65	90	142.00	0.24
10	41.00	50.04	37	76.00	0.64	64	108.00	5.21	91	143.00	0.33
11	42.00	2.29	38	77.00	25.08	65	109.00	1.22	92	145.00	1.04
12	43.00	19.70	39	78.00	5.53	66	110.00	1.45	93	146.00	0.52
13	48.00	0.47	40	79.00	21.17	67	111.00	0.22	94	147.00	1.27
14	49.00	0.29	41	80.00	6.23	68	114.00	0.36	95	148.00	1.42
15	50.00	1.83	42	81.00	8.41	69	115.00	2.73	96	149.00	0.69
16	51.00	5.67	43	82.00	1.13	70	116.00	1.19	97	159.00	0.31
17	52.00	2.60	44	83.00	0.29	71	117.00	2.78	98	161.00	23.13
18	53.00	16.00	45	84.00	0.70	72	118.00	0.96	99	162.00	4.41
19	54.00	1.38	46	85.00	0.39	73	119.00	7.49	100	163.00	0.56
20	55.00	13.54	47	86.00	0.80	74	121.00	100.00	101	175.00	0.51
21	56.00	0.94	48	87.00	0.28	75	122.00	10.21	102	176.00	0.35
22	57.00	0.97	49	91.00	35.91	76	123.00	1.42	103	189.00	2.69
23	58.00	0.25	50	92.00	10.12	77	125.00	0.18	104	190.00	0.32
24	59.00	0.44	51	93.00	88.87	78	128.00	1.38	105	204.00	4.77
25	62.00	0.68	52	94.00	12.49	79	129.00	1.05	106	205.00	0.68
26	63.00	2.14	53	95.00	2.82	80	130.00	0.66			
27	64.00	1.27	54	96.00	0.29	81	131.00	1.61			

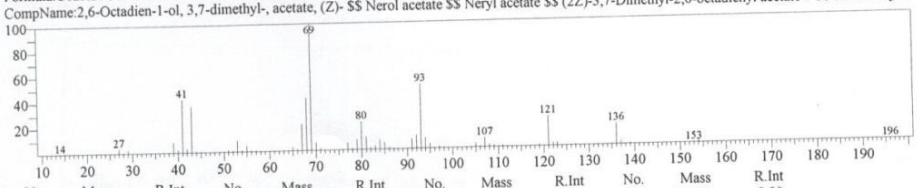


Compound Information

Entry:41462 Library:NIST11.LIB

Formula:C12H20O2 CAS:141-12-8 MolWeight:196 RetIndex:1352

CompName:2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)- $$ Nerol acetate $$ Neryl acetate $$ (2Z)-3,7-Dimethyl-2,6-octadienyl acetate # $$ cis-Geranyl a



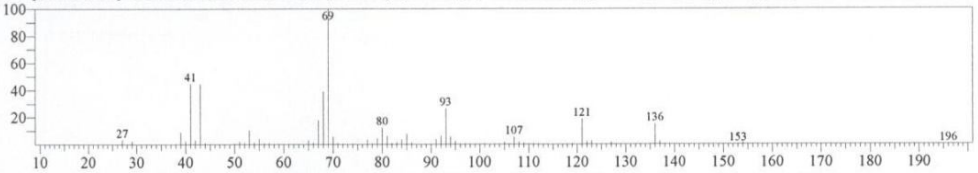
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	0.10	27	59.00	0.30	53	86.00	1.30	79	115.00	0.30
2	15.00	0.70	28	60.00	0.40	54	87.00	0.10	80	116.00	0.10
3	26.00	0.20	29	61.00	0.40	55	89.00	0.10	81	117.00	0.30
4	27.00	3.60	30	62.00	0.10	56	91.00	7.71	82	118.00	0.10
5	28.00	0.70	31	63.00	0.50	57	92.00	10.61	83	119.00	1.20
6	29.00	2.80	32	64.00	0.10	58	93.00	50.56	84	120.00	0.40
7	30.00	0.10	33	65.00	3.10	59	94.00	8.21	85	121.00	23.52
8	31.00	0.10	34	66.00	1.30	60	95.00	3.60	86	122.00	2.40
9	37.00	0.10	35	67.00	20.92	61	96.00	0.50	87	123.00	2.60
10	38.00	0.30	36	68.00	41.54	62	97.00	1.70	88	124.00	0.30
11	39.00	8.21	37	69.00	100.00	63	98.00	0.80	89	125.00	0.10
12	40.00	2.40	38	70.00	6.11	64	99.00	0.20	90	126.00	0.60
13	41.00	41.74	39	71.00	1.50	65	101.00	0.40	91	127.00	1.10
14	42.00	3.00	40	72.00	0.30	66	102.00	0.10	92	128.00	0.10
15	43.00	36.23	41	73.00	0.10	67	103.00	0.50	93	134.00	0.10
16	44.00	1.10	42	74.00	0.10	68	104.00	0.20	94	135.00	0.40
17	45.00	0.60	43	75.00	0.10	69	105.00	3.30	95	136.00	16.41
18	50.00	0.50	44	77.00	5.30	70	106.00	0.80	96	137.00	2.60
19	51.00	1.70	45	78.00	1.10	71	107.00	7.21	97	138.00	0.40
20	52.00	1.00	46	79.00	7.61	72	108.00	2.00	98	139.00	1.00
21	53.00	9.11	47	80.00	21.92	73	109.00	1.50	99	140.00	0.10
22	54.00	1.20	48	81.00	10.01	74	110.00	0.40	100	153.00	0.20
23	55.00	4.50	49	82.00	1.50	75	111.00	1.10	101	154.00	2.60
24	56.00	1.00	50	83.00	2.70	76	112.00	0.30	102	155.00	0.30
25	57.00	0.80	51	84.00	7.21	77	113.00	0.10	103	196.00	0.10
26	58.00	0.10	52	85.00	5.30	78	114.00	0.10			

Compound Information

Entry:41457 Library:NIST11.LIB

Formula:C12H20O2 CAS:105-87-3 MolWeight:196 RetIndex:1352

CompName:Geranyl acetate $$ 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)- $$ Acetic acid, geraniol ester $$ Bay pine (oyster) oil $$ Geraniol acetate $$ t



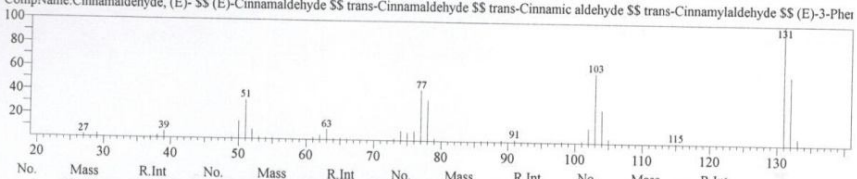
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.70	25	59.00	0.20	49	86.00	1.50	73	113.00	0.10
2	26.00	0.20	26	60.00	0.10	50	87.00	0.10	74	114.00	0.10
3	27.00	3.50	27	61.00	0.40	51	89.00	0.10	75	115.00	0.10
4	29.00	2.60	28	62.00	0.10	52	91.00	3.90	76	117.00	0.10
5	30.00	0.10	29	63.00	0.50	53	92.00	6.30	77	119.00	0.70
6	31.00	0.10	30	64.00	0.10	54	93.00	26.50	78	121.00	18.60
7	37.00	0.10	31	65.00	3.00	55	94.00	5.60	79	122.00	2.00
8	38.00	0.30	32	66.00	1.20	56	95.00	2.40	80	123.00	2.90
9	39.00	9.20	33	67.00	17.60	57	96.00	0.30	81	124.00	0.30
10	40.00	2.50	34	68.00	39.10	58	97.00	0.60	82	125.00	0.10
11	41.00	44.70	35	69.00	100.00	59	98.00	0.40	83	126.00	0.30
12	42.00	3.30	36	70.00	5.90	60	99.00	0.20	84	127.00	1.70
13	43.00	44.70	37	71.00	1.10	61	101.00	0.60	85	128.00	0.20
14	44.00	1.20	38	72.00	0.20	62	102.00	0.10	86	135.00	0.30
15	45.00	0.40	39	73.00	0.10	63	103.00	0.30	87	136.00	15.10
16	50.00	0.60	40	77.00	3.50	64	104.00	0.10	88	137.00	2.40
17	51.00	2.00	41	78.00	0.70	65	105.00	1.70	89	138.00	0.50
18	52.00	1.20	42	79.00	4.70	66	106.00	0.50	90	139.00	0.50
19	53.00	10.40	43	80.00	12.20	67	107.00	5.50	91	140.00	0.10
20	54.00	1.40	44	81.00	6.30	68	108.00	1.80	92	153.00	0.30
21	55.00	4.50	45	82.00	1.10	69	109.00	1.30	93	154.00	1.70
22	56.00	0.90	46	83.00	1.50	70	110.00	0.30	94	155.00	0.20
23	57.00	1.00	47	84.00	3.40	71	111.00	0.60	95	196.00	0.10
24	58.00	0.10	48	85.00	7.80	72	112.00	0.20			

Compound Information

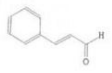
Entry:8563 Library:NIST11.LIB

Formula:C9H8O CAS:14371-10-9 MolWeight:132 RetIndex:1189

CompName:Cinnamaldehyde, (E)- $$ (E)-Cinnamaldehyde $$ trans-Cinnamaldehyde $$ trans-Cinnamic aldehyde $$ trans-Cinnamylaldehyde $$ (E)-3-Phen



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	25.00	0.10	18	52.00	7.90	35	77.00	42.60	52	101.00	1.60
2	26.00	0.70	19	53.00	1.90	36	78.00	34.30	53	102.00	12.40
3	27.00	2.00	20	54.00	1.20	37	79.00	2.30	54	103.00	58.50
4	28.00	0.10	21	55.00	1.20	38	80.00	0.10	55	104.00	27.80
5	29.00	3.00	22	57.00	0.10	39	84.00	0.10	56	105.00	3.60
6	36.00	0.10	23	60.00	0.20	40	85.00	0.50	57	106.00	0.20
7	37.00	1.00	24	61.00	1.90	41	86.00	0.80	58	109.00	0.10
8	38.00	2.00	25	62.00	4.10	42	87.00	1.10	59	110.00	0.10
9	39.00	5.40	26	63.00	8.60	43	88.00	0.30	60	113.00	0.20
10	40.00	0.20	27	64.00	1.00	44	89.00	1.50	61	114.00	0.10
11	41.00	0.20	28	65.00	1.50	45	90.00	0.20	62	115.00	0.90
12	42.00	0.10	29	66.00	1.00	46	91.00	2.20	63	116.00	0.10
13	43.00	0.10	30	72.00	0.10	47	92.00	0.20	64	129.00	0.20
14	48.00	0.10	31	73.00	1.40	48	97.00	0.30	65	131.00	100.00
15	49.00	1.30	32	74.00	8.10	49	98.00	1.20	66	132.00	57.60
16	50.00	14.60	33	75.00	6.60	50	99.00	0.30	67	133.00	5.70
17	51.00	32.70	34	76.00	7.80	51	100.00	0.10	68	134.00	0.40

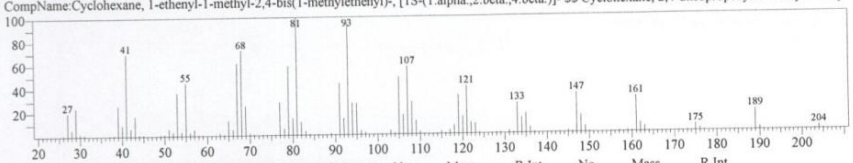


Compound Information

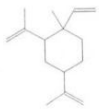
Entry:18058 Library:NIST11S.LIB

Formula:C15H24 CAS:515-13-9 MolWeight:204 RetIndex:1398

CompName:Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1.alpha.,2.beta.,4.beta.)]- $$ Cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl

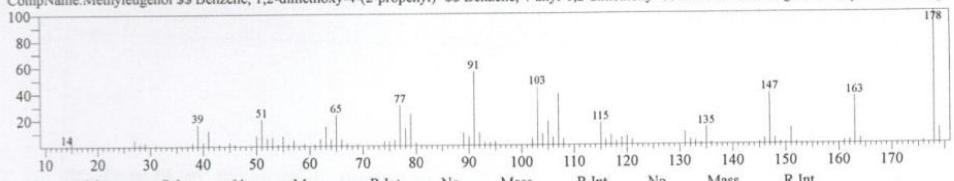


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	1.00	32	67.00	61.34	63	103.00	3.32	94	143.00	0.52
2	27.00	19.88	33	68.00	72.00	64	104.00	1.44	95	144.00	0.47
3	28.00	5.58	34	69.00	25.19	65	105.00	48.85	96	145.00	1.80
4	29.00	24.13	35	70.00	1.76	66	106.00	16.71	97	146.00	0.92
5	30.00	2.13	36	71.00	0.72	67	107.00	57.45	98	147.00	33.74
6	31.00	1.49	37	73.00	0.68	68	108.00	27.68	99	148.00	14.86
7	37.00	0.47	38	74.00	0.43	69	109.00	11.36	100	149.00	5.36
8	38.00	0.82	39	75.00	0.40	70	110.00	2.15	101	150.00	0.88
9	39.00	26.00	40	76.00	0.64	71	111.00	0.36	102	155.00	0.37
10	40.00	9.31	41	77.00	27.92	72	115.00	2.35	103	157.00	0.73
11	41.00	69.62	42	78.00	5.36	73	116.00	0.58	104	159.00	1.50
12	42.00	6.43	43	79.00	58.51	74	117.00	3.18	105	160.00	1.09
13	43.00	16.96	44	80.00	14.52	75	118.00	7.37	106	161.00	30.40
14	44.00	1.20	45	81.00	100.00	76	119.00	33.03	107	162.00	7.70
15	45.00	0.95	46	82.00	11.12	77	120.00	14.94	108	163.00	4.77
16	49.00	1.15	47	83.00	3.43	78	121.00	40.61	109	164.00	0.69
17	50.00	1.43	48	84.00	0.87	79	122.00	9.68	110	173.00	0.55
18	51.00	5.80	49	85.00	0.30	80	123.00	8.60	111	175.00	5.90
19	52.00	3.41	50	86.00	0.54	81	124.00	1.08	112	176.00	2.59
20	53.00	36.56	51	87.00	0.30	82	127.00	0.37	113	177.00	0.66
21	54.00	3.34	52	89.00	1.63	83	128.00	0.85	114	187.00	0.30
22	55.00	44.70	53	90.00	0.37	84	129.00	1.09	115	189.00	18.12
23	56.00	3.08	54	91.00	43.79	85	131.00	2.39	116	190.00	2.91
24	57.00	5.52	55	92.00	14.25	86	132.00	1.09	117	191.00	0.61
25	58.00	1.07	56	93.00	94.84	87	133.00	25.81	118	193.00	0.44
26	59.00	0.71	57	94.00	27.37	88	134.00	13.25	119	203.00	0.36
27	62.00	0.41	58	95.00	26.76	89	135.00	16.97	120	204.00	3.43
28	63.00	2.13	59	96.00	3.54	90	136.00	4.98	121	205.00	0.66
29	64.00	1.17	60	97.00	2.22	91	137.00	0.76			
30	65.00	12.70	61	99.00	0.30	92	141.00	0.47			
31	66.00	5.06	62	102.00	0.43	93	142.00	0.35			

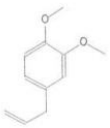


Compound Information

Entry:14052 Library:NIST11S.LIB
Formula:C11H14O2 CAS:93-15-2 MolWeight:178 RetIndex:1361
CompName:Methyleugenol $$ Benzene, 1,2-dimethoxy-4-(2-propenyl)- $$ Benzene, 4-allyl-1,2-dimethoxy- $$ Ent 21040 $$ Eugenol methyl ether $$ Euge

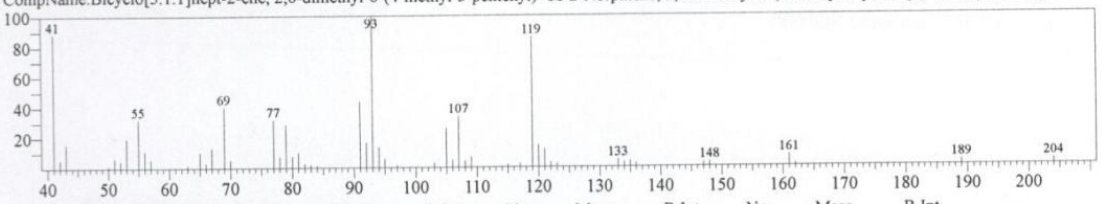


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	14.00	0.59	21	56.00	1.38	41	91.00	56.01	61	132.00	4.09
2	15.00	8.42	22	57.00	4.61	42	92.00	9.70	62	133.00	2.95
3	27.00	5.03	23	59.00	1.95	43	93.00	2.11	63	134.00	1.29
4	28.00	1.86	24	61.00	1.45	44	94.00	1.72	64	135.00	13.09
5	29.00	2.94	25	62.00	5.39	45	95.00	2.72	65	136.00	1.64
6	31.00	0.99	26	63.00	14.72	46	102.00	5.13	66	145.00	1.45
7	32.00	0.27	27	64.00	5.37	47	103.00	43.99	67	146.00	4.15
8	38.00	2.90	28	65.00	23.43	48	104.00	8.40	68	147.00	38.83
9	39.00	16.59	29	66.00	5.16	49	105.00	18.25	69	148.00	4.46
10	40.00	3.06	30	67.00	2.01	50	106.00	5.76	70	149.00	1.81
11	41.00	11.91	31	69.00	1.32	51	107.00	39.25	71	150.00	1.29
12	43.00	1.47	32	74.00	3.45	52	108.00	4.53	72	151.00	12.47
13	45.00	3.11	33	75.00	3.39	53	115.00	16.87	73	152.00	1.31
14	46.00	1.38	34	76.00	4.20	54	116.00	4.03	74	161.00	2.29
15	50.00	8.10	35	77.00	30.75	55	117.00	7.42	75	162.00	2.83
16	51.00	20.40	36	78.00	13.39	56	118.00	3.04	76	163.00	35.60
17	52.00	6.06	37	79.00	24.08	57	119.00	5.33	77	164.00	4.01
18	53.00	6.67	38	80.00	2.28	58	120.00	6.92	78	176.00	1.72
19	54.00	1.42	39	89.00	9.57	59	121.00	3.58	79	178.00	100.00
20	55.00	7.55	40	90.00	6.60	60	131.00	9.63	80	179.00	11.24



Compound Information

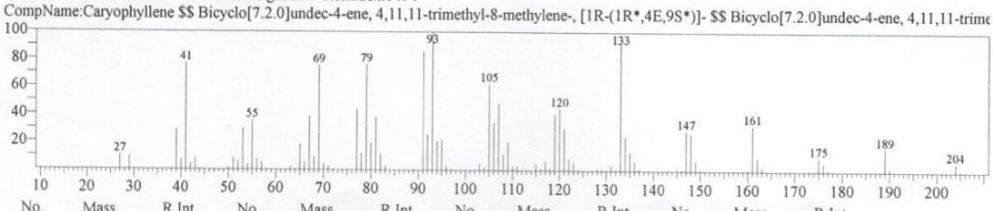
Entry:46623 Library:NIST11.LIB
Formula:C15H24 CAS:17699-05-7 MolWeight:204 RetIndex:1430
CompName:Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)- $$ 2-Norpinene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)- $$ .alpha.-Bergamoten



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	41.00	88.49	15	69.00	40.36	29	95.00	5.84	43	123.00	2.19
2	42.00	5.44	16	70.00	5.39	30	97.00	1.39	44	133.00	4.84
3	43.00	15.85	17	77.00	31.91	31	103.00	3.09	45	134.00	3.24
4	50.00	1.44	18	78.00	7.54	32	105.00	25.90	46	135.00	3.84
5	51.00	6.39	19	79.00	28.60	33	106.00	4.99	47	136.00	2.34
6	52.00	4.54	20	80.00	7.54	34	107.00	34.01	48	147.00	2.69
7	53.00	19.65	21	81.00	9.74	35	108.00	4.69	49	148.00	2.99
8	55.00	32.16	22	82.00	2.69	36	109.00	6.99	50	161.00	7.34
9	56.00	11.10	23	83.00	2.04	37	115.00	2.04	51	162.00	1.79
10	57.00	5.54	24	84.00	1.44	38	117.00	2.39	52	189.00	3.34
11	63.00	1.79	25	91.00	43.76	39	119.00	85.69	53	204.00	3.59
12	65.00	10.30	26	92.00	16.55	40	120.00	14.40	54	205.00	0.60
13	66.00	3.19	27	93.00	100.00	41	121.00	11.90			
14	67.00	13.10	28	94.00	13.30	42	122.00	2.99			

Compound Information

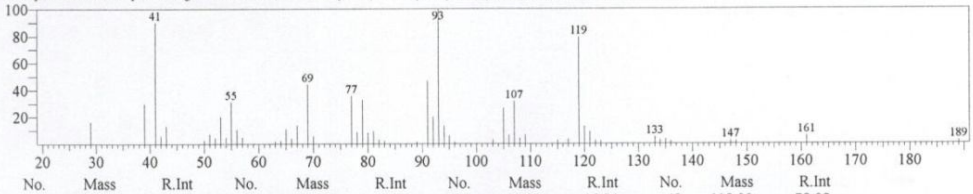
Entry:46636 Library:NIST11.LIB
Formula:C15H24 CAS:87-44-5 MolWeight:204 RetIndex:1494
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trime



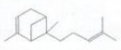
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	15.00	0.20	31	68.00	9.50	61	105.00	62.40	91	136.00	6.60
2	26.00	0.30	32	69.00	75.50	62	106.00	34.20	92	137.00	1.80
3	27.00	10.30	33	70.00	4.70	63	107.00	48.30	93	138.00	0.20
4	29.00	9.40	34	71.00	3.10	64	108.00	11.80	94	141.00	0.30
5	30.00	0.20	35	72.00	0.20	65	109.00	20.50	95	142.00	0.20
6	37.00	0.10	36	74.00	0.20	66	110.00	3.20	96	143.00	0.20
7	38.00	0.70	37	75.00	0.30	67	111.00	3.40	97	144.00	0.10
8	39.00	28.80	38	77.00	43.90	68	112.00	0.50	98	145.00	1.50
9	40.00	7.10	39	78.00	12.00	69	113.00	0.10	99	146.00	1.10
10	41.00	77.00	40	79.00	76.40	70	114.00	0.10	100	147.00	28.90
11	42.00	4.60	41	80.00	19.20	71	115.00	5.00	101	148.00	26.70
12	43.00	8.50	42	81.00	38.60	72	116.00	1.90	102	149.00	7.40
13	44.00	0.30	43	82.00	11.40	73	117.00	6.90	103	150.00	1.00
14	50.00	1.70	44	83.00	3.50	74	118.00	1.90	104	151.00	0.10
15	51.00	8.20	45	84.00	0.50	75	119.00	40.60	105	159.00	0.40
16	52.00	6.30	46	85.00	0.10	76	120.00	44.70	106	160.00	1.00
17	53.00	29.90	47	87.00	0.10	77	121.00	30.50	107	161.00	33.00
18	54.00	4.00	48	89.00	1.00	78	122.00	8.70	108	162.00	9.40
19	55.00	35.60	49	91.00	85.90	79	123.00	6.00	109	163.00	2.80
20	56.00	7.60	50	92.00	25.90	80	124.00	0.90	110	164.00	0.30
21	57.00	5.80	51	93.00	100.00	81	125.00	0.10	111	173.00	0.10
22	58.00	0.60	52	94.00	20.60	82	127.00	0.50	112	174.00	0.10
23	59.00	0.30	53	95.00	21.60	83	128.00	1.60	113	175.00	9.90
24	60.00	0.10	54	96.00	3.00	84	129.00	1.50	114	176.00	6.10
25	62.00	0.40	55	97.00	1.20	85	130.00	0.60	115	177.00	0.80
26	63.00	2.50	56	98.00	0.10	86	131.00	4.20	116	189.00	16.60
27	64.00	1.00	57	101.00	0.10	87	132.00	0.90	117	190.00	2.50
28	65.00	18.30	58	102.00	0.60	88	133.00	92.20	118	191.00	0.20
29	66.00	5.70	59	103.00	5.10	89	134.00	24.40	119	204.00	6.50
30	67.00	38.70	60	104.00	2.50	90	135.00	13.20	120	205.00	1.10

Compound Information

Entry:46622 Library:NIST11.LIB
Formula:C15H24 CAS:13474-59-4 MolWeight:204 RetIndex:1430
CompName:trans-.alpha.-Bergamotene $$ 2,6-Dimethyl-6-(4-methyl-3-pentenyl)bicyclo[3.1.1]hept-2-ene # $$



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	29.00	16.31	15	64.00	2.20	29	91.00	46.84	43	119.00	79.08
2	39.00	29.83	16	65.00	11.21	30	92.00	20.02	44	120.00	12.91
3	41.00	90.09	17	66.00	3.80	31	93.00	100.00	45	121.00	9.01
4	42.00	5.81	18	67.00	13.81	32	94.00	13.31	46	122.00	2.60
5	43.00	13.31	19	69.00	44.24	33	95.00	6.31	47	123.00	2.20
6	50.00	2.60	20	70.00	5.81	34	96.00	1.60	48	133.00	5.10
7	51.00	7.31	21	77.00	35.73	35	103.00	3.10	49	134.00	2.80
8	52.00	4.50	22	78.00	8.61	36	105.00	26.42	50	135.00	3.50
9	53.00	20.02	23	79.00	32.63	37	106.00	6.41	51	136.00	2.00
10	54.00	4.90	24	80.00	8.11	38	107.00	31.53	52	147.00	2.40
11	55.00	31.13	25	81.00	9.51	39	108.00	4.20	53	148.00	2.10
12	56.00	10.71	26	82.00	3.20	40	109.00	6.61	54	161.00	5.81
13	57.00	4.80	27	83.00	2.20	41	115.00	2.70	55	189.00	2.30
14	63.00	2.10	28	89.00	1.70	42	117.00	3.50			

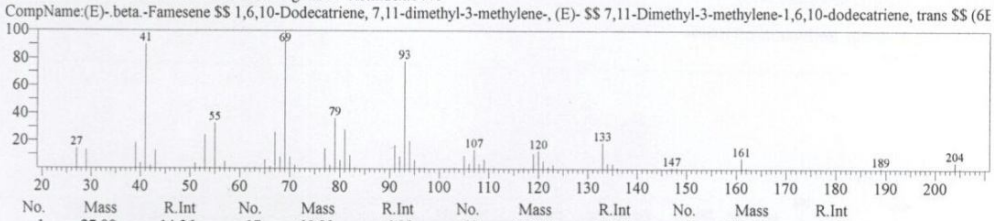


Compound Information

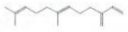
Entry:18051 Library:NIST11S.LIB

Formula:C15H24 CAS:18794-84-8 MolWeight:204 RetIndex:1440

CompName:(E)-.beta.-Famesene $$ 1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (E)- $$ 7,11-Dimethyl-3-methylene-1,6,10-dodecatriene, trans $$ (6E



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	27.00	14.36	17	65.00	6.38	33	93.00	78.19	49	121.00	5.85
2	29.00	13.30	18	66.00	1.60	34	94.00	20.21	50	122.00	1.60
3	39.00	18.62	19	67.00	26.59	35	95.00	6.38	51	123.00	3.19
4	40.00	3.72	20	68.00	8.51	36	96.00	1.06	52	133.00	19.15
5	41.00	90.43	21	69.00	100.00	37	97.00	1.06	53	134.00	4.25
6	42.00	2.13	22	70.00	8.51	38	103.00	1.06	54	135.00	3.72
7	43.00	13.30	23	71.00	2.66	39	105.00	9.57	55	136.00	1.06
8	51.00	3.72	24	77.00	14.89	40	106.00	3.72	56	147.00	1.06
9	52.00	1.06	25	78.00	2.66	41	107.00	13.83	57	148.00	1.06
10	53.00	24.47	26	79.00	36.70	42	108.00	3.72	58	161.00	7.98
11	54.00	1.06	27	80.00	6.38	43	109.00	6.91	59	162.00	1.06
12	55.00	32.98	28	81.00	28.72	44	110.00	0.53	60	189.00	1.06
13	56.00	1.06	29	82.00	9.57	45	111.00	1.06	61	204.00	5.32
14	57.00	5.32	30	83.00	1.06	46	117.00	1.06	62	205.00	1.06
15	58.00	0.53	31	91.00	17.02	47	119.00	11.17			
16	63.00	1.06	32	92.00	9.04	48	120.00	13.30			

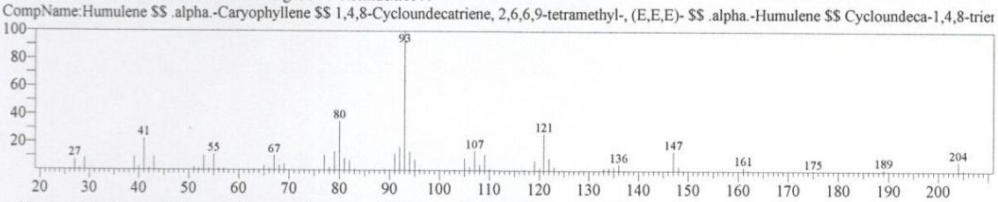


Compound Information

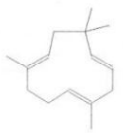
Entry:18070 Library:NIST11S.LIB

Formula:C15H24 CAS:6753-98-6 MolWeight:204 RetIndex:1579

CompName:Humulene $$ .alpha.-Caryophyllene $$ 1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)- $$ .alpha.-Humulene $$ Cycloundeca-1,4,8-trien



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.70	19	65.00	3.50	37	93.00	100.00	55	123.00	2.60
2	27.00	7.61	20	66.00	1.60	38	94.00	13.51	56	133.00	1.90
3	28.00	1.40	21	67.00	10.51	39	95.00	7.81	57	134.00	2.10
4	29.00	8.51	22	68.00	3.40	40	96.00	1.00	58	135.00	2.70
5	39.00	9.21	23	69.00	4.60	41	103.00	0.80	59	136.00	4.60
6	40.00	2.30	24	70.00	0.60	42	105.00	8.71	60	137.00	0.60
7	41.00	22.62	25	75.00	0.50	43	106.00	2.90	61	146.00	0.80
8	42.00	1.70	26	77.00	10.81	44	107.00	14.11	62	147.00	14.11
9	43.00	9.91	27	78.00	2.50	45	108.00	4.30	63	148.00	3.20
10	50.00	0.50	28	79.00	13.51	46	109.00	11.41	64	149.00	0.70
11	51.00	2.00	29	80.00	35.13	47	110.00	1.50	65	161.00	2.80
12	52.00	1.30	30	81.00	8.71	48	111.00	0.50	66	162.00	0.80
13	53.00	10.31	31	82.00	7.31	49	115.00	0.70	67	175.00	0.50
14	54.00	1.30	32	83.00	1.10	50	117.00	0.80	68	189.00	1.70
15	55.00	11.21	33	89.00	0.80	51	119.00	7.31	69	204.00	7.31
16	56.00	1.30	34	90.00	0.50	52	120.00	1.80	70	205.00	1.20
17	57.00	1.00	35	91.00	11.91	53	121.00	26.52			
18	63.00	0.60	36	92.00	16.82	54	122.00	8.91			

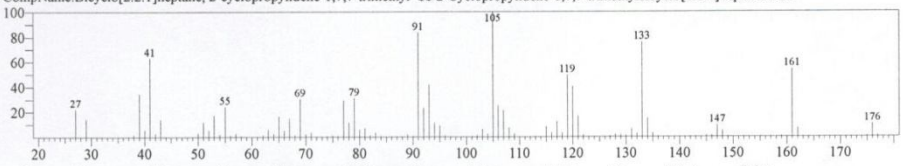


Compound Information

Entry:29328 Library:NIST11.LIB

Formula:C13H20 CAS:0-00-0 MolWeight:176 RetIndex:1251

CompName:Bicyclo[2.2.1]heptane, 2-cyclopropylidene-1,7,7-trimethyl- $$ 2-Cyclopropylidene-1,7,7-trimethylbicyclo[2.2.1]heptane # $$



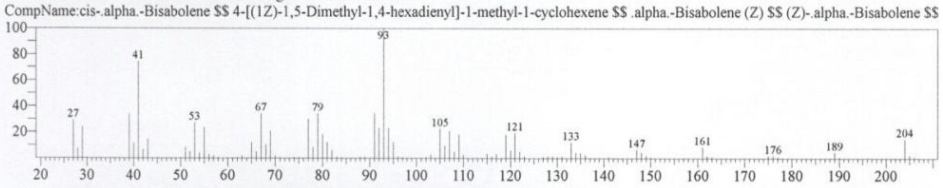
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	27.00	22.21	32	66.00	5.21	63	97.00	0.18	94	129.00	2.28
2	29.00	14.16	33	67.00	14.59	64	98.00	0.10	95	130.00	1.24
3	30.00	0.29	34	68.00	1.62	65	99.00	0.09	96	131.00	6.55
4	36.00	0.02	35	69.00	30.46	66	100.00	0.11	97	132.00	2.78
5	37.00	0.49	36	70.00	2.20	67	101.00	0.45	98	133.00	75.99
6	38.00	1.76	37	71.00	3.86	68	102.00	1.27	99	134.00	14.82
7	39.00	34.82	38	72.00	0.70	69	103.00	6.09	100	135.00	3.12
8	40.00	5.58	39	73.00	0.14	70	104.00	2.69	101	136.00	0.57
9	41.00	63.01	40	74.00	0.84	71	105.00	100.00	102	137.00	0.04
10	42.00	3.11	41	75.00	1.40	72	106.00	25.00	103	139.00	0.04
11	43.00	14.26	42	76.00	0.94	73	107.00	21.31	104	141.00	0.28
12	44.00	0.33	43	77.00	29.60	74	108.00	7.32	105	142.00	0.12
13	45.00	0.05	44	78.00	11.41	75	109.00	2.75	106	143.00	0.27
14	46.00	0.06	45	79.00	31.21	76	110.00	0.35	107	144.00	0.25
15	49.00	0.14	46	80.00	5.74	77	111.00	0.07	108	145.00	1.46
16	50.00	3.31	47	81.00	6.94	78	112.00	0.05	109	146.00	1.37
17	51.00	11.88	48	82.00	1.37	79	113.00	0.18	110	147.00	9.21
18	52.00	5.43	49	83.00	3.39	80	114.00	0.23	111	148.00	5.06
19	53.00	17.37	50	84.00	0.57	81	115.00	8.23	112	149.00	0.58
20	54.00	2.02	51	85.00	0.12	82	116.00	3.36	113	157.00	0.05
21	55.00	24.35	52	86.00	0.22	83	117.00	12.18	114	159.00	0.77
22	56.00	1.46	53	87.00	0.45	84	118.00	3.41	115	160.00	0.28
23	57.00	2.74	54	88.00	0.39	85	119.00	49.35	116	161.00	54.16
24	58.00	0.98	55	89.00	1.94	86	120.00	40.43	117	162.00	7.01
25	59.00	0.30	56	90.00	0.86	87	121.00	16.55	118	163.00	0.43
26	60.00	0.11	57	91.00	83.35	88	122.00	1.88	119	175.00	0.83
27	61.00	0.27	58	92.00	23.04	89	123.00	0.23	120	176.00	10.21
28	62.00	1.36	59	93.00	41.68	90	124.00	0.03	121	177.00	1.50
29	63.00	5.64	60	94.00	11.49	91	126.00	0.12	122	178.00	0.07
30	64.00	2.70	61	95.00	9.12	92	127.00	0.80			
31	65.00	16.50	62	96.00	1.13	93	128.00	2.21			

Compound Information

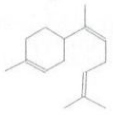
Entry:46619 Library:NIST11.LIB

Formula:C15H24 CAS:29837-07-8 MolWeight:204 RetIndex:1518

CompName:cis-.alpha.-Bisabolene $$ 4-[(1Z)-1,5-Dimethyl-1,4-hexadienyl]-1-methyl-1-cyclohexene $$ .alpha.-Bisabolene (Z) $$ (Z)-.alpha.-Bisabolene $$



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	27.00	29.03	23	67.00	34.43	45	96.00	1.90	67	131.00	1.80
2	28.00	7.51	24	68.00	10.41	46	97.00	0.90	68	133.00	12.51
3	29.00	24.12	25	69.00	21.12	47	102.00	1.00	69	134.00	4.70
4	30.00	0.80	26	70.00	2.00	48	103.00	2.90	70	135.00	4.20
5	39.00	34.23	27	71.00	0.90	49	105.00	22.72	71	136.00	2.80
6	40.00	11.71	28	74.00	0.90	50	106.00	9.51	72	141.00	0.90
7	41.00	74.78	29	75.00	0.90	51	107.00	21.12	73	147.00	6.91
8	42.00	6.71	30	77.00	30.33	52	108.00	5.00	74	148.00	4.60
9	43.00	14.81	31	78.00	8.71	53	109.00	18.52	75	149.00	2.50
10	50.00	0.70	32	79.00	34.43	54	110.00	2.60	76	150.00	1.10
11	51.00	8.41	33	80.00	18.62	55	115.00	3.60	77	161.00	8.91
12	52.00	5.30	34	81.00	12.31	56	116.00	1.60	78	162.00	2.30
13	53.00	27.22	35	82.00	6.21	57	117.00	3.50	79	163.00	1.10
14	54.00	4.00	36	83.00	1.30	58	119.00	18.22	80	175.00	2.20
15	55.00	23.62	37	84.00	0.90	59	120.00	6.21	81	176.00	2.30
16	56.00	3.00	38	88.00	1.00	60	121.00	19.72	82	177.00	1.10
17	57.00	2.10	39	89.00	1.30	61	122.00	5.20	83	189.00	4.80
18	58.00	0.90	40	91.00	34.83	62	123.00	1.60	84	190.00	1.00
19	62.00	0.70	41	92.00	23.32	63	127.00	1.20	85	204.00	15.01
20	63.00	2.30	42	93.00	100.00	64	128.00	1.90	86	205.00	2.60
21	65.00	12.31	43	94.00	23.32	65	129.00	1.60	87	206.00	1.00
22	66.00	5.00	44	95.00	12.71	66	130.00	1.10			

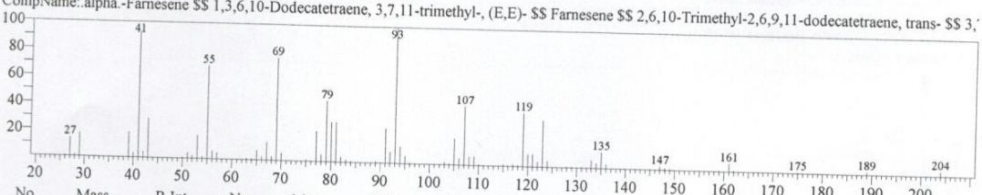


Compound Information

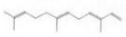
Entry:18064 Library:NIST11S.LIB

Formula:C15H24 CAS:502-61-4 MolWeight:204 RetIndex:1458

CompName:.alpha.-Farnesene $$ 1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (E,E)- $$ Farnesene $$ 2,6,10-Trimethyl-2,6,9,11-dodecatetraene, trans- $$ 3,



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.80	22	66.00	2.80	43	94.00	12.61	64	123.00	34.43
2	27.00	13.91	23	67.00	13.31	44	95.00	5.71	65	124.00	4.70
3	28.00	1.60	24	68.00	2.90	45	96.00	0.80	66	128.00	0.60
4	29.00	17.42	25	69.00	75.68	46	97.00	0.70	67	129.00	0.60
5	32.00	0.70	26	70.00	5.40	47	103.00	1.90	68	131.00	0.80
6	39.00	18.72	27	71.00	0.50	48	104.00	1.10	69	133.00	6.11
7	40.00	3.50	28	75.00	1.20	49	105.00	19.32	70	134.00	3.80
8	41.00	92.89	29	76.00	0.50	50	106.00	5.00	71	135.00	11.91
9	42.00	4.20	30	77.00	22.22	51	107.00	43.24	72	136.00	3.20
10	43.00	28.93	31	78.00	5.00	52	108.00	6.41	73	145.00	0.60
11	50.00	0.90	32	79.00	44.74	53	109.00	6.41	74	147.00	2.60
12	51.00	4.30	33	80.00	29.33	54	110.00	1.00	75	148.00	1.70
13	52.00	2.10	34	81.00	29.13	55	111.00	0.60	76	149.00	1.00
14	53.00	17.32	35	82.00	3.80	56	115.00	1.40	77	159.00	0.70
15	54.00	1.90	36	83.00	1.80	57	116.00	0.70	78	161.00	5.91
16	55.00	68.77	37	84.00	0.70	58	117.00	1.90	79	162.00	1.00
17	56.00	6.11	38	89.00	1.40	59	118.00	1.00	80	175.00	0.70
18	57.00	4.60	39	90.00	0.70	60	119.00	39.44	81	189.00	2.10
19	63.00	1.10	40	91.00	25.42	61	120.00	9.01	82	204.00	3.50
20	64.00	0.90	41	92.00	8.31	62	121.00	9.21	83	205.00	0.60
21	65.00	7.11	42	93.00	100.00	63	122.00	3.80			

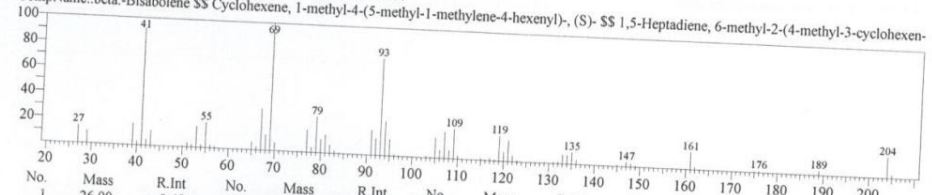


Compound Information

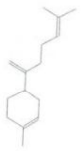
Entry:18054 Library:NIST11S.LIB

Formula:C15H24 CAS:495-61-4 MolWeight:204 RetIndex:1500

CompName:.beta.-Bisabolene $$ Cyclohexene, 1-methyl-4-(5-methyl-1-methylene-4-hexenyl)-, (S)- $$ 1,5-Heptadiene, 6-methyl-2-(4-methyl-3-cyclohexen-



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	26.00	0.48	25	67.00	32.66	49	103.00	1.43	73	133.00	7.10
2	27.00	14.20	26	68.00	12.17	50	104.00	1.02	74	134.00	6.79
3	28.00	0.60	27	69.00	100.00	51	105.00	16.13	75	135.00	9.29
4	29.00	10.14	28	70.00	6.33	52	106.00	6.50	76	136.00	3.59
5	30.00	0.40	29	71.00	0.57	53	107.00	20.67	77	137.00	0.46
6	37.00	0.37	30	75.00	0.38	54	108.00	6.43	78	143.00	0.16
7	38.00	0.35	31	76.00	0.41	55	109.00	23.23	79	145.00	1.29
8	39.00	17.25	32	77.00	17.60	56	110.00	2.54	80	146.00	0.22
9	40.00	3.23	33	78.00	4.08	57	111.00	0.47	81	147.00	3.70
10	41.00	92.00	34	79.00	28.02	58	115.00	1.53	82	148.00	2.77
11	42.00	4.80	35	80.00	10.52	59	116.00	0.55	83	149.00	0.94
12	43.00	12.07	36	81.00	14.24	60	117.00	2.19	84	157.00	0.59
13	50.00	0.78	37	82.00	6.56	61	118.00	1.29	85	159.00	0.38
14	51.00	3.84	38	83.00	2.28	62	119.00	19.68	86	160.00	0.59
15	52.00	2.26	39	84.00	0.33	63	120.00	7.26	87	161.00	13.53
16	53.00	16.67	40	89.00	0.69	64	121.00	16.70	88	162.00	2.22
17	54.00	2.14	41	90.00	0.40	65	122.00	4.78	89	163.00	0.60
18	55.00	19.86	42	91.00	19.66	66	123.00	1.07	90	175.00	1.05
19	56.00	2.43	43	92.00	13.37	67	127.00	0.27	91	176.00	1.39
20	57.00	1.60	44	93.00	76.17	68	128.00	0.27	92	189.00	3.37
21	63.00	0.82	45	94.00	26.99	69	129.00	0.75	93	190.00	0.50
22	64.00	0.33	46	95.00	13.02	70	130.00	0.41	94	202.00	0.47
23	65.00	6.51	47	96.00	1.53	71	131.00	1.29	95	204.00	16.23
24	66.00	2.77	48	97.00	1.04	72	132.00	1.58	96	205.00	2.48

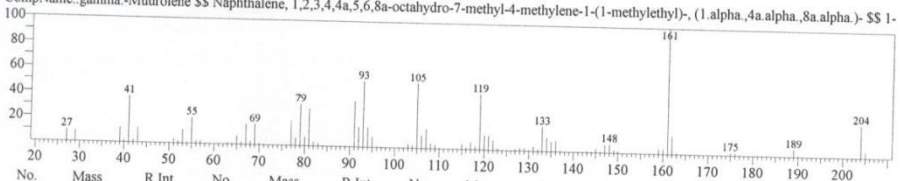


Compound Information

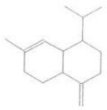
Entry:18125 Library:NIST11S.LIB

Formula:C15H24 CAS:30021-74-0 MolWeight:204 RetIndex:1435

CompName:.gamma.-Muurolene $$ Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1.alpha.,4a.alpha.,8a.alpha.)- $$ 1-



No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	25.00	0.30	27	71.00	0.49	53	107.00	15.46	79	142.00	0.67
2	27.00	9.40	28	75.00	0.59	54	108.00	3.88	80	143.00	0.73
3	29.00	8.81	29	76.00	0.44	55	109.00	2.90	81	144.00	0.63
4	39.00	11.86	30	77.00	19.87	56	110.00	0.77	82	145.00	2.80
5	40.00	1.86	31	78.00	6.15	57	115.00	3.97	83	146.00	1.00
6	41.00	37.01	32	79.00	33.14	58	116.00	1.87	84	147.00	6.40
7	42.00	2.19	33	80.00	7.21	59	117.00	5.82	85	148.00	6.87
8	43.00	11.92	34	81.00	29.76	60	118.00	2.58	86	149.00	2.50
9	44.00	0.17	35	82.00	3.34	61	119.00	44.09	87	150.00	1.65
10	50.00	0.54	36	83.00	2.36	62	120.00	11.62	88	157.00	0.58
11	51.00	3.34	37	84.00	0.47	63	121.00	11.35	89	159.00	3.68
12	52.00	1.86	38	88.00	0.35	64	122.00	8.09	90	160.00	3.67
13	53.00	10.88	39	89.00	0.89	65	123.00	1.77	91	161.00	100.00
14	54.00	1.15	40	90.00	0.52	66	124.00	0.32	92	162.00	14.27
15	55.00	20.68	41	91.00	36.21	67	127.00	1.33	93	163.00	1.09
16	56.00	2.40	42	92.00	15.87	68	128.00	2.25	94	175.00	2.13
17	57.00	2.56	43	93.00	52.57	69	129.00	2.41	95	176.00	1.84
18	58.00	0.36	44	94.00	15.82	70	130.00	1.03	96	177.00	0.35
19	63.00	1.39	45	95.00	8.43	71	131.00	3.39	97	183.00	0.41
20	64.00	0.88	46	96.00	1.06	72	132.00	1.38	98	187.00	0.48
21	65.00	6.89	47	97.00	0.52	73	133.00	19.47	99	189.00	5.82
22	66.00	2.01	48	102.00	0.64	74	134.00	10.80	100	190.00	0.94
23	67.00	16.17	49	103.00	3.34	75	135.00	7.63	101	202.00	0.36
24	68.00	2.67	50	104.00	2.32	76	136.00	8.62	102	204.00	25.77
25	69.00	16.34	51	105.00	51.55	77	137.00	1.12	103	205.00	4.34
26	70.00	1.61	52	106.00	10.21	78	141.00	0.52	104	206.00	0.36

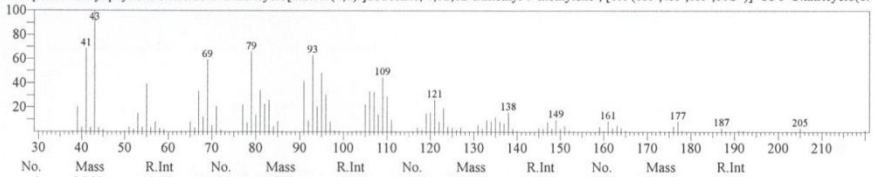


Compound Information

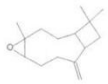
Entry:20008 Library:NIST11S.LIB

Formula:C15H24O CAS:1139-30-6 MolWeight:220 RetIndex:1507

CompName:Caryophyllene oxide $$ 5-Oxatricyclo[8.2.0.0(4,6)-]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- $$ 5-Oxatricyclo(8.

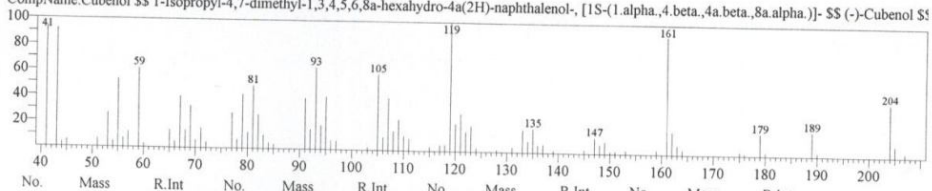


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	36.00	0.13	34	76.00	0.48	67	115.00	0.54	100	150.00	2.67
2	38.00	0.70	35	77.00	22.33	68	116.00	0.42	101	151.00	5.03
3	39.00	20.54	36	78.00	7.54	69	117.00	3.40	102	152.00	1.62
4	40.00	3.69	37	79.00	66.08	70	118.00	2.04	103	153.00	0.52
5	41.00	68.73	38	80.00	14.04	71	119.00	15.21	104	159.00	4.44
6	42.00	3.72	39	81.00	34.24	72	120.00	15.99	105	160.00	1.29
7	43.00	100.00	40	82.00	22.88	73	121.00	26.48	106	161.00	8.92
8	44.00	3.67	41	83.00	26.40	74	122.00	8.53	107	162.00	3.27
9	45.00	2.07	42	84.00	4.57	75	123.00	19.70	108	163.00	5.48
10	46.00	0.19	43	85.00	8.72	76	124.00	4.32	109	164.00	3.64
11	50.00	0.78	44	86.00	0.84	77	125.00	3.42	110	165.00	1.50
12	51.00	3.84	45	89.00	0.22	78	126.00	1.77	111	166.00	0.15
13	52.00	2.46	46	91.00	42.08	79	127.00	3.57	112	173.00	1.06
14	53.00	15.21	47	92.00	9.38	80	128.00	0.46	113	174.00	0.54
15	54.00	3.81	48	93.00	63.26	81	129.00	0.60	114	175.00	0.76
16	55.00	39.39	49	94.00	21.20	82	130.00	0.21	115	176.00	4.53
17	56.00	3.79	50	95.00	48.47	83	131.00	5.77	116	177.00	8.72
18	57.00	8.06	51	96.00	30.82	84	132.00	2.62	117	178.00	1.36
19	58.00	3.01	52	97.00	8.53	85	133.00	9.68	118	179.00	0.18
20	59.00	2.10	53	98.00	1.26	86	134.00	8.69	119	187.00	3.16
21	60.00	0.10	54	99.00	1.08	87	135.00	12.08	120	188.00	0.54
22	63.00	0.88	55	102.00	0.10	88	136.00	8.48	121	189.00	0.37
23	64.00	0.40	56	103.00	1.20	89	137.00	7.30	122	190.00	0.04
24	65.00	8.00	57	104.00	1.23	90	138.00	16.12	123	191.00	1.45
25	66.00	3.45	58	105.00	22.42	91	139.00	2.65	124	192.00	1.30
26	67.00	33.50	59	106.00	33.76	92	140.00	1.15	125	202.00	0.43
27	68.00	12.20	60	107.00	33.10	93	143.00	0.18	126	203.00	0.09
28	69.00	59.50	61	108.00	14.19	94	144.00	0.10	127	204.00	0.07
29	70.00	5.51	62	109.00	44.97	95	145.00	3.34	128	205.00	3.00
30	71.00	20.89	63	110.00	29.26	96	146.00	2.58	129	206.00	0.42
31	72.00	1.78	64	111.00	10.01	97	147.00	7.96	130	220.00	1.59
32	73.00	0.31	65	112.00	0.97	98	148.00	3.10			
33	75.00	0.13	66	113.00	0.27	99	149.00	10.10			

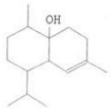


Compound Information

Entry:59424 Library:NIST11.LIB
Formula:C15H26O CAS:21284-22-0 MolWeight:222 RetIndex:1580
CompName:Cubenol $$ 1-Isopropyl-4,7-dimethyl-1,3,4,5,6,8a-hexahydro-4a(2H)-naphthalenol-, [1S-(1.alpha.,4.beta.,4a.beta.,8a.alpha.)]- $$ (-)-Cubenol $$

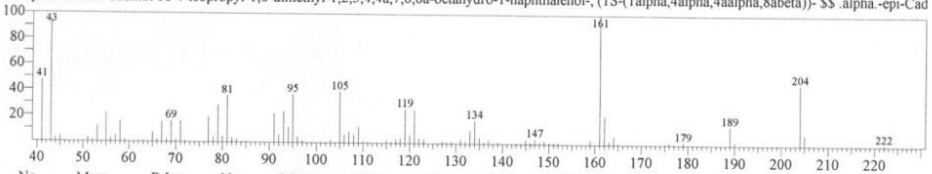


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	41.00	93.74	22	78.00	6.82	43	110.00	11.30	64	148.00	7.01
2	43.00	91.97	23	79.00	42.06	44	111.00	9.15	65	149.00	9.28
3	44.00	3.60	24	80.00	12.19	45	115.00	3.34	66	150.00	1.83
4	45.00	5.49	25	81.00	48.57	46	117.00	4.86	67	151.00	2.08
5	51.00	6.63	26	82.00	26.02	47	118.00	5.05	68	153.00	2.84
6	53.00	26.40	27	83.00	10.67	48	119.00	100.00	69	159.00	3.22
7	54.00	4.61	28	84.00	4.73	49	120.00	21.28	70	161.00	90.96
8	55.00	52.81	29	85.00	3.53	50	121.00	28.86	71	162.00	17.24
9	56.00	6.88	30	91.00	39.28	51	122.00	15.34	72	163.00	7.07
10	57.00	12.06	31	92.00	15.28	52	123.00	19.77	73	164.00	3.60
11	59.00	61.46	32	93.00	63.49	53	124.00	3.03	74	175.00	2.77
12	60.00	2.77	33	94.00	18.44	54	128.00	1.76	75	176.00	1.64
13	65.00	13.64	34	95.00	40.67	55	131.00	3.72	76	179.00	16.73
14	66.00	5.11	35	96.00	7.20	56	133.00	17.18	77	180.00	2.71
15	67.00	40.04	36	97.00	6.82	57	134.00	8.84	78	189.00	18.44
16	68.00	13.70	37	103.00	2.46	58	135.00	18.19	79	190.00	2.90
17	69.00	32.34	38	105.00	58.69	59	136.00	5.74	80	204.00	40.61
18	70.00	6.00	39	106.00	10.04	60	137.00	6.37	81	205.00	8.59
19	71.00	15.22	40	107.00	40.48	61	139.00	2.02	82	207.00	3.28
20	72.00	4.61	41	108.00	14.71	62	145.00	2.96			
21	77.00	27.35	42	109.00	23.62	63	147.00	12.12			

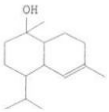


Compound Information

Entry:59439 Library:NIST11.LIB
Formula:C15H26O CAS:5937-11-1 MolWeight:222 RetIndex:1580
CompName:.tau.-Cadinol $$ 4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7,8,8a-octahydro-1-naphthalenol-, (1S-(1alpha,4alpha,4aalpha,8abeta))- $$ .alpha.-epi-Cad

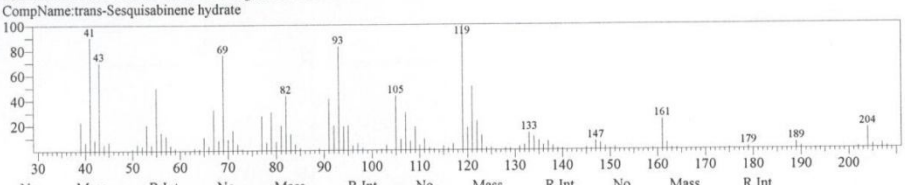


No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	41.00	47.23	25	79.00	28.69	49	116.00	1.01	73	147.00	4.17
2	43.00	94.46	26	80.00	4.67	50	117.00	3.66	74	148.00	1.81
3	44.00	2.84	27	81.00	35.83	51	118.00	3.83	75	149.00	2.55
4	45.00	4.14	28	82.00	3.68	52	119.00	26.31	76	150.00	1.14
5	50.00	0.47	29	83.00	2.41	53	120.00	6.33	77	151.00	1.33
6	51.00	3.16	30	84.00	0.68	54	121.00	25.61	78	152.00	1.48
7	52.00	1.78	31	85.00	0.90	55	122.00	4.29	79	159.00	3.73
8	53.00	12.00	32	91.00	21.89	56	123.00	2.92	80	161.00	100.00
9	55.00	22.37	33	92.00	6.16	57	127.00	1.59	81	162.00	21.71
10	56.00	2.80	34	93.00	23.81	58	128.00	1.24	82	163.00	2.70
11	57.00	4.93	35	94.00	11.86	59	129.00	1.31	83	164.00	6.48
12	58.00	15.68	36	95.00	37.22	60	131.00	3.28	84	165.00	1.07
13	59.00	2.08	37	96.00	4.82	61	132.00	1.60	85	175.00	1.07
14	63.00	0.92	38	97.00	1.72	62	133.00	10.29	86	176.00	1.72
15	65.00	7.27	39	103.00	2.10	63	134.00	17.87	87	177.00	0.85
16	66.00	1.98	40	105.00	39.29	64	135.00	4.50	88	179.00	2.08
17	67.00	14.98	41	106.00	6.71	65	136.00	1.47	89	189.00	14.27
18	68.00	2.34	42	107.00	8.71	66	137.00	3.15	90	190.00	2.46
19	69.00	16.16	43	108.00	6.55	67	138.00	0.68	91	204.00	46.58
20	70.00	2.27	44	109.00	12.53	68	139.00	1.42	92	205.00	8.14
21	71.00	15.85	45	110.00	1.90	69	143.00	0.53	93	206.00	0.77
22	72.00	1.13	46	111.00	1.11	70	144.00	0.53	94	222.00	1.40
23	77.00	18.81	47	113.00	0.49	71	145.00	3.47			
24	78.00	3.90	48	115.00	2.44	72	146.00	1.62			

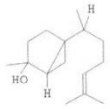


Compound Information

Entry:59425 Library:NIST11.LIB
Formula:C15H26O CAS:0-00-0 MolWeight:222 RetIndex:1523
CompName:trans-Sesquisabinene hydrate

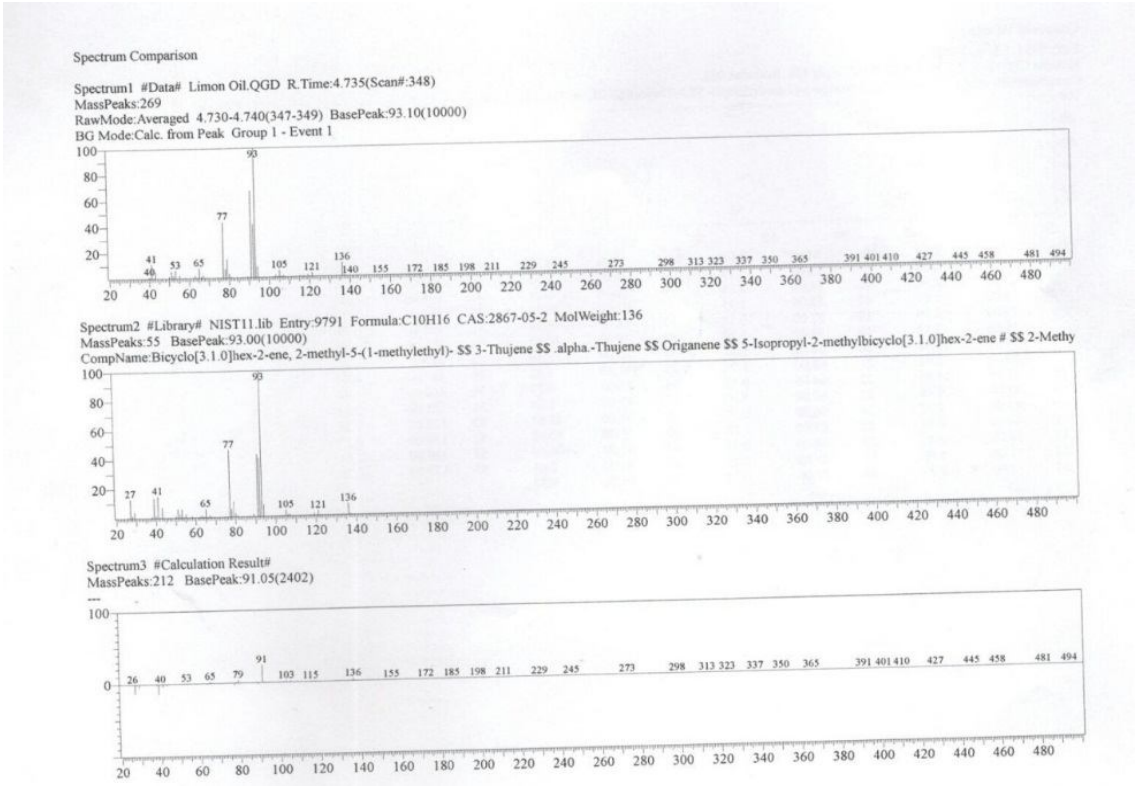


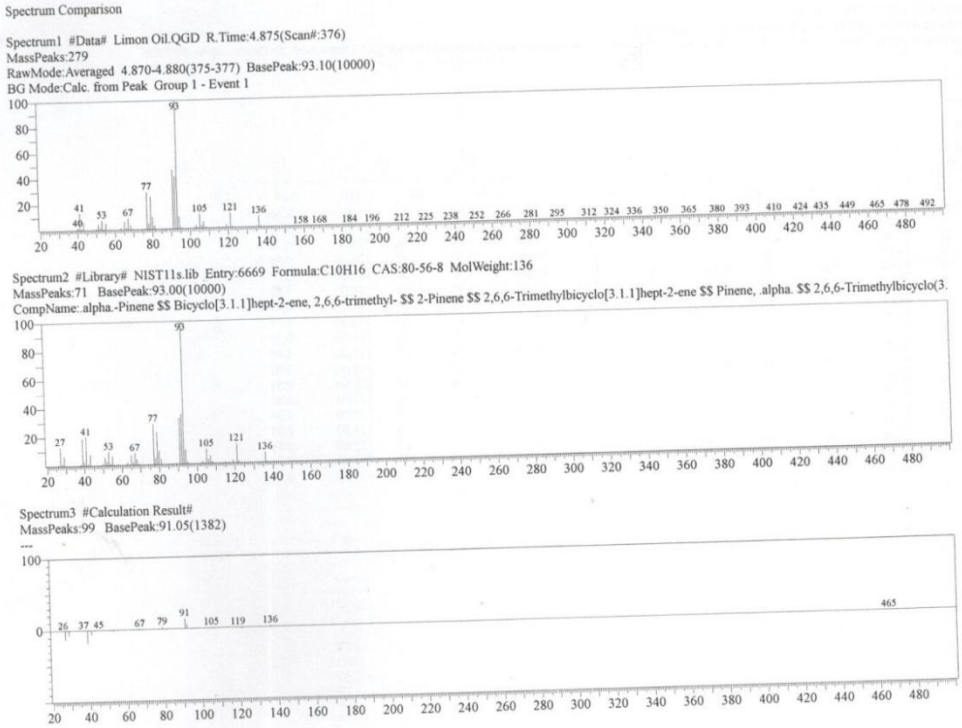
No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int	No.	Mass	R.Int
1	39.00	22.77	26	71.00	15.94	51	107.00	29.79	76	137.00	6.64
2	40.00	6.83	27	72.00	4.93	52	108.00	7.21	77	138.00	3.41
3	41.00	90.14	28	73.00	1.13	53	109.00	18.41	78	139.00	1.33
4	42.00	8.35	29	77.00	27.51	54	110.00	3.99	79	140.00	1.13
5	43.00	70.02	30	78.00	6.45	55	111.00	8.54	80	145.00	1.90
6	44.00	4.93	31	79.00	30.17	56	112.00	1.90	81	146.00	0.94
7	45.00	6.83	32	80.00	6.83	57	113.00	0.94	82	147.00	6.64
8	50.00	1.33	33	81.00	19.74	58	115.00	3.41	83	148.00	5.31
9	51.00	5.31	34	82.00	43.45	59	116.00	1.33	84	149.00	2.65
10	52.00	3.41	35	83.00	12.91	60	117.00	4.93	85	150.00	0.94
11	53.00	20.12	36	84.00	4.74	61	119.00	100.00	86	151.00	2.47
12	54.00	4.37	37	85.00	1.71	62	120.00	17.65	87	159.00	1.13
13	55.00	49.52	38	89.00	1.52	63	121.00	50.86	88	161.00	23.90
14	56.00	14.23	39	91.00	40.99	64	122.00	22.96	89	162.00	5.31
15	57.00	11.39	40	92.00	19.35	65	123.00	11.39	90	163.00	1.13
16	58.00	3.99	41	93.00	82.74	66	124.00	1.90	91	164.00	1.13
17	59.00	1.90	42	94.00	18.78	67	125.00	1.90	92	175.00	1.13
18	63.00	1.71	43	95.00	19.74	68	128.00	1.52	93	179.00	1.90
19	64.00	1.13	44	96.00	3.80	69	129.00	1.33	94	189.00	5.12
20	65.00	10.44	45	97.00	5.69	70	131.00	2.84	95	190.00	1.90
21	66.00	3.61	46	98.00	1.90	71	132.00	3.99	96	202.00	1.13
22	67.00	32.63	47	102.00	0.94	72	133.00	13.66	97	204.00	16.13
23	68.00	7.96	48	103.00	3.99	73	134.00	10.44	98	205.00	2.84
24	69.00	75.91	49	105.00	43.26	74	135.00	7.40	99	207.00	3.61
25	70.00	8.92	50	106.00	8.73	75	136.00	3.80	100	208.00	1.33



Appendix 3

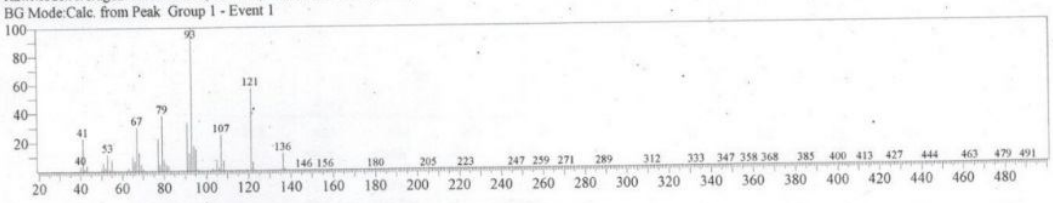
Comparison of mass spectra of the components of the essential oil of C. Limon peels. With standard spectra from the instrument library



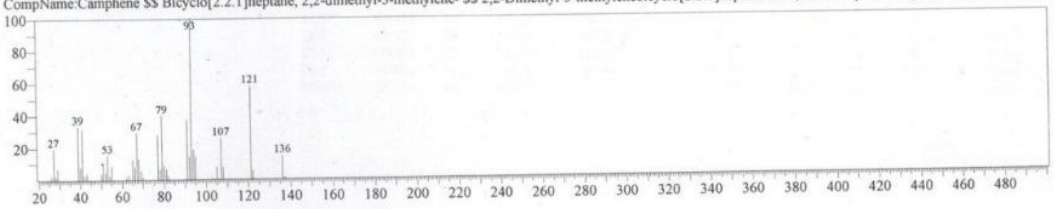


Spectrum Comparison

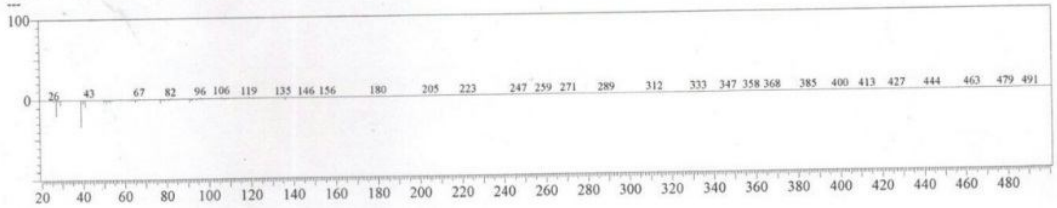
Spectrum1 #Data# Limon Oil.QGD R.Time:5.160(Scan#:433)
MassPeaks:302
RawMode:Averaged 5.155-5.165(432-434) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:9817 Formula:C10H16 CAS:79-92-5 MolWeight:136
MassPeaks:44 BasePeak:93.00(10000)
CompName:Camphene $$ Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene- $$ 2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane $$ 2,2-Dimethyl-3-methylenenorbornane $$ 3,

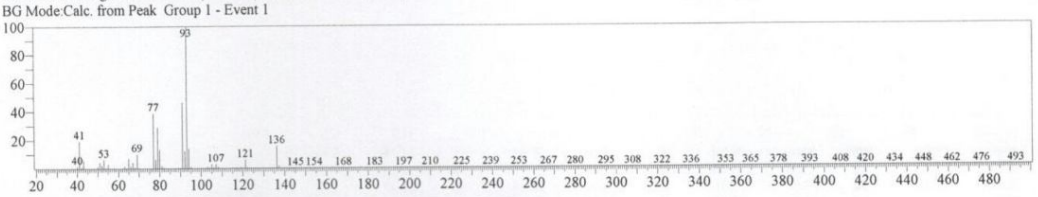


Spectrum3 #Calculation Result#
MassPeaks:298 BasePeak:106.10(190)

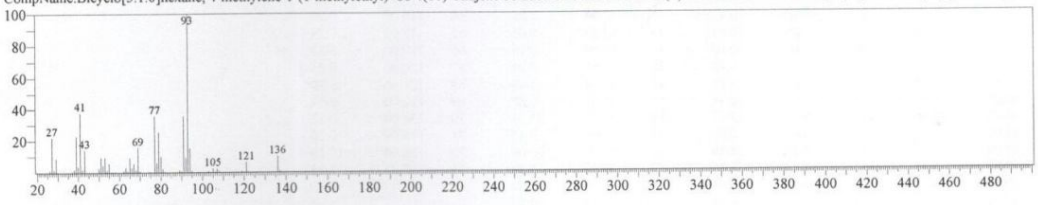


Spectrum Comparison

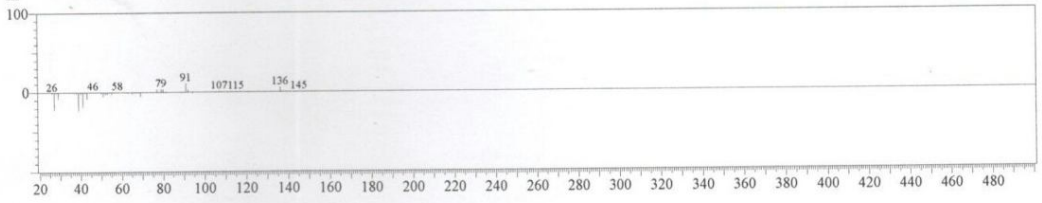
Spectrum1 #Data# Limon Oil.QGD R.Time:5.610(Scan#:523)
MassPeaks:272
RawMode:Averaged 5.605-5.615(522-524) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:9781 Formula:C10H16 CAS:3387-41-5 MolWeight:136
MassPeaks:73 BasePeak:93.00(10000)
CompName:Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- $$ 4(10)-Thujene $$ Sabinen $$ Sabinene $$ (+)-Sabinene $$ THUJENE, 4(10)- $$ 1-Isopropyl-4-methylene

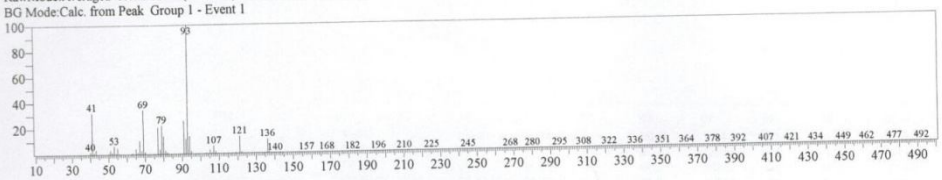


Spectrum3 #Calculation Result#
MassPeaks:96 BasePeak:91.05(1077)

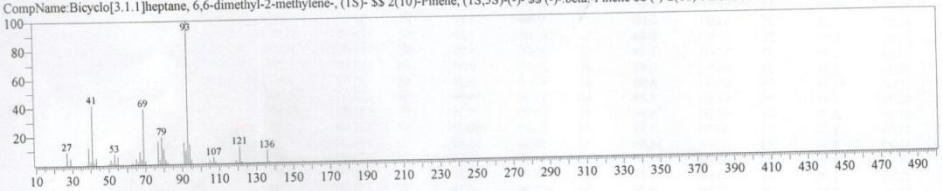


Spectrum Comparison

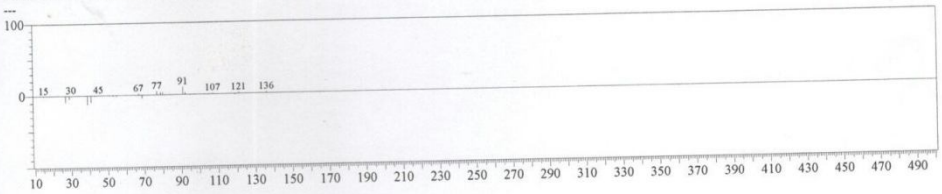
Spectrum1 #Data# Limon Oil.QGD R.Time:5.695(Scan#:540)
MassPeaks:274
RawMode:Averaged 5.690-5.700(539-541) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:9776 Formula:C10H16 CAS:18172-67-3 MolWeight:136
MassPeaks:72 BasePeak:93.00(10000)
CompName:Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)- $$ 2(10)-Pinene, (1S,5S)-(-)- $$ (-)-.beta.-Pinene $$ (-)-2(10)-Pinene $$ L-.beta.-Pinene $$ (1S)-(-)-.beta.-

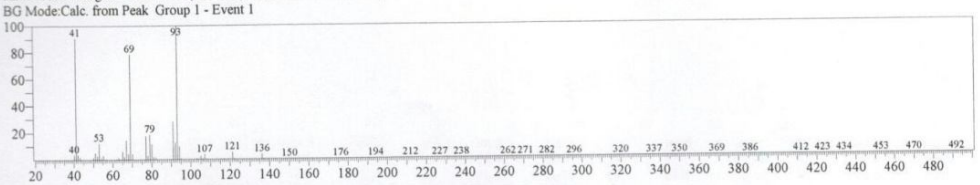


Spectrum3 #Calculation Result#
MassPeaks:93 BasePeak:91.05(1067)

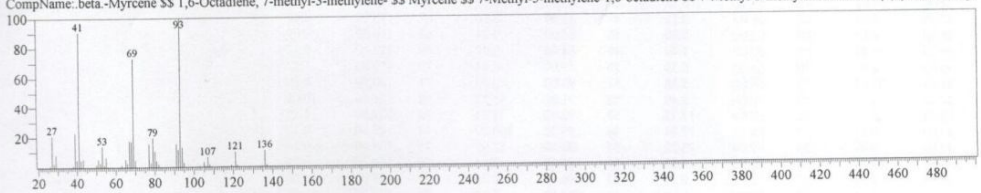


Spectrum Comparison

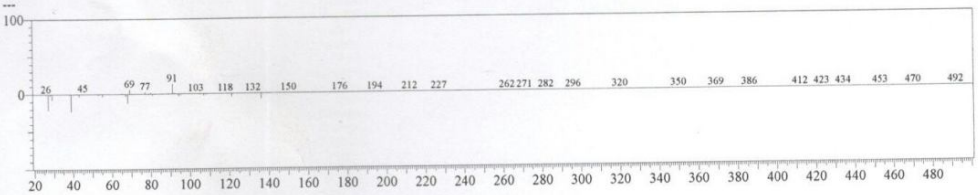
Spectrum1 #Data# Limon Oil.QGD R.Time:5.900(Scan#:581)
MassPeaks:271
RawMode:Averaged 5.895-5.905(580-582) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:6636 Formula:C10H16 CAS:123-35-3 MolWeight:136
MassPeaks:80 BasePeak:93.00(10000)
CompName:.beta.-Myrcene $$ 1,6-Octadiene, 7-methyl-3-methylene- $$ Myrcene $$ 7-Methyl-3-methylene-1,6-octadiene $$ 7-Methyl-3-methyleneoctadiene-(1,6) $$ 2-Methyl

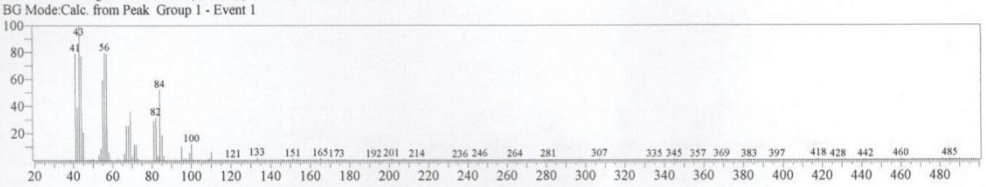


Spectrum3 #Calculation Result#
MassPeaks:144 BasePeak:91.05(1301)

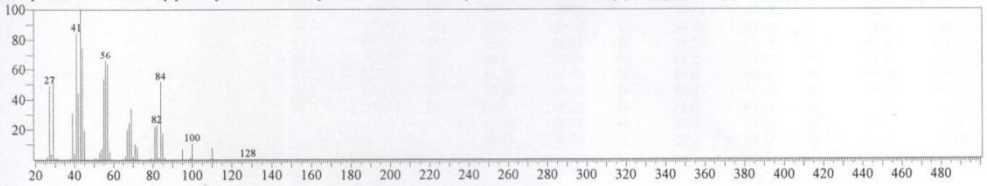


Spectrum Comparison

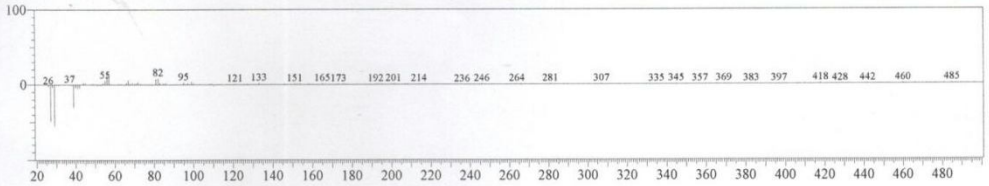
Spectrum1 #Data# Limon Oil.QGD R.Time:6.145(Scan#:630)
MassPeaks:237
RawMode:Averaged 6.140-6.150(629-631) BasePeak:43.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:5153 Formula:C8H16O CAS:124-13-0 MolWeight:128
MassPeaks:58 BasePeak:43.00(10000)
CompName:Octanal $$ n-Caprylaldehyde $$ n-Octaldehyde $$ n-Octanal $$ n-Octylal $$ Antifoam-LF $$ Caprylaldehyde $$ Caprylic aldehyde $$ Octaldehyde $$ Octanaldeh

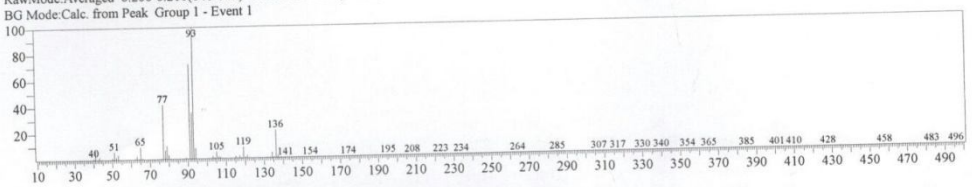


Spectrum3 #Calculation Result#
MassPeaks:255 BasePeak:57.05(1503)

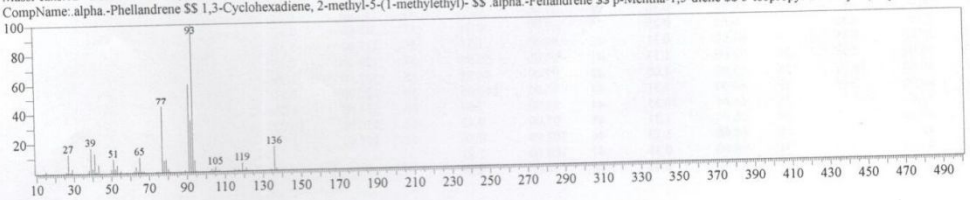


Spectrum Comparison

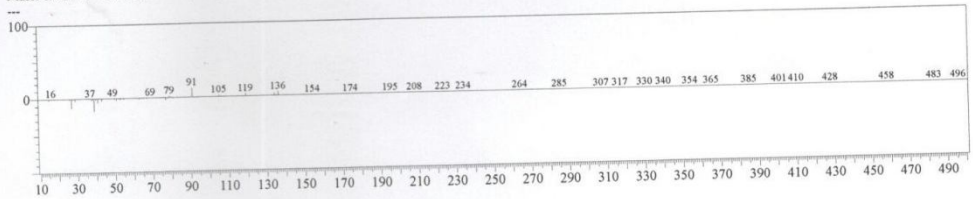
Spectrum1 #Data# Limon Oil.QGD R.Time:6.205(Scan#:642)
MassPeaks:224
RawMode:Averaged 6.200-6.210(641-643) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:6660 Formula:C10H16 CAS:99-83-2 MolWeight:136
MassPeaks:62 BasePeak:93.00(10000)
CompName:.alpha.-Phellandrene $$ 1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)- $$ .alpha.-Fellandrene $$ p-Mentha-1,5-diene $$ 5-Isopropyl-2-methyl-1,3-cyclohexadien

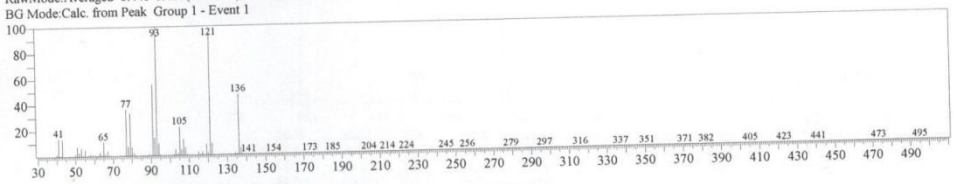


Spectrum3 #Calculation Result#
MassPeaks:218 BasePeak:91.05(1219)

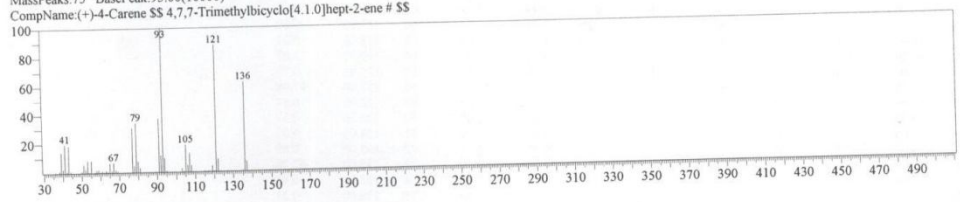


Spectrum Comparison

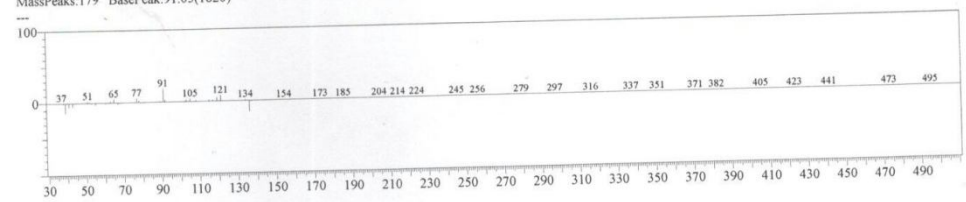
Spectrum1 #Data# Limon Oil.QGD R.Time:6.450(Scan#:691)
MassPeaks:235
RawMode:Averaged 6.445-6.455(690-692) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:9827 Formula:C10H16 CAS:29050-33-7 MolWeight:136
MassPeaks:75 BasePeak:93.00(10000)
CompName:(+)-4-Carene $$ 4,7,7-Trimethylbicyclo[4.1.0]hept-2-ene # $$

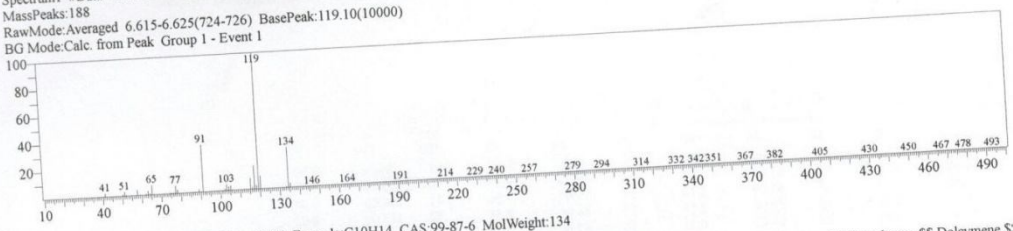


Spectrum3 #Calculation Result#
MassPeaks:179 BasePeak:91.05(1820)

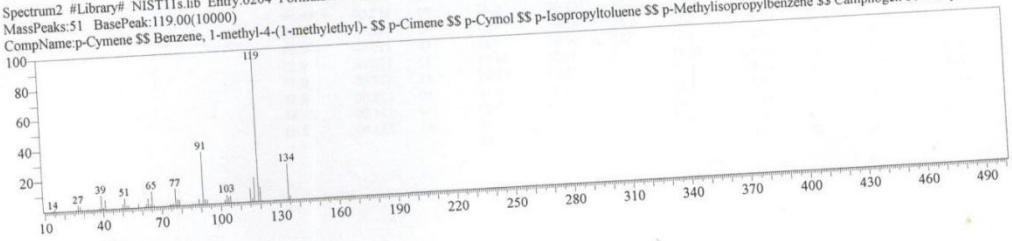


Spectrum Comparison

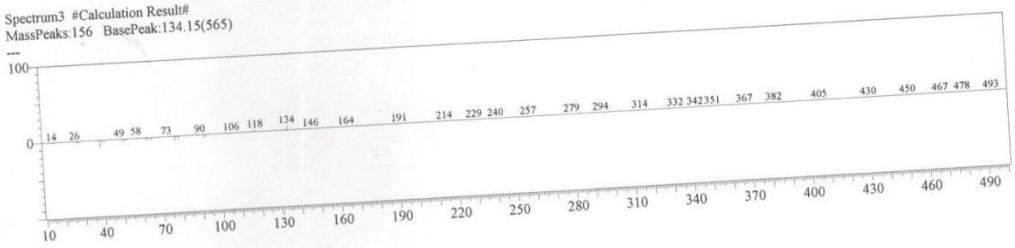
Spectrum1 #Data# Limon Oil.QGD R.Time:6.620(Scan#:725)
MassPeaks:188
RawMode:Averaged 6.615-6.625(724-726) BasePeak:119.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:6204 Formula:C10H14 CAS:99-87-6 MolWeight:134
MassPeaks:51 BasePeak:119.00(10000)
CompName:p-Cymene $$ Benzene, 1-methyl-4-(1-methylethyl)- $$ p-Cimene $$ p-Cymol $$ p-Isopropyltoluene $$ p-Methylisopropylbenzene $$ Camphogen $$ Dolcymene $:

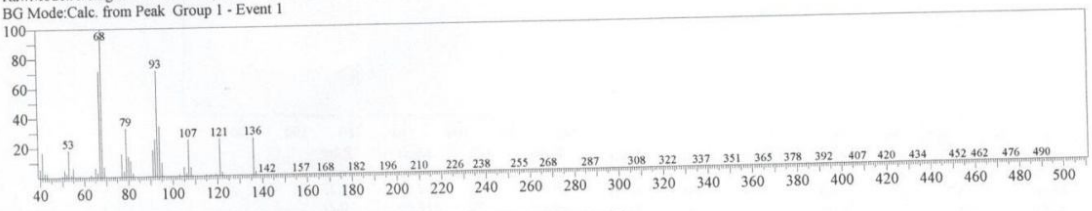


Spectrum3 #Calculation Result#
MassPeaks:156 BasePeak:134.15(565)

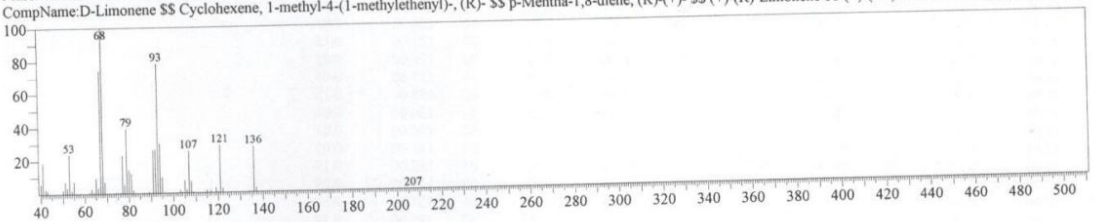


Spectrum Comparison

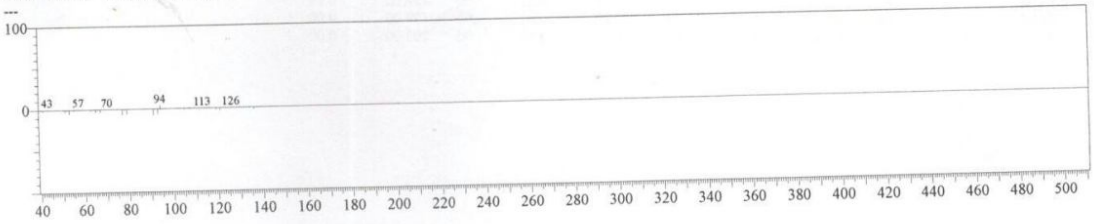
Spectrum1 #Data# Limon Oil.QGD R.Time:6.720(Scan#:745)
MassPeaks:288
RawMode:Averaged 6.715-6.725(744-746) BasePeak:68.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:6621 Formula:C10H16 CAS:5989-27-5 MolWeight:136
MassPeaks:92 BasePeak:68.00(10000)
CompName:D-Limonene $$ Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- $$ p-Mentha-1,8-diene, (R)-(+)- $$ (+)-(R)-Limonene $$ (+)-(4R)-Limonene $$ (+)-p-Mentha-1,

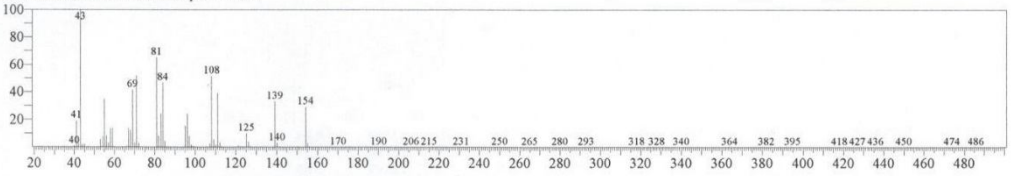


Spectrum3 #Calculation Result#
MassPeaks:85 BasePeak:94.10(374)

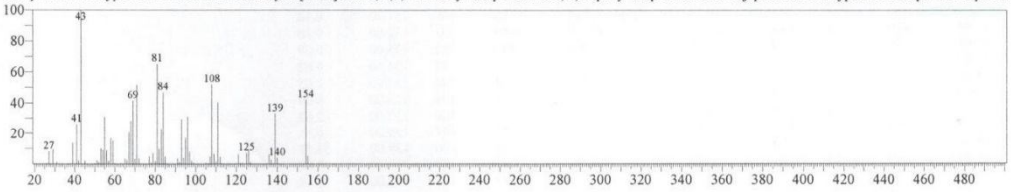


Spectrum Comparison

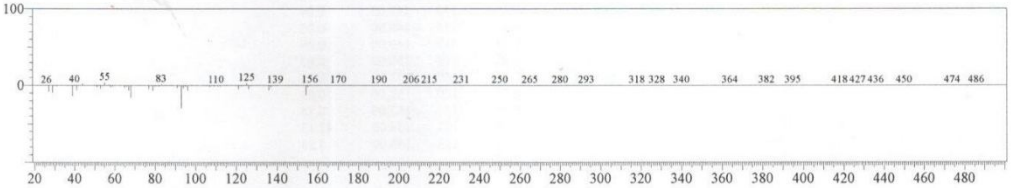
Spectrum1 #Data# Limon Oil.QGD R.Time:6.785(Scan#:758)
MassPeaks:209
RawMode:Averaged 6.780-6.790(757-759) BasePeak:43.00(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:9939 Formula:C10H18O CAS:470-82-6 MolWeight:154
MassPeaks:123 BasePeak:43.00(10000)
CompName:Eucalyptol $$ Cineole $$ 2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- $$ p-Menthane, 1,8-epoxy- $$ p-Cineole $$ Cajeputol $$ Cucalyptol $$ Eucapur $$ Terpan $:

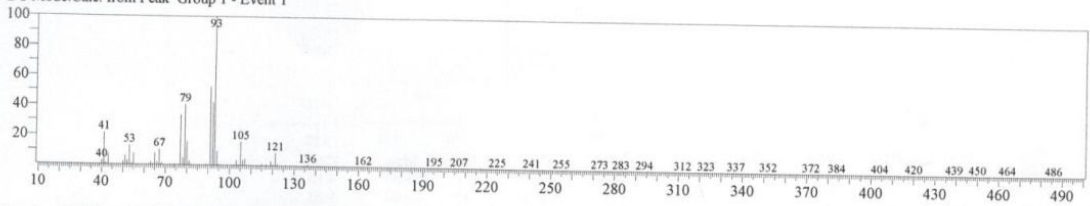


Spectrum3 #Calculation Result#
MassPeaks:246 BasePeak:55.05(368)

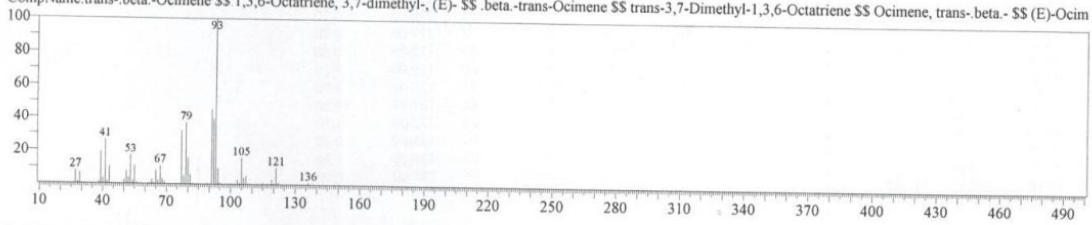


Spectrum Comparison

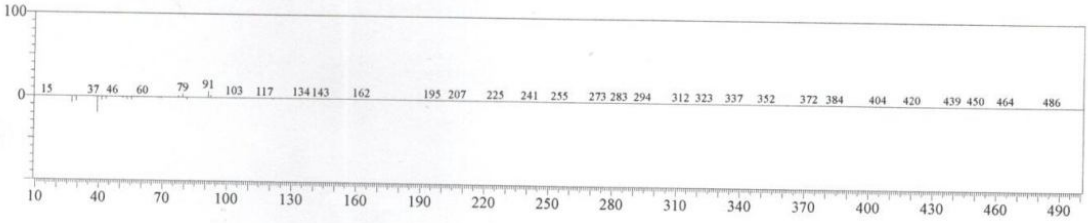
Spectrum1 #Data# Limon Oil.QGD R.Time:6.840(Scan#:769)
MassPeaks:245
RawMode:Averaged 6.835-6.845(768-770) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:6664 Formula:C10H16 CAS:3779-61-1 MolWeight:136
MassPeaks:66 BasePeak:93.00(10000)
CompName:trans-.beta.-Ocimene $$ 1,3,6-Octatriene, 3,7-dimethyl-, (E)- $$ .beta.-trans-Ocimene $$ trans-3,7-Dimethyl-1,3,6-Octatriene $$ Ocimene, trans-.beta.- $$ (E)-Ocim

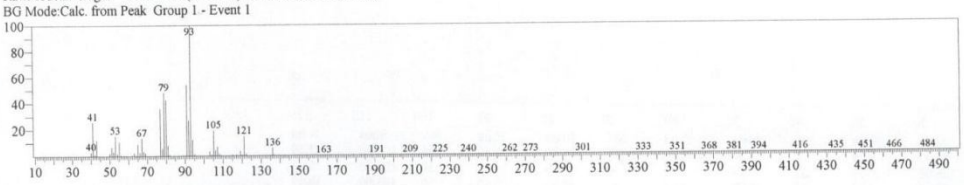


Spectrum3 #Calculation Result#
MassPeaks:231 BasePeak:91.05(774)

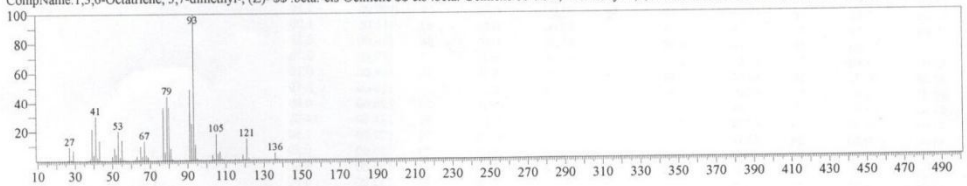


Spectrum Comparison

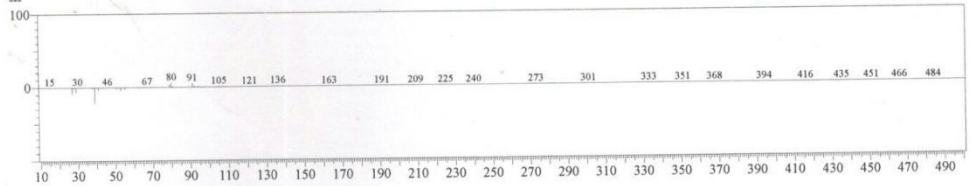
Spectrum1 #Data# Limon Oil.QGD R.Time:7.060(Scan#:813)
MassPeaks:240
RawMode:Averaged 7.055-7.065(812-814) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:6662 Formula:C10H16 CAS:3338-55-4 MolWeight:136
MassPeaks:76 BasePeak:93.00(10000)
CompName:1,3,6-Octatriene, 3,7-dimethyl-, (Z)- $$ .beta.-cis-Ocimene $$ cis-.beta.-Ocimene $$ cis-3,7-Dimethyl-1,3,6-octatriene $$ Ocimene, cis-.beta.- $$ (Z)-Ocimene $$ ci

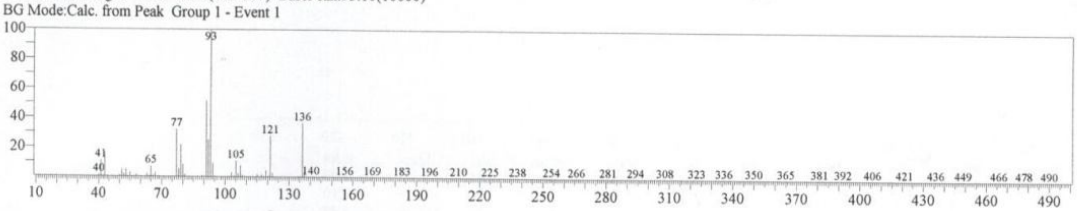


Spectrum3 #Calculation Result#
MassPeaks:174 BasePeak:80.05(604)

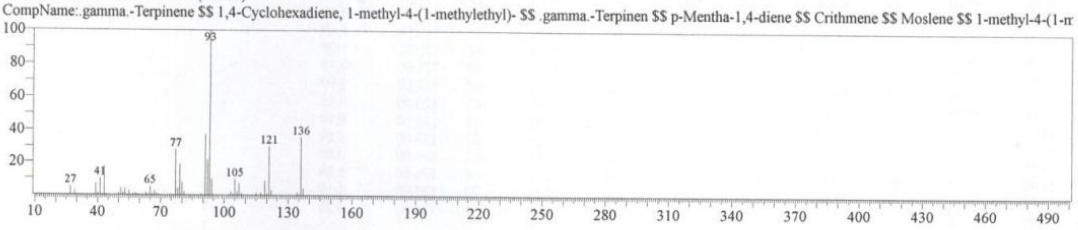


Spectrum Comparison

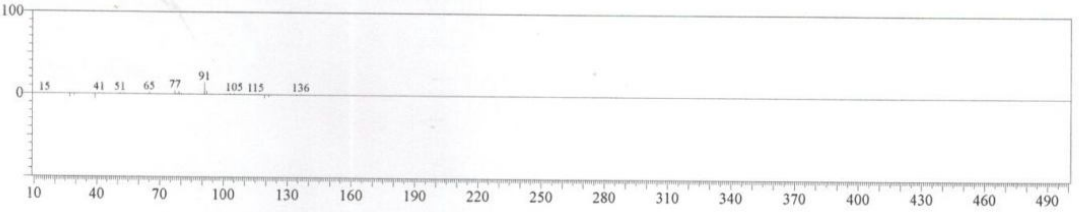
Spectrum1 #Data# Limon Oil.QGD R.Time:7.325(Scan#:866)
MassPeaks:324
RawMode:Averaged 7.320-7.330(865-867) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:9811 Formula:C10H16 CAS:99-85-4 MolWeight:136
MassPeaks:71 BasePeak:93.00(10000)
CompName:.gamma.-Terpinene $$ 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- $$ .gamma.-Terpinen $$ p-Mentha-1,4-diene $$ Crithmene $$ Moslene $$ 1-methyl-4-(1-m

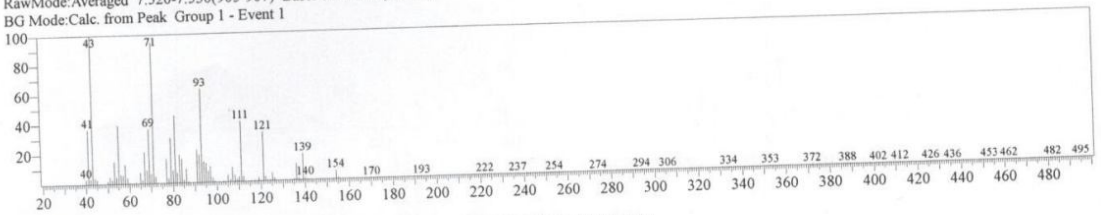


Spectrum3 #Calculation Result#
MassPeaks:93 BasePeak:91.05(1430)

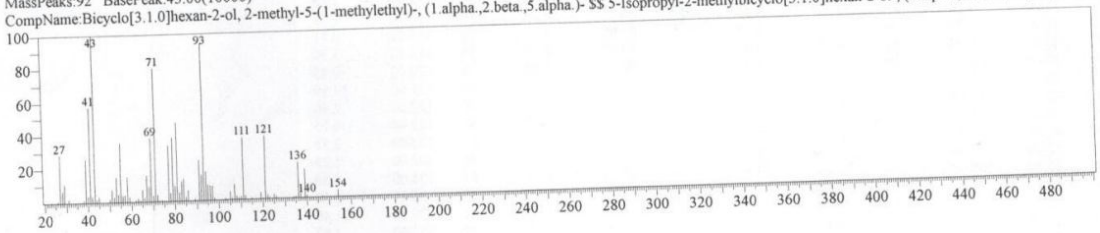


Spectrum Comparison

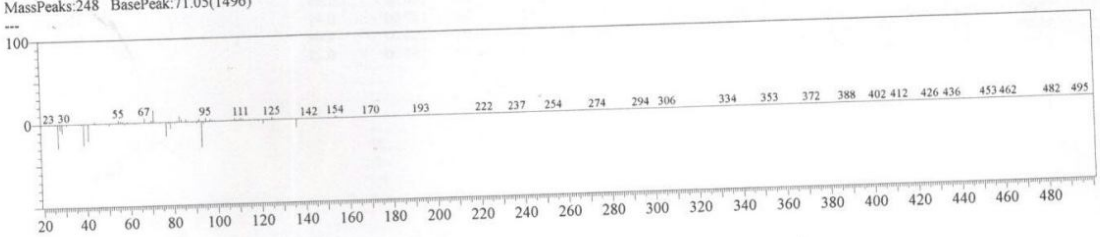
Spectrum1 #Data# Limon Oil.QGD R.Time:7.525(Scan#:906)
MassPeaks:237
RawMode:Averaged 7.520-7.530(905-907) BasePeak:43.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:17480 Formula:C10H18O CAS:15537-55-0 MolWeight:154
MassPeaks:92 BasePeak:43.00(10000)
CompName:Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1.alpha.,2.beta.,5.alpha.)- $$ 5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol-, (1.alpha.,2.beta.,5.alpha.)- $$ (

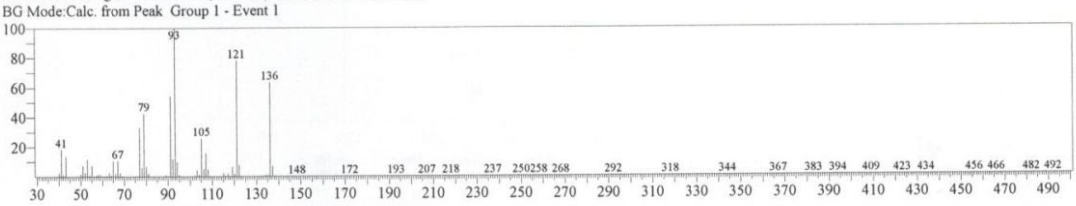


Spectrum3 #Calculation Result#
MassPeaks:248 BasePeak:71.05(1496)

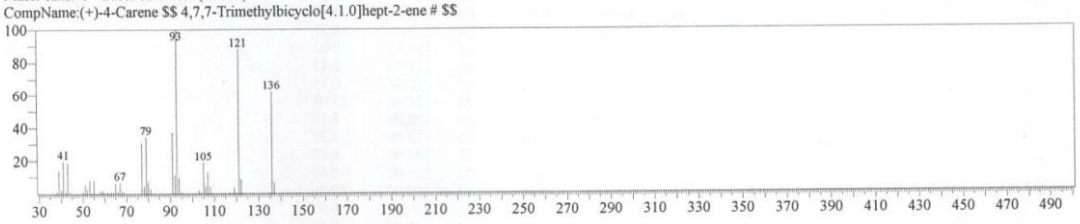


Spectrum Comparison

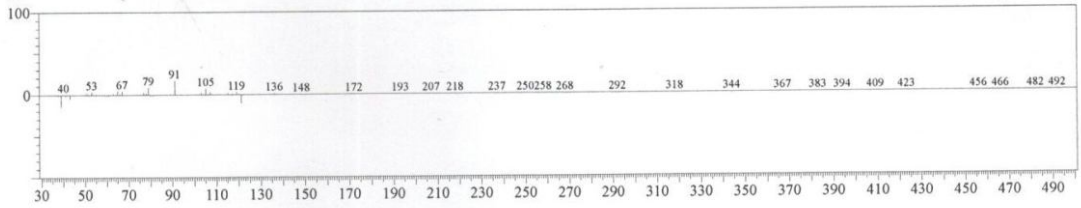
Spectrum1 #Data# Limon Oil.QGD R.Time:7.950(Scan#:991)
MassPeaks:260
RawMode:Averaged 7.945-7.955(990-992) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:9827 Formula:C10H16 CAS:29050-33-7 MolWeight:136
MassPeaks:75 BasePeak:93.00(10000)
CompName:(+)-4-Carene $$ 4,7,7-Trimethylbicyclo[4.1.0]hept-2-ene # $$

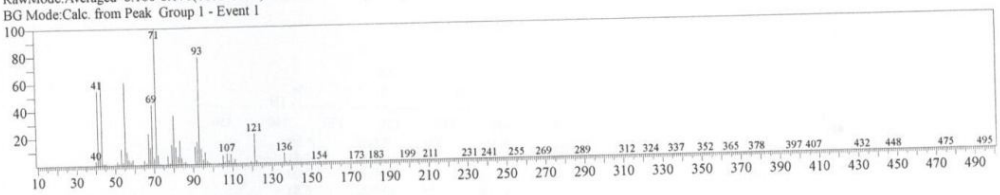


Spectrum3 #Calculation Result#
MassPeaks:195 BasePeak:91.05(1690)

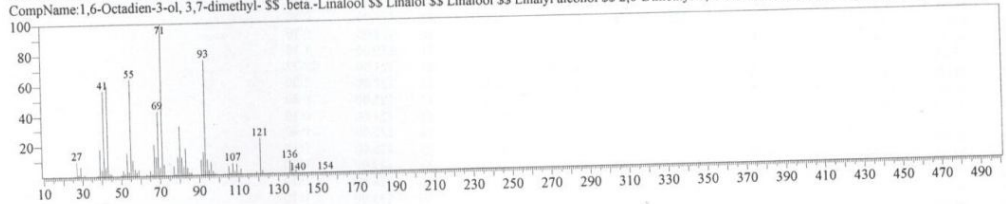


Spectrum Comparison

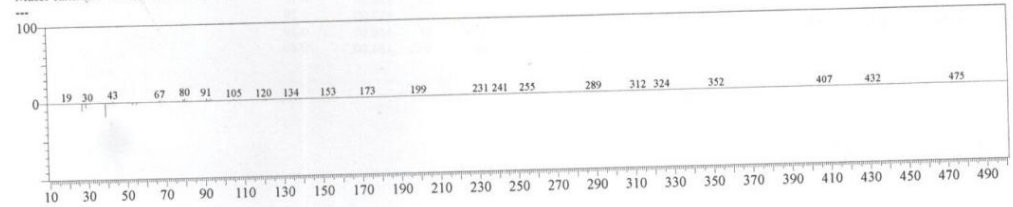
Spectrum1 #Data# Limon Oil.QGD R.Time:8.165(Scan#:1034)
MassPeaks:255
RawMode:Averaged 8.160-8.170(1033-1035) BasePeak:71.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:17562 Formula:C10H18O CAS:78-70-6 MolWeight:154
MassPeaks:96 BasePeak:71.00(10000)
CompName:1,6-Octadien-3-ol, 3,7-dimethyl- $$ .beta.-Linalool $$ Linalol $$ Linalool $$ Linalyl alcohol $$ 2,6-Dimethyl-2,7-octadien-6-ol $$ allo-Ocimenol $$ 2,6-Dimethyl-7

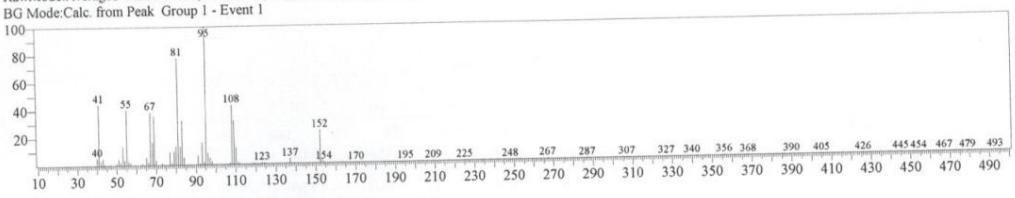


Spectrum3 #Calculation Result#
MassPeaks:126 BasePeak:80.05(386)

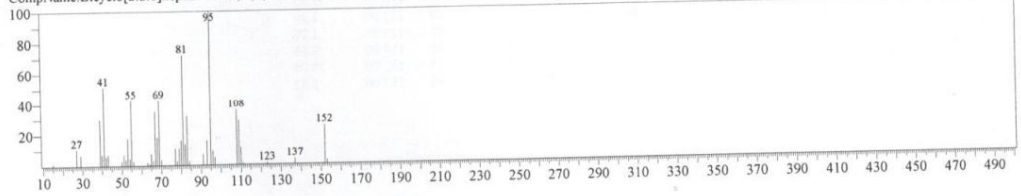


Spectrum Comparison

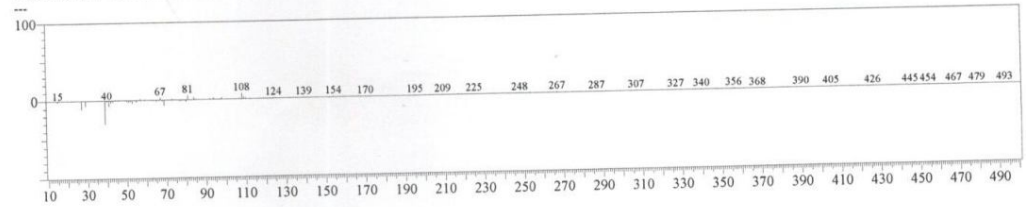
Spectrum1 #Data# Limon Oil.QGD R.Time:9.225(Scan#:1246)
MassPeaks:308
RawMode:Averaged 9.220-9.230(1245-1247) BasePeak:95.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:16453 Formula:C10H16O CAS:464-48-2 MolWeight:152
MassPeaks:44 BasePeak:95.00(10000)
CompName:Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- $$ (-)-Alcanfor $$ (-)-Camphor $$ Camphor, (1S,4S)-(-)- $$ L-camphor $$ Levo-(-)-camphor $$ (1S)-(-)-Campl

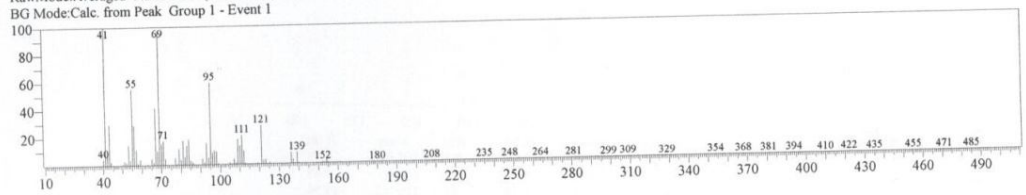


Spectrum3 #Calculation Result#
MassPeaks:310 BasePeak:108.10(702)

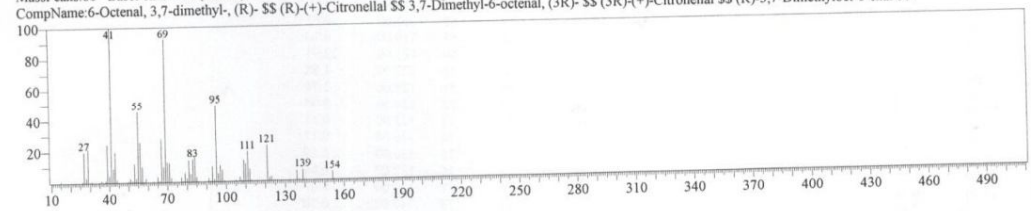


Spectrum Comparison

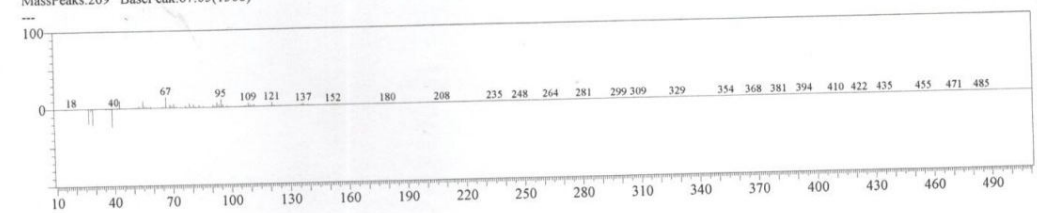
Spectrum1 #Data# Limon Oil.QGD R.Time:9.295(Scan#:1260)
MassPeaks:257
RawMode:Averaged 9.290-9.300(1259-1261) BasePeak:41.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:17443 Formula:C10H18O CAS:2385-77-5 MolWeight:154
MassPeaks:80 BasePeak:41.00(10000)
CompName:6-Octenal, 3,7-dimethyl-, (R)- $$ (R)-(+)-Citronellal $$ 3,7-Dimethyl-6-octenal, (3R)- $$ (3R)-(+)-Citronellal $$ (R)-3,7-Dimethyloct-6-enal $$

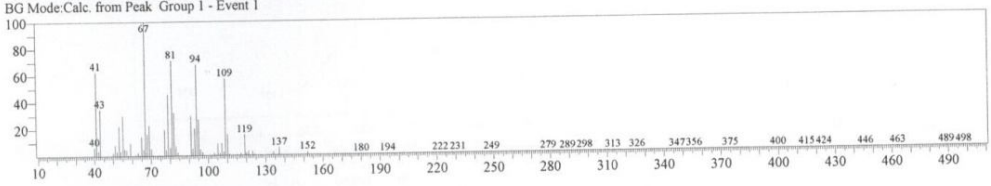


Spectrum3 #Calculation Result#
MassPeaks:269 BasePeak:67.05(1368)

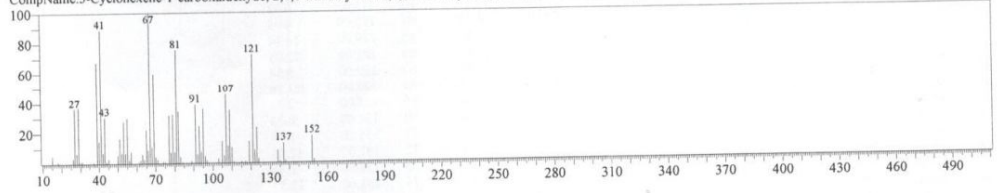


Spectrum Comparison

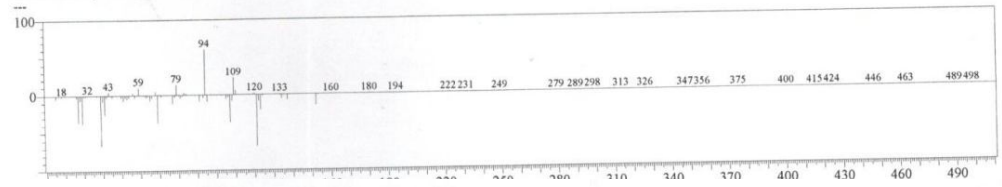
Spectrum1 #Data# Limon Oil.QGD R.Time:9.540(Scan#:1309)
MassPeaks:264
RawMode:Averaged 9.535-9.545(1308-1310) BasePeak:67.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:16340 Formula:C10H16O CAS:1423-46-7 MolWeight:152
MassPeaks:75 BasePeak:67.00(10000)
CompName:3-Cyclohexene-1-carboxaldehyde, 2,4,6-trimethyl- $$ 2,4,6-Trimethyl-3-cyclohexene-1-carboxaldehyde $$ 2,4,6-Trimethyl-4-cyclohexene-1-carboxaldehyde $$ 2,4

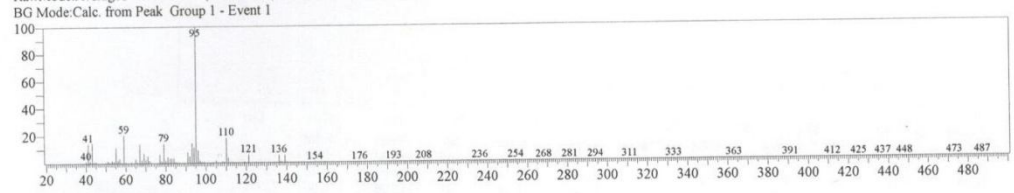


Spectrum3 #Calculation Result#
MassPeaks:275 BasePeak:94.10(6033)

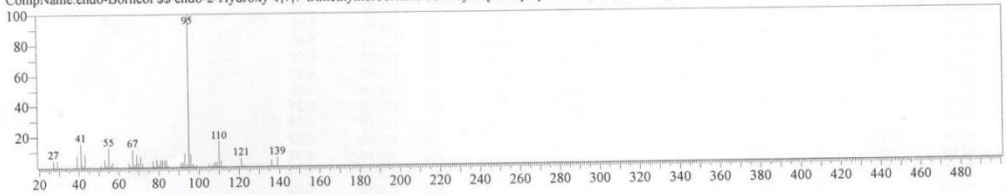


Spectrum Comparison

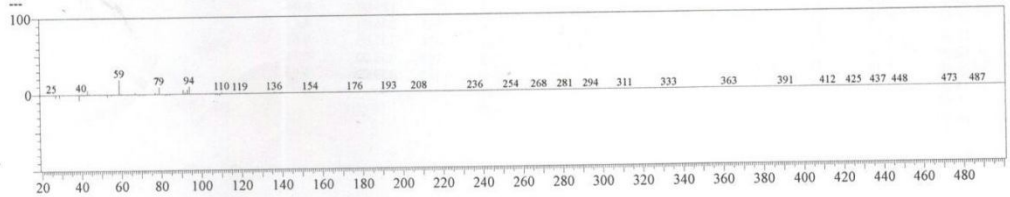
Spectrum1 #Data# Limon Oil.QGD R.Time:9.675(Scan#:1336)
MassPeaks:274
RawMode:Averaged 9.670-9.680(1335-1337) BasePeak:95.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:10018 Formula:C10H18O CAS:507-70-0 MolWeight:154
MassPeaks:110 BasePeak:95.00(10000)
CompName:endo-Borneol $$ endo-2-Hydroxy-1,7,7-trimethylnorbornane $$ Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, endo- $$ 1,7,7-Trimethyl-bicyclo(2.2.1)heptan-2-ol, en

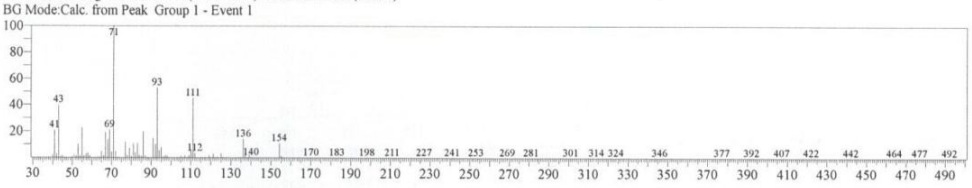


Spectrum3 #Calculation Result#
MassPeaks:289 BasePeak:59.05(1924)

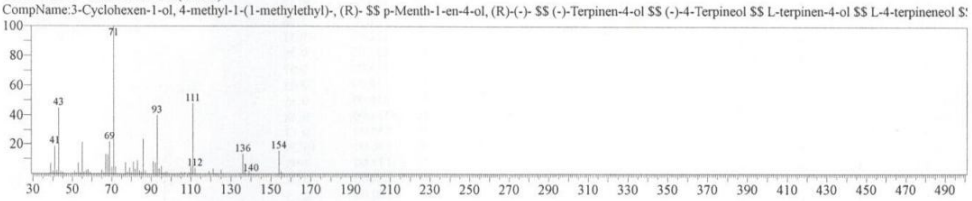


Spectrum Comparison

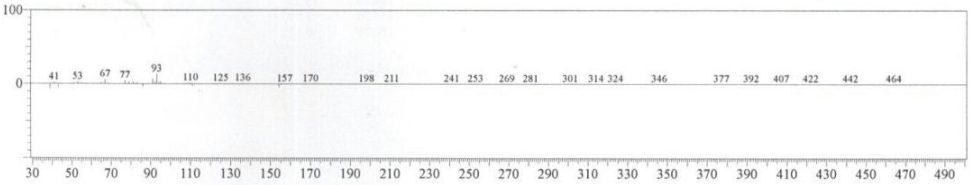
Spectrum1 #Data# Limon Oil.QGD R.Time:9.895(Scan#:1380)
MassPeaks:300
RawMode:Averaged 9.890-9.900(1379-1381) BasePeak:71.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:17565 Formula:C10H18O CAS:20126-76-5 MolWeight:154
MassPeaks:95 BasePeak:71.00(10000)
CompName:3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)- $$ p-Menth-1-en-4-ol, (R)-(-)- $$ (-)-Terpinen-4-ol $$ (-)-4-Terpineol $$ L-terpinen-4-ol $$ L-4-terpineneol $:

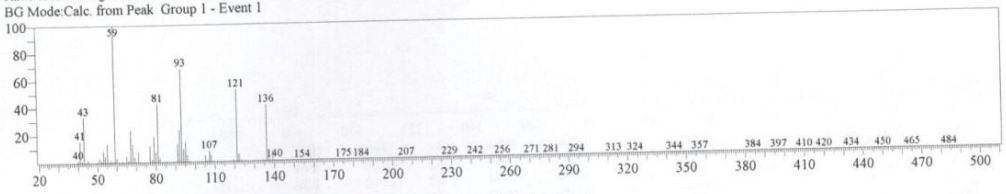


Spectrum3 #Calculation Result#
MassPeaks:158 BasePeak:93.10(1335)

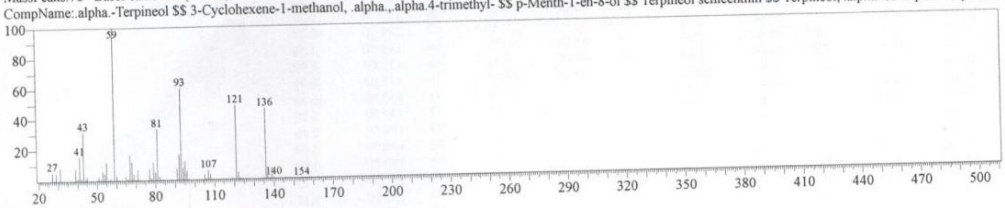


Spectrum Comparison

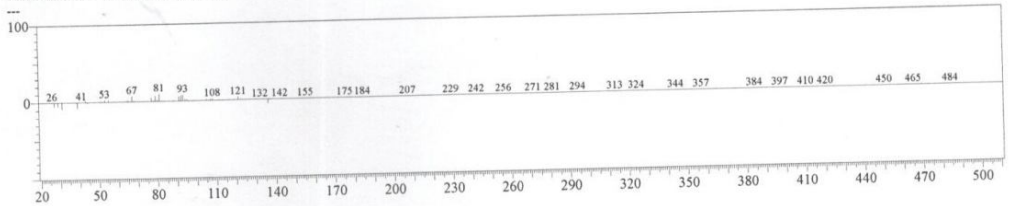
Spectrum1 #Data# Limon Oil.QGD R.Time:10.175(Scan#:1436)
MassPeaks:264
RawMode:Averaged 10.170-10.180(1435-1437) BasePeak:59.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:9958 Formula:C10H18O CAS:98-55-5 MolWeight:154
MassPeaks:78 BasePeak:59.00(10000)
CompName:.alpha.-Terpineol $$ 3-Cyclohexene-1-methanol, .alpha.,.alpha.4-trimethyl- $$ p-Menth-1-en-8-ol $$ Terpineol schlechthin $$ Terpineol, .alpha. $$ .alpha.-Terpinol $

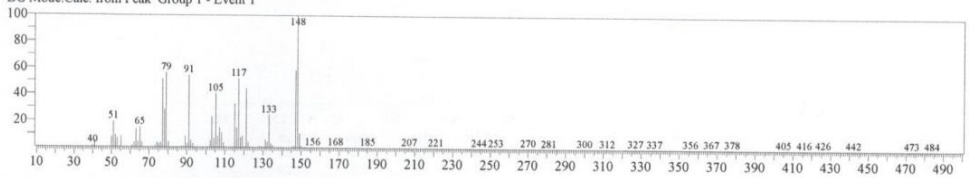


Spectrum3 #Calculation Result#
MassPeaks:169 BasePeak:81.05(926)

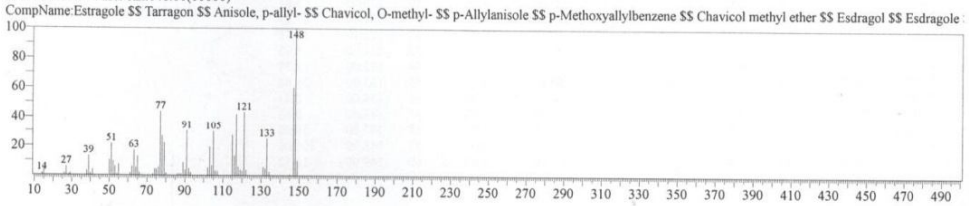


Spectrum Comparison

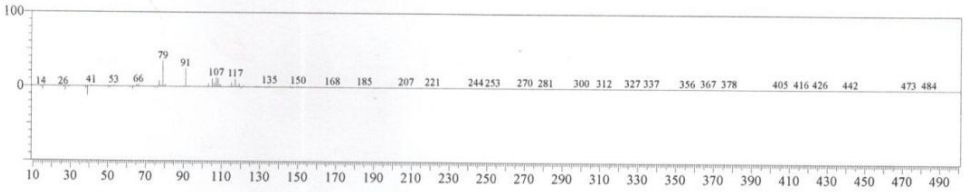
Spectrum1 #Data# Limon Oil.QGD R.Time:10.320(Scan#:1465)
MassPeaks:254
RawMode:Averaged 10.315-10.325(1464-1466) BasePeak:148.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:14629 Formula:C10H12O CAS:140-67-0 MolWeight:148
MassPeaks:60 BasePeak:148.00(10000)
CompName:Estragole $$ Tarragon $$ Anisole, p-allyl- $$ Chavicol, O-methyl- $$ p-Allylanisole $$ p-Methoxyallylbenzene $$ Chavicol methyl ether $$ Esdragol $$ Esdragole

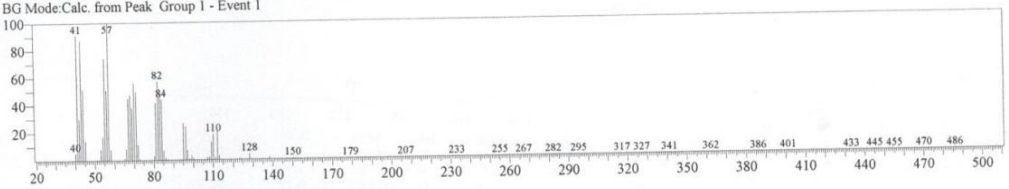


Spectrum3 #Calculation Result#
MassPeaks:260 BasePeak:79.05(3423)

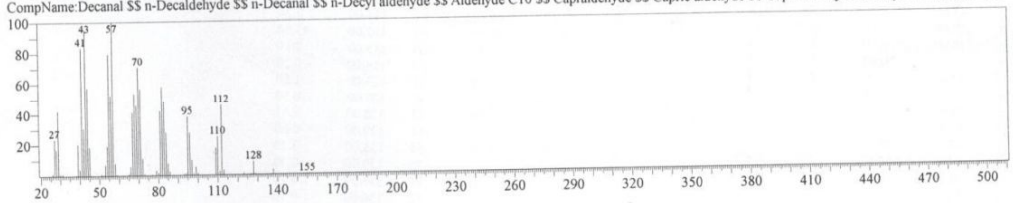


Spectrum Comparison

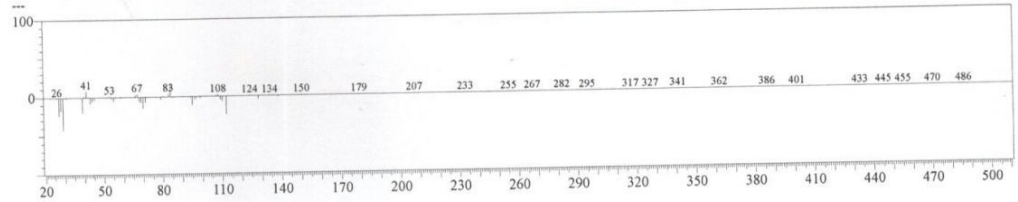
Spectrum1 #Data# Limon Oil.QGD R.Time:10.395(Scan#:1480)
MassPeaks:257
RawMode:Averaged 10.390-10.400(1479-1481) BasePeak:57.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:10329 Formula:C10H20O CAS:112-31-2 MolWeight:156
MassPeaks:72 BasePeak:57.00(10000)
CompName:Decanal $$ n-Decaldehyde $$ n-Decanal $$ n-Decyl aldehyde $$ Aldehyde C10 $$ Capraldehyde $$ Capric aldehyde $$ Caprinaldehyde $$ Caprinic aldehyde $$ D

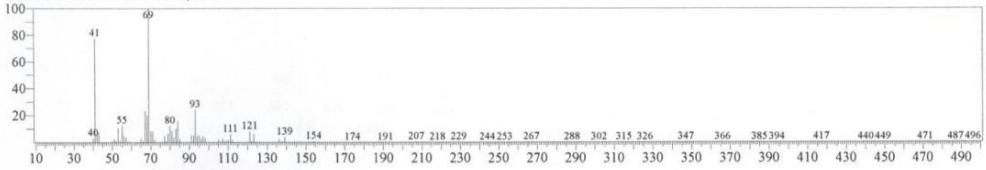


Spectrum3 #Calculation Result#
MassPeaks:274 BasePeak:84.05(1619)

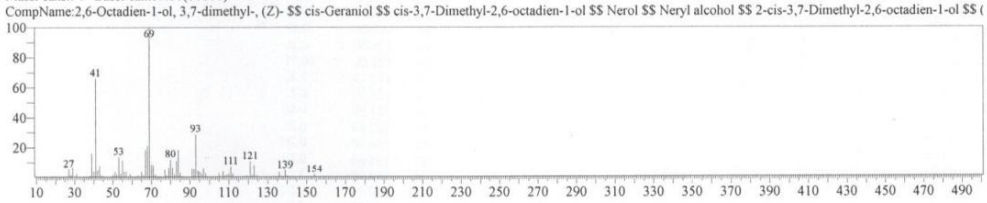


Spectrum Comparison

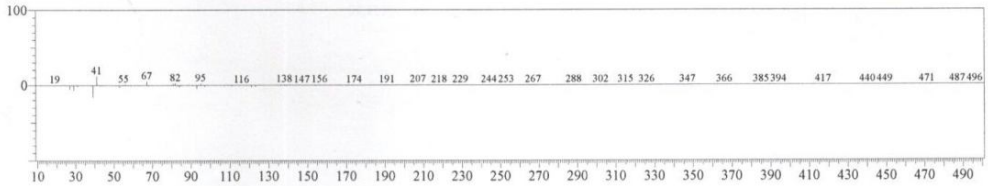
Spectrum1 #Data# Limon Oil.QGD R.Time:10.910(Scan#:1583)
MassPeaks:290
RawMode:Averaged 10.905-10.915(1582-1584) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:17537 Formula:C10H18O CAS:106-25-2 MolWeight:154
MassPeaks:94 BasePeak:69.00(10000)
CompName:2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- $$ cis-Geraniol $$ cis-3,7-Dimethyl-2,6-octadien-1-ol $$ Nerol $$ Neryl alcohol $$ 2-cis-3,7-Dimethyl-2,6-octadien-1-ol $$ (

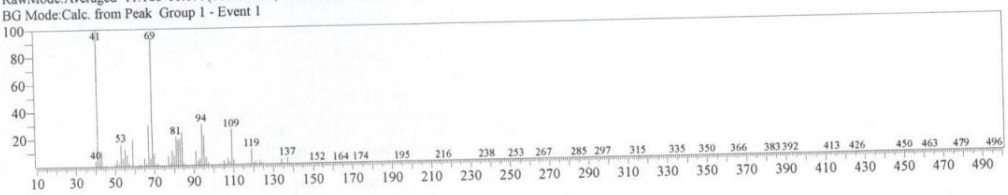


Spectrum3 #Calculation Result#
MassPeaks:291 BasePeak:41.05(1161)

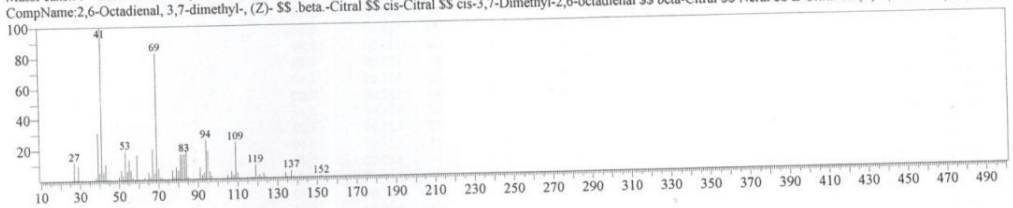


Spectrum Comparison

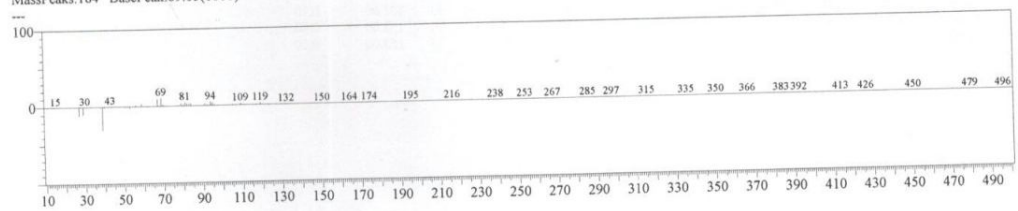
Spectrum1 #Data# Limon Oil.QGD R.Time:11.190(Scan#:1639)
MassPeaks:296
RawMode:Averaged 11.185-11.195(1638-1640) BasePeak:41.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:9466 Formula:C10H16O CAS:106-26-3 MolWeight:152
MassPeaks:95 BasePeak:41.00(10000)
CompName:2,6-Octadienal, 3,7-dimethyl-, (Z)- $$ .beta.-Citral $$ cis-Citral $$ cis-3,7-Dimethyl-2,6-octadienal $$ beta-Citral $$ Neral $$ Z-Citral $$ (Z)-3,7-Dimethyl-2,6-octa

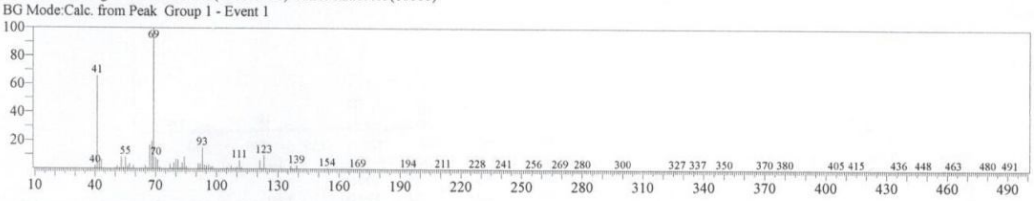


Spectrum3 #Calculation Result#
MassPeaks:184 BasePeak:69.05(1060)

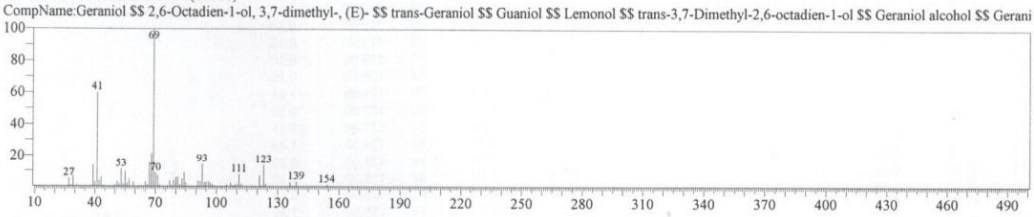


Spectrum Comparison

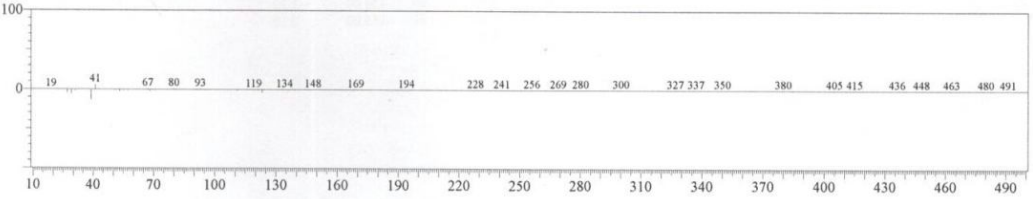
Spectrum1 #Data# Limon Oil.QGD R.Time:11.440(Scan#:1689)
MassPeaks:276
RawMode:Averaged 11.435-11.445(1688-1690) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:17535 Formula:C10H18O CAS:106-24-1 MolWeight:154
MassPeaks:91 BasePeak:69.00(10000)
CompName:Geraniol $$ 2,6-Octadien-1-ol, 3,7-dimethyl-, (E)- $$ trans-Geraniol $$ Guaniol $$ Lemonol $$ trans-3,7-Dimethyl-2,6-octadien-1-ol $$ Geraniol alcohol $$ Gerani

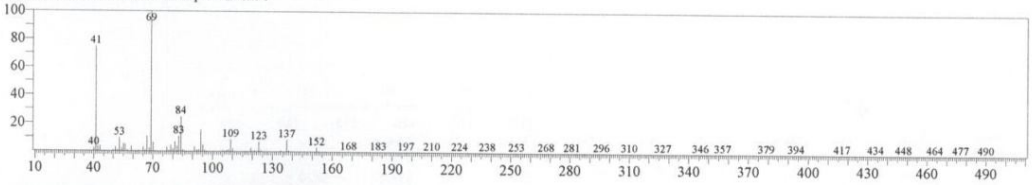


Spectrum3 #Calculation Result#
MassPeaks:190 BasePeak:41.05(587)

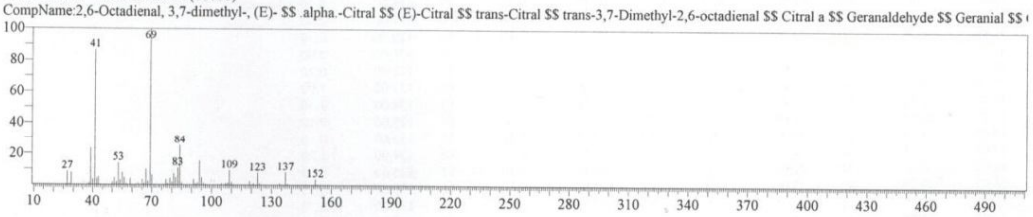


Spectrum Comparison

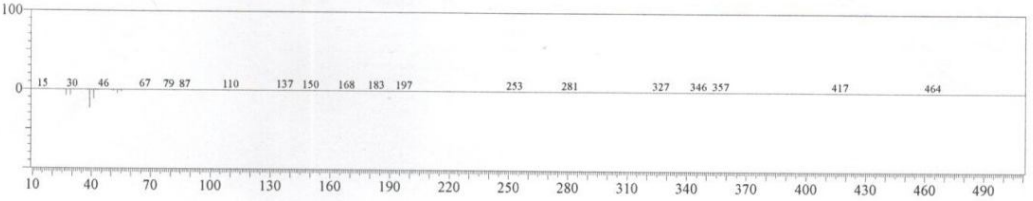
Spectrum1 #Data# Limon Oil.QGD R.Time:11.795(Scan#:1760)
MassPeaks:311
RawMode:Averaged 11.790-11.800(1759-1761) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:9502 Formula:C10H16O CAS:141-27-5 MolWeight:152
MassPeaks:93 BasePeak:69.00(10000)
CompName:2,6-Octadienal, 3,7-dimethyl-, (E)- $$ .alpha.-Citral $$ (E)-Citral $$ trans-Citral $$ trans-3,7-Dimethyl-2,6-octadienal $$ Citral a $$ Geranaldehyde $$ Geranial $$

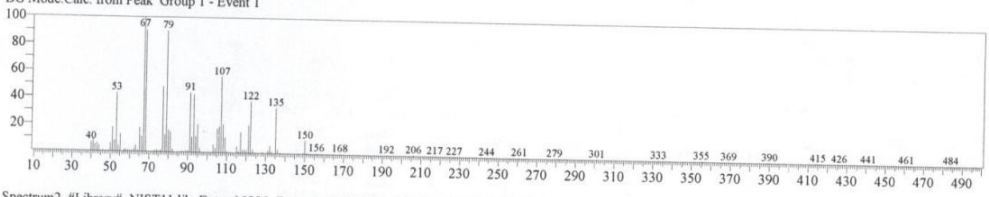


Spectrum3 #Calculation Result#
MassPeaks:133 BasePeak:67.05(41)

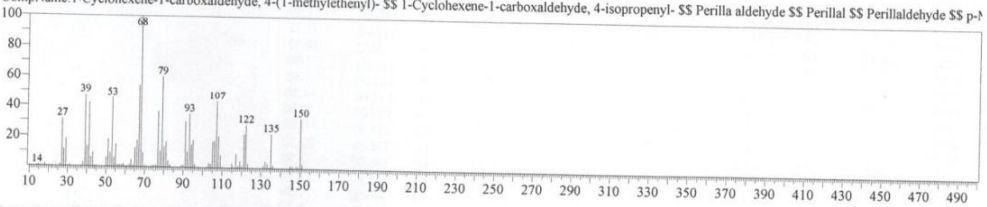


Spectrum Comparison

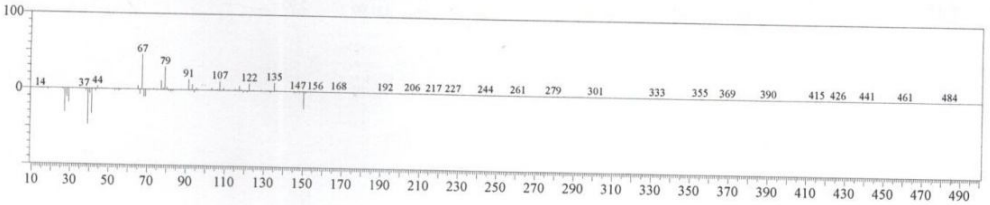
Spectrum1 #Data# Limon Oil.QGD R.Time:11.955(Scan#:1792)
MassPeaks:274
RawMode:Averaged 11.950-11.960(1791-1793) BasePeak:67.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:15335 Formula:C10H14O CAS:2111-75-3 MolWeight:150
MassPeaks:88 BasePeak:68.00(10000)
CompName:1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)- $$ 1-Cyclohexene-1-carboxaldehyde, 4-isopropenyl- $$ Perilla aldehyde $$ Perillal $$ Perillaldehyde $$ p-M

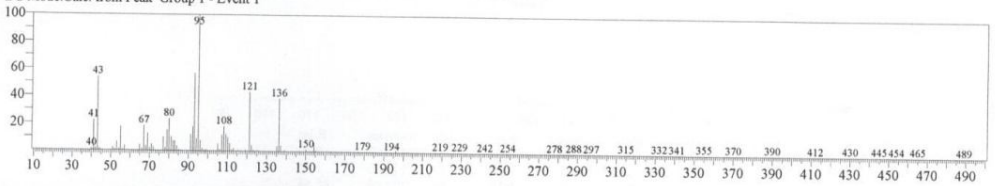


Spectrum3 #Calculation Result#
MassPeaks:294 BasePeak:67.05(4574)

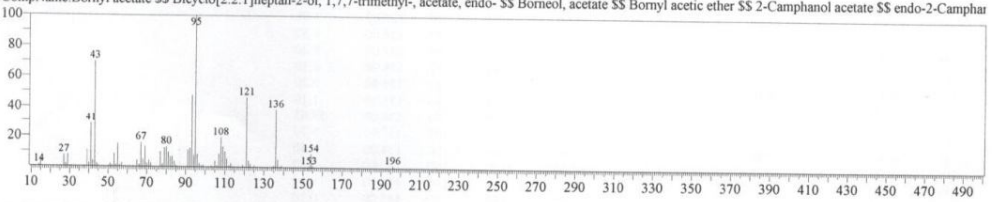


Spectrum Comparison

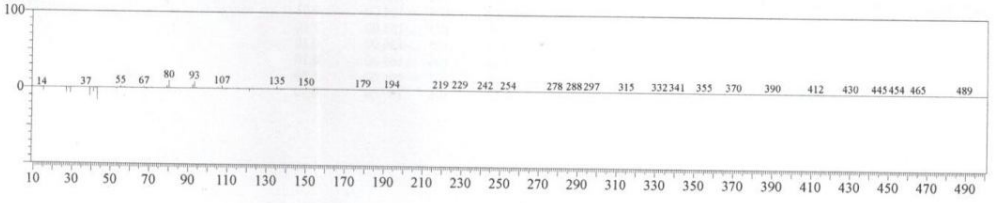
Spectrum1 #Data# Limon Oil.QGD R.Time:12.150(Scan#:1831)
MassPeaks:223
RawMode:Averaged 12.145-12.155(1830-1832) BasePeak:95.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:41489 Formula:C12H20O2 CAS:76-49-3 MolWeight:196
MassPeaks:108 BasePeak:95.00(10000)
CompName:Bornyl acetate $$ Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, endo- $$ Borneol, acetate $$ Bornyl acetic ether $$ 2-Camphanol acetate $$ endo-2-Camphar

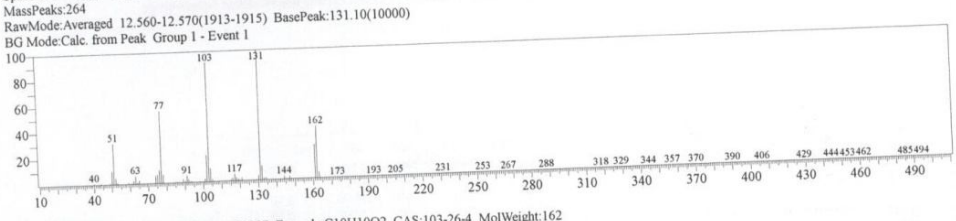


Spectrum3 #Calculation Result#
MassPeaks:231 BasePeak:80.05(1008)

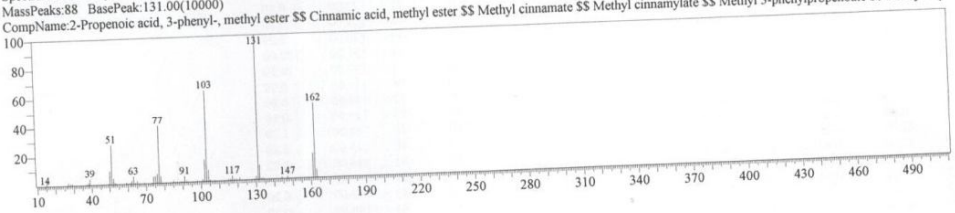


Spectrum Comparison

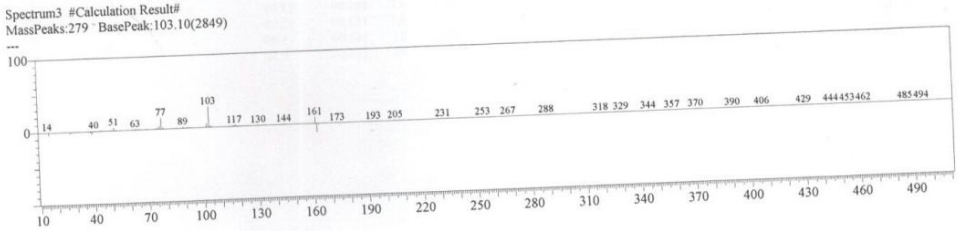
Spectrum1 #Data# Limon Oil.QGD R.Time:12.565(Scan#:1914)
MassPeaks:264
RawMode:Averaged 12.560-12.570(1913-1915) BasePeak:131.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:21207 Formula:C10H10O2 CAS:103-26-4 MolWeight:162
MassPeaks:88 BasePeak:131.00(10000)
CompName:2-Propenoic acid, 3-phenyl-, methyl ester $$ Cinnamic acid, methyl ester $$ Methyl cinnamate $$ Methyl cinnamylate $$ Methyl 3-phenylpropenoate $$ Methyl 3-p

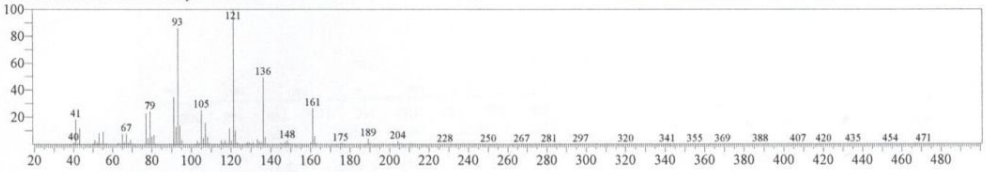


Spectrum3 #Calculation Result#
MassPeaks:279 BasePeak:103.10(2849)

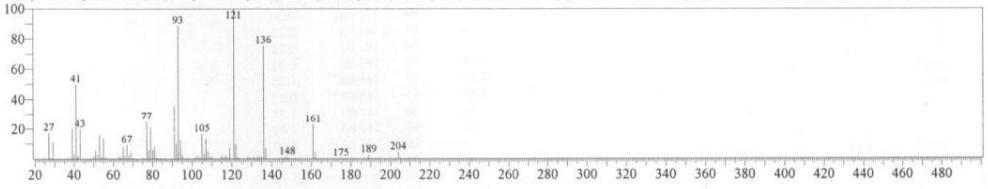


Spectrum Comparison

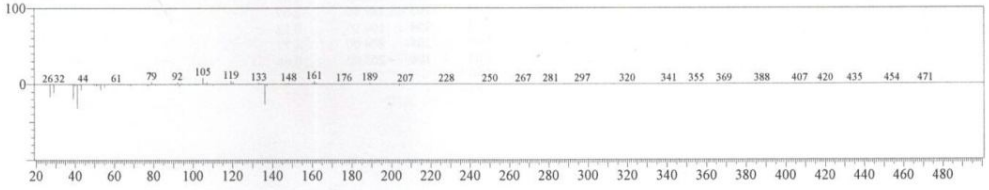
Spectrum1 #Data# Limon Oil.QGD R.Time:13.190(Scan#:2039)
MassPeaks:305
RawMode:Averaged 13.185-13.195(2038-2040) BasePeak:121.15(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:46695 Formula:C15H24 CAS:20307-84-0 MolWeight:204
MassPeaks:106 BasePeak:121.00(10000)
CompName:Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R-trans)- $$ p-Menth-3-ene, 2-isopropenyl-1-vinyl-, (1S,2R)-(-)- $$ .delta.-Elemene $$

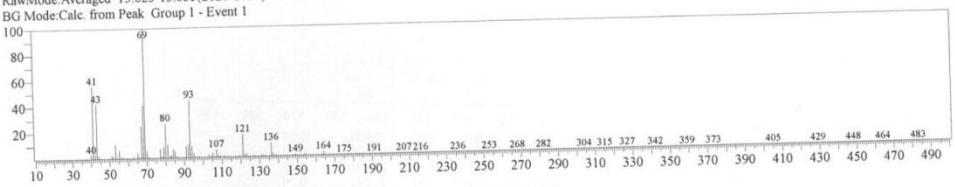


Spectrum3 #Calculation Result#
MassPeaks:288 BasePeak:105.10(850)

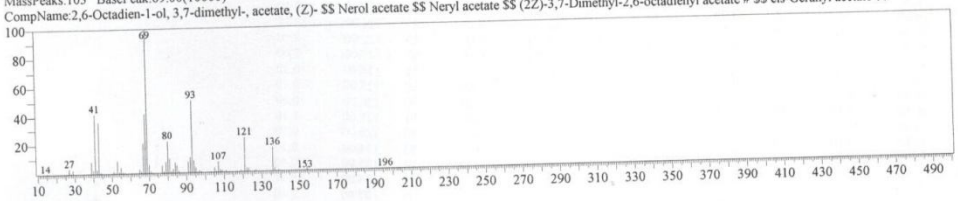


Spectrum Comparison

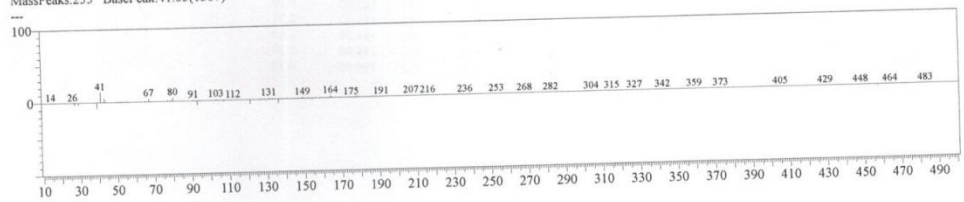
Spectrum1 #Data# Limon Oil.QGD R.Time:13.630(Scan#:2127)
MassPeaks:263
RawMode:Averaged 13.625-13.635(2126-2128) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:41462 Formula:C12H20O2 CAS:141-12-8 MolWeight:196
MassPeaks:103 BasePeak:69.00(10000)
CompName:2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)- $$ Nerol acetate $$ Neryl acetate $$ (2Z)-3,7-Dimethyl-2,6-octadienyl acetate # $$ cis-Geranyl acetate $$

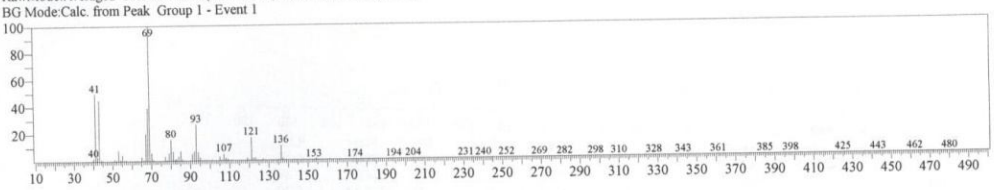


Spectrum3 #Calculation Result#
MassPeaks:255 BasePeak:41.05(1387)

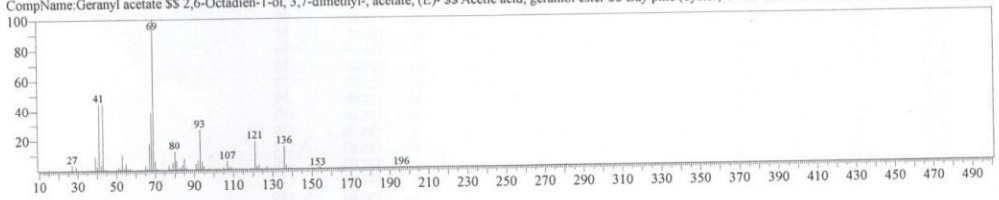


Spectrum Comparison

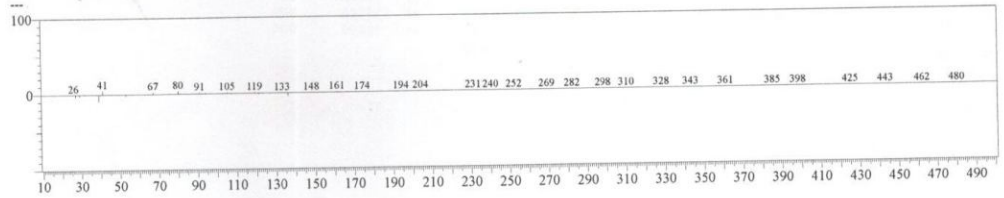
Spectrum1 #Data# Limon Oil.QGD R.Time:14.005(Scan#:2202)
MassPeaks:308
RawMode:Averaged 14.000-14.010(2201-2203) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:41457 Formula:C12H20O2 CAS:105-87-3 MolWeight:196
MassPeaks:95 BasePeak:69.00(10000)
CompName:Geranyl acetate $$ 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)- $$ Acetic acid, geraniol ester $$ Bay pine (oyster) oil $$ Geraniol acetate $$ trans-3,7-Dimethyl-2,

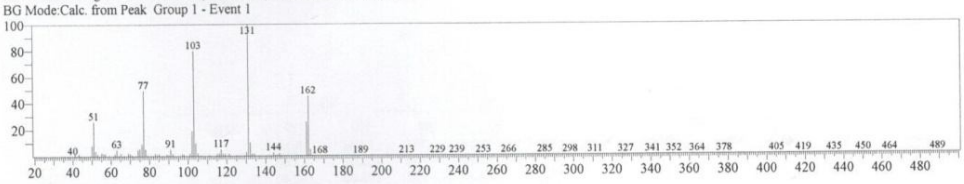


Spectrum3 #Calculation Result#
MassPeaks:258 BasePeak:41.05(493)

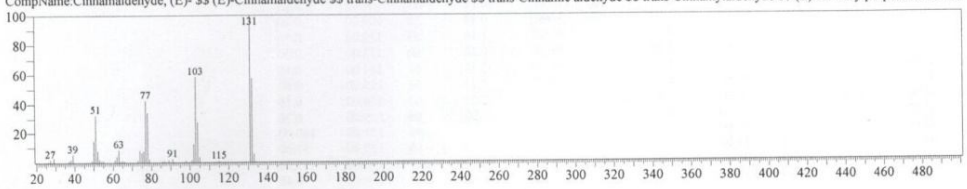


Spectrum Comparison

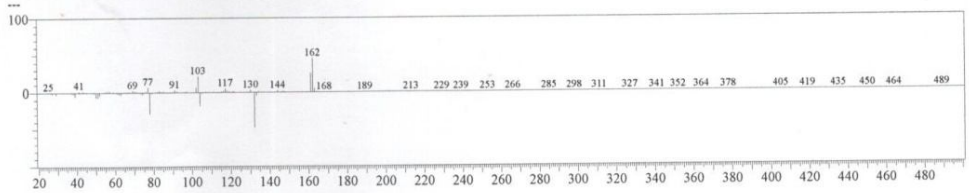
Spectrum1 #Data# Limon Oil.QGD R.Time:14.130(Scan#:2227)
MassPeaks:308
RawMode:Averaged 14.125-14.135(2226-2228) BasePeak:131.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:8563 Formula:C9H8O CAS:14371-10-9 MolWeight:132
MassPeaks:68 BasePeak:131.00(10000)
CompName:Cinnamaldehyde, (E)- $$ (E)-Cinnamaldehyde $$ trans-Cinnamaldehyde $$ trans-Cinnamic aldehyde $$ trans-Cinnamylaldehyde $$ (E)-3-Phenylpropenal $$ 2-Pro

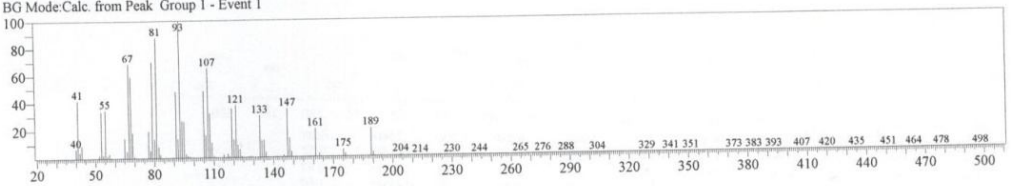


Spectrum3 #Calculation Result#
MassPeaks:254 BasePeak:162.10(4514)

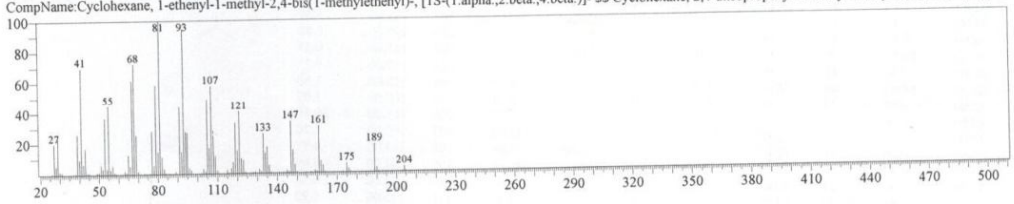


Spectrum Comparison

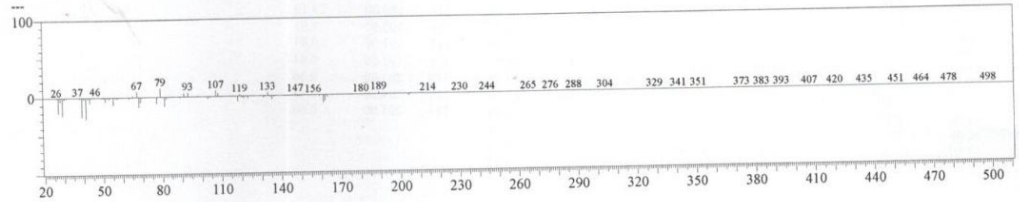
Spectrum1 #Data# Limon Oil.QGD R.Time:14.290(Scan#:2259)
MassPeaks:226
RawMode:Averaged 14.285-14.295(2258-2260) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:18058 Formula:C15H24 CAS:515-13-9 MolWeight:204
MassPeaks:121 BasePeak:81.00(10000)
CompName:Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1.alpha.,2.beta.,4.beta.)]- $$ Cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl-, (1S,2R,4R)- (-)- $

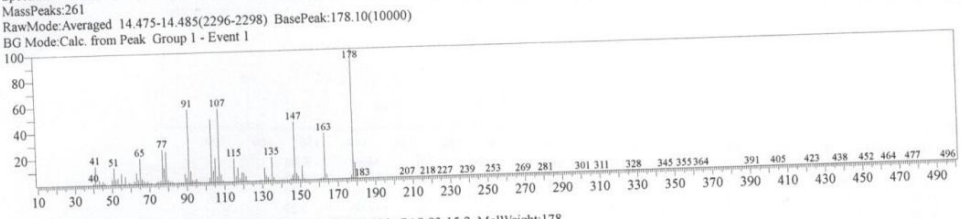


Spectrum3 #Calculation Result#
MassPeaks:243 BasePeak:79.05(1147)

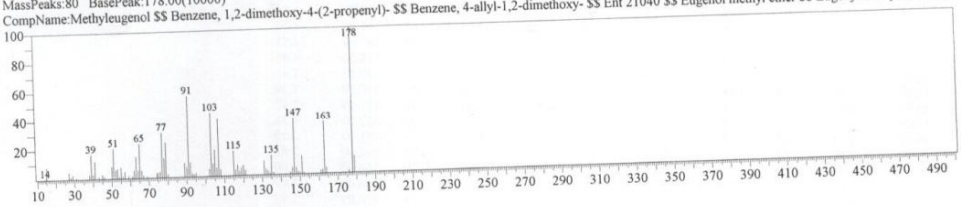


Spectrum Comparison

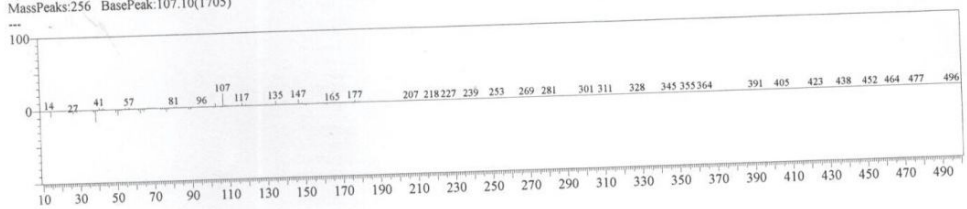
Spectrum1 #Data# Limon Oil.QGD R.Time:14.480(Scan#:2297)
MassPeaks:261
RawMode:Averaged 14.475-14.485(2296-2298) BasePeak:178.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:14052 Formula:C11H14O2 CAS:93-15-2 MolWeight:178
MassPeaks:80 BasePeak:178.00(10000)
CompName:Methyleugenol $$ Benzene, 1,2-dimethoxy-4-(2-propenyl)- $$ Benzene, 4-allyl-1,2-dimethoxy- $$ Ent 21040 $$ Eugenol methyl ether $$ Eugenyl methyl ether $$ 1

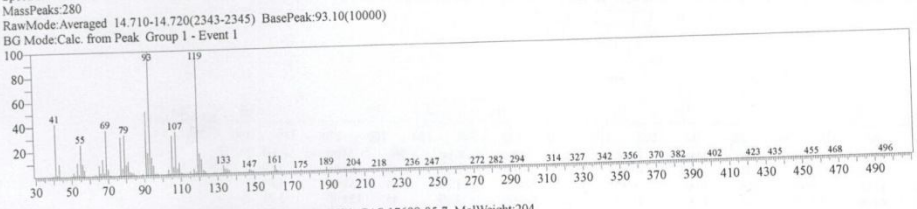


Spectrum3 #Calculation Result#
MassPeaks:256 BasePeak:107.10(1705)

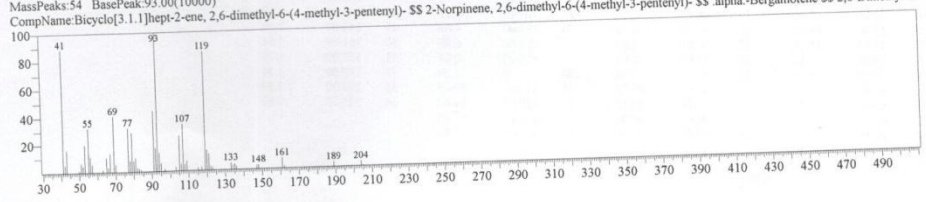


Spectrum Comparison

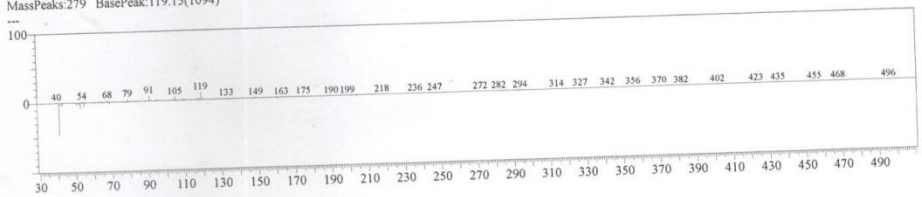
Spectrum1 #Data# Limon Oil.QGD R.Time:14.715(Scan#:2344)
MassPeaks:280
RawMode:Averaged 14.710-14.720(2343-2345) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:46623 Formula:C15H24 CAS:17699-05-7 MolWeight:204
MassPeaks:54 BasePeak:93.00(10000)
CompName:Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)- $$ 2-Norpinene, 2,6-dimethyl-6-(4-methyl-3-pentenyl)- $$ .alpha.-Bergamotene $$ 2,6-Dimethyl-6

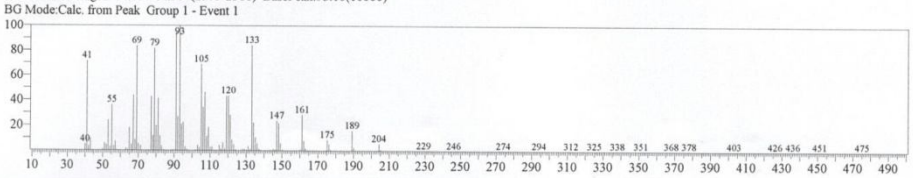


Spectrum3 #Calculation Result#
MassPeaks:279 BasePeak:119.15(1094)

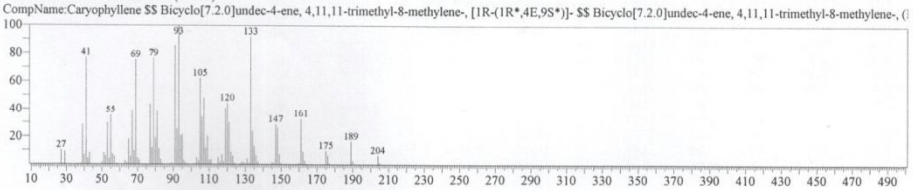


Spectrum Comparison

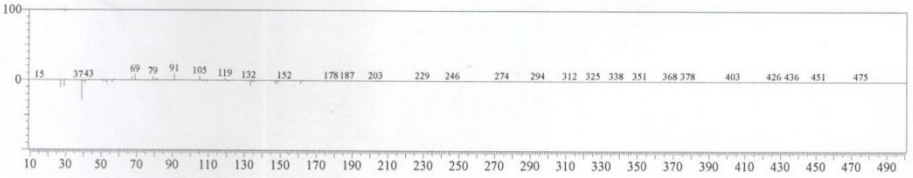
Spectrum1 #Data# Limon Oil.QGD R.Time:14.895(Scan#:2380)
MassPeaks:291
RawMode:Averaged 14.890-14.900(2379-2381) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:46636 Formula:C15H24 CAS:87-44-5 MolWeight:204
MassPeaks:120 BasePeak:93.00(10000)
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (

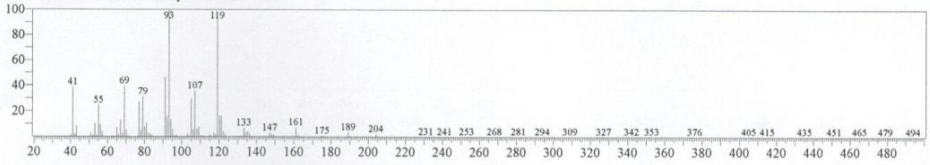


Spectrum3 #Calculation Result#
MassPeaks:239 BasePeak:91.05(935)

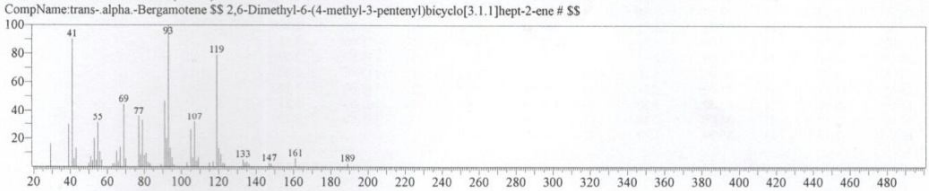


Spectrum Comparison

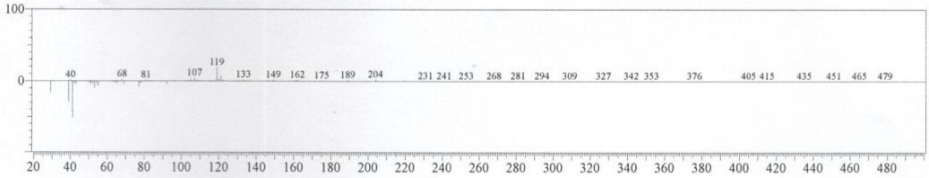
Spectrum1 #Data# Limon Oil.QGD R.Time:15.105(Scan#:2422)
MassPeaks:309
RawMode:Averaged 15.100-15.110(2421-2423) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:46622 Formula:C15H24 CAS:13474-59-4 MolWeight:204
MassPeaks:55 BasePeak:93.00(10000)
CompName:trans-.alpha.-Bergamotene $$ 2,6-Dimethyl-6-(4-methyl-3-pentenyl)bicyclo[3.1.1]hept-2-ene # $$

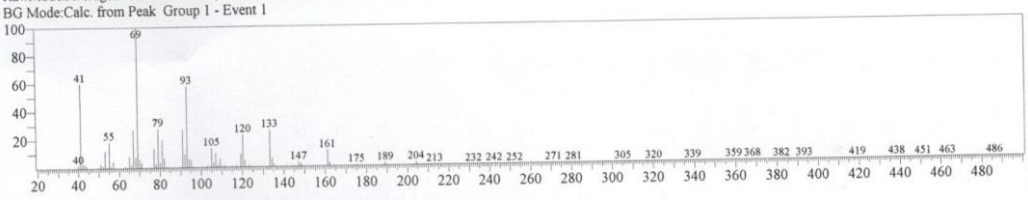


Spectrum3 #Calculation Result#
MassPeaks:213 BasePeak:119.10(1873)

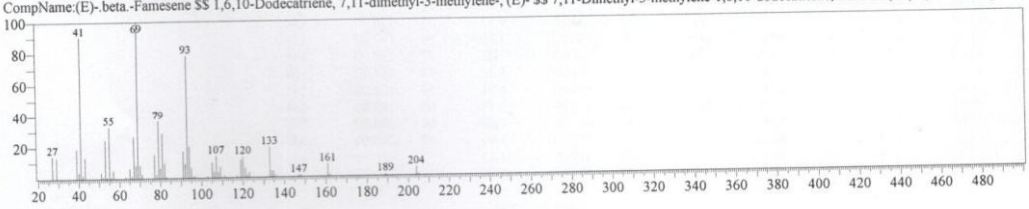


Spectrum Comparison

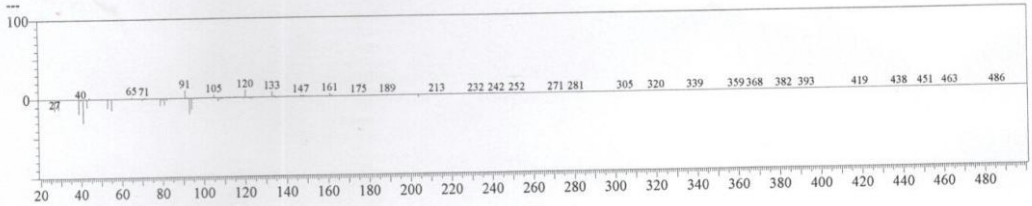
Spectrum1 #Data# Limon Oil.QGD R.Time:15.420(Scan#:2485)
MassPeaks:245
RawMode:Averaged 15.415-15.425(2484-2486) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:18051 Formula:C15H24 CAS:18794-84-8 MolWeight:204
MassPeaks:62 BasePeak:69.00(10000)
CompName:(E)-.beta.-Famesene $$ 1,6,10-Dodecatriene, 7,11-dimethyl-3-methylene-, (E)- $$ 7,11-Dimethyl-3-methylene-1,6,10-dodecatriene, trans $$ (6E)-7,11-Dimethyl-3-n

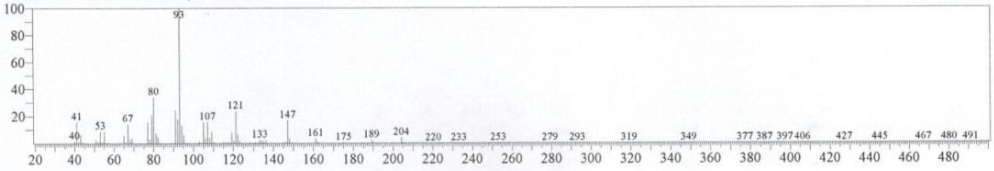


Spectrum3 #Calculation Result#
MassPeaks:237 BasePeak:91.10(973)

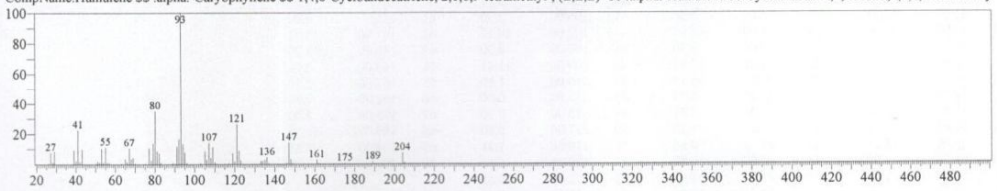


Spectrum Comparison

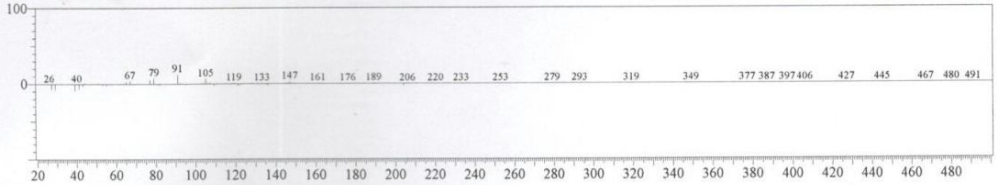
Spectrum1 #Data# Limon Oil.QGD R.Time:15.550(Scan#:2511)
MassPeaks:296
RawMode:Averaged 15.545-15.555(2510-2512) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:18070 Formula:C15H24 CAS:6753-98-6 MolWeight:204
MassPeaks:70 BasePeak:93.00(10000)
CompName:Humulene $$ .alpha.-Caryophyllene $$ 1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)- $$ .alpha.-Humulene $$ Cycloundeca-1,4,8-triene,2,6,6,9-tetramethy

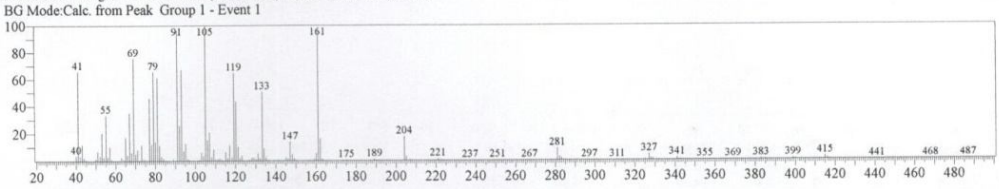


Spectrum3 #Calculation Result#
MassPeaks:280 BasePeak:91.05(1251)

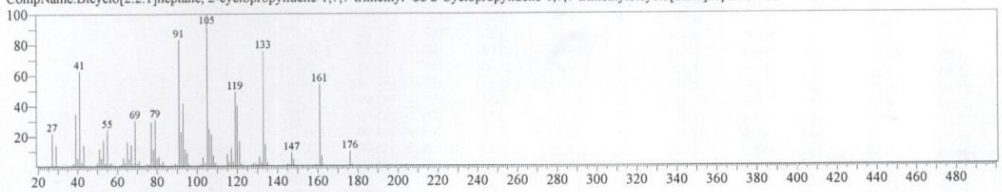


Spectrum Comparison

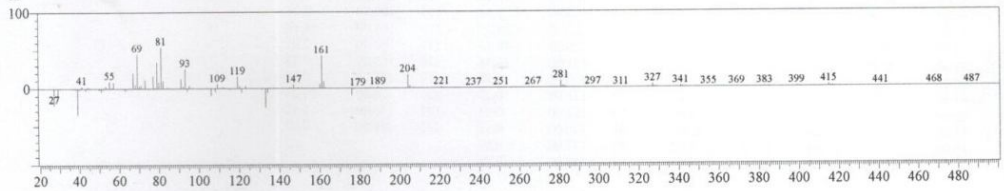
Spectrum1 #Data# Limon Oil.QGD R.Time:16.060(Scan#:2613)
MassPeaks:337
RawMode:Averaged 16.055-16.065(2612-2614) BasePeak:105.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:29328 Formula:C13H20 CAS:0-00-0 MolWeight:176
MassPeaks:122 BasePeak:105.00(10000)
CompName:Bicyclo[2.2.1]heptane, 2-cyclopropylidene-1,7,7-trimethyl- $$ 2-Cyclopropylidene-1,7,7-trimethylbicyclo[2.2.1]heptane # $$

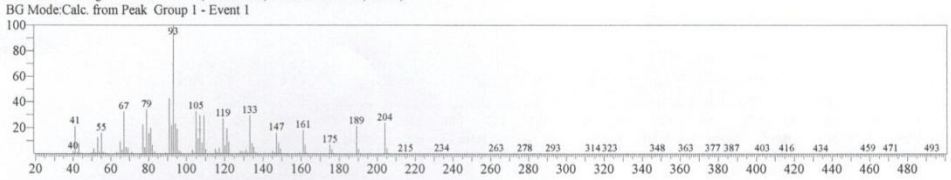


Spectrum3 #Calculation Result#
MassPeaks:332 BasePeak:81.10(5412)

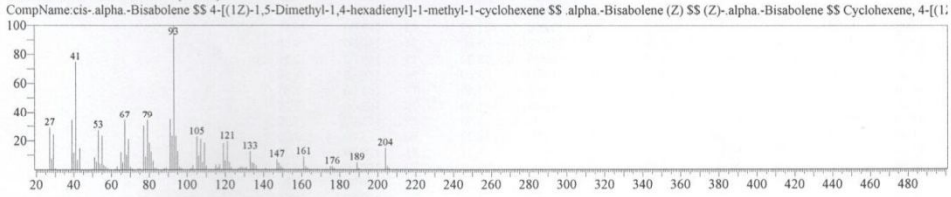


Spectrum Comparison

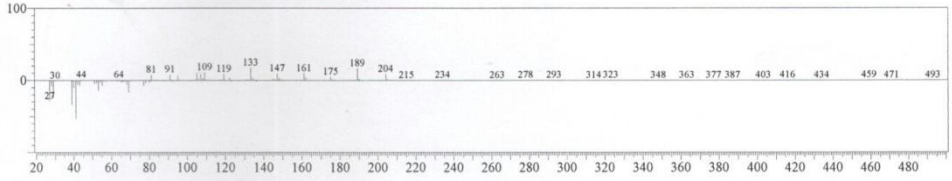
Spectrum1 #Data# Limon Oil.QGD R.Time:16.330(Scan#:2667)
MassPeaks:284
RawMode:Averaged 16.325-16.335(2666-2668) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:46619 Formula:C15H24 CAS:29837-07-8 MolWeight:204
MassPeaks:87 BasePeak:93.00(10000)
CompName:cis-.alpha.-Bisabolene $$ 4-[(1Z)-1,5-Dimethyl-1,4-hexadienyl]-1-methyl-1-cyclohexene $$ .alpha.-Bisabolene (Z) $$ (Z)-.alpha.-Bisabolene $$ Cyclohexene, 4-[(1

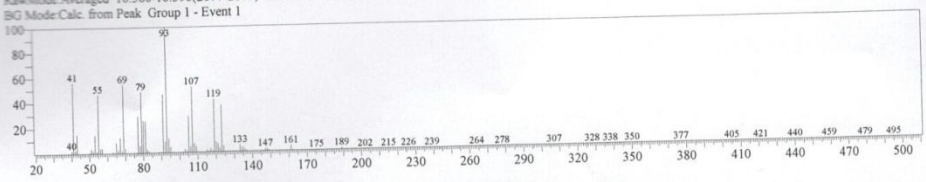


Spectrum3 #Calculation Result#
MassPeaks:289 BasePeak:133.15(1708)

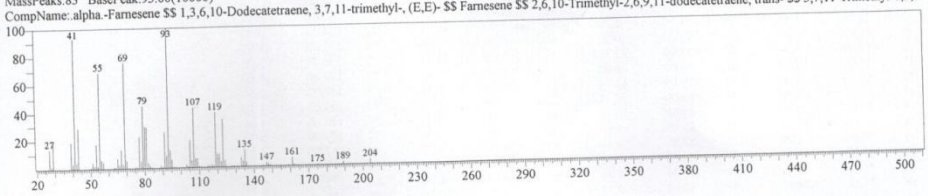


Spectrum Comparison

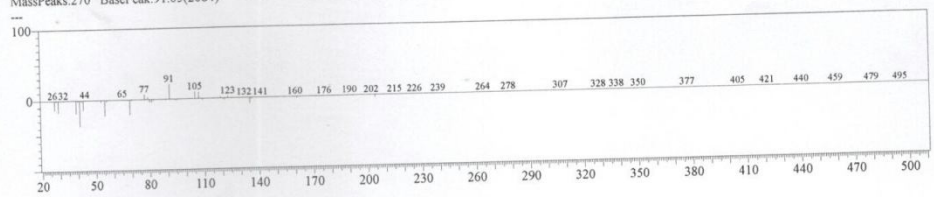
Spectrum1 #Data# Limon Oil.QGD R.Time:16.385(Scan#:2678)
MassPeaks:299
RawMode:Averaged 16.380-16.390(2677-2679) BasePeak:93.10(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:18064 Formula:C15H24 CAS:502-61-4 MolWeight:204
MassPeaks:83 BasePeak:93.00(10000)
CompName:.alpha.-Farnesene $$ 1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (E,E)- $$ Farnesene $$ 2,6,10-Trimethyl-2,6,9,11-dodecatetraene, trans- $$ 3,7,11-Trimethyl-1,3,6

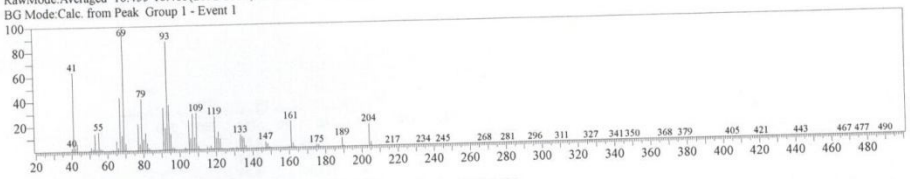


Spectrum3 #Calculation Result#
MassPeaks:270 BasePeak:91.05(2084)

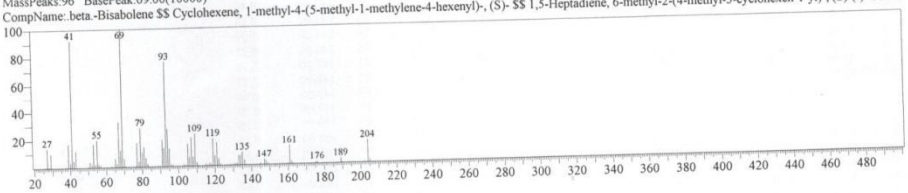


Spectrum Comparison

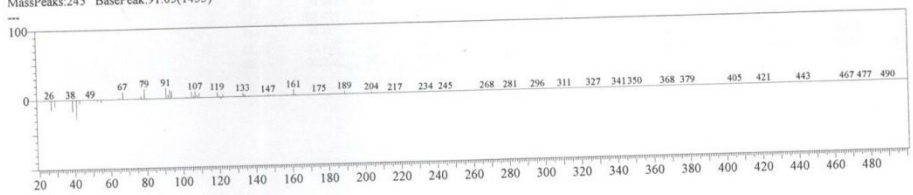
Spectrum1 #Data# Limon Oil.QGD R.Time:16.460(Scan#:2693)
MassPeaks:331
RawMode:Averaged 16.455-16.465(2692-2694) BasePeak:69.05(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:18054 Formula:C15H24 CAS:495-61-4 MolWeight:204
MassPeaks:96 BasePeak:69.00(10000)
CompName:.beta.-Bisabolene $$ Cyclohexene, 1-methyl-4-(5-methyl-1-methylene-4-hexenyl)-, (S)- $$ 1,5-Heptadiene, 6-methyl-2-(4-methyl-3-cyclohexen-1-yl)-, (S)-(-)- $$ l-.l

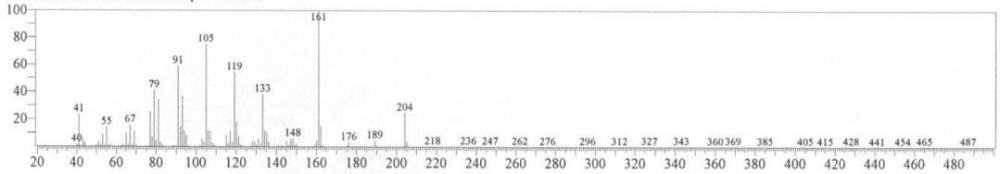


Spectrum3 #Calculation Result#
MassPeaks:245 BasePeak:91.05(1433)

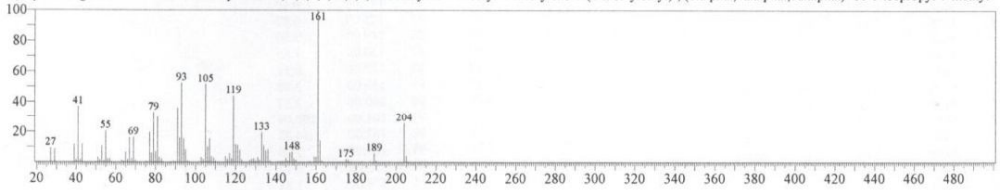


Spectrum Comparison

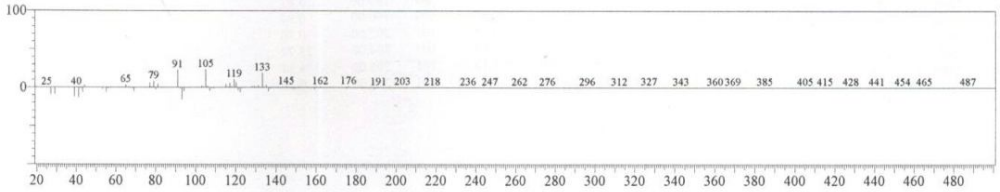
Spectrum1 #Data# Limon Oil.QGD R.Time:16.655(Scan#:2732)
MassPeaks:312
RawMode:Averaged 16.650-16.660(2731-2733) BasePeak:161.15(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:18125 Formula:C15H24 CAS:30021-74-0 MolWeight:204
MassPeaks:104 BasePeak:161.00(10000)
CompName:.gamma.-Muurolene $$ Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1.alpha.,4a.alpha.,8a.alpha.)- $$ 1-Isopropyl-7-methyl-

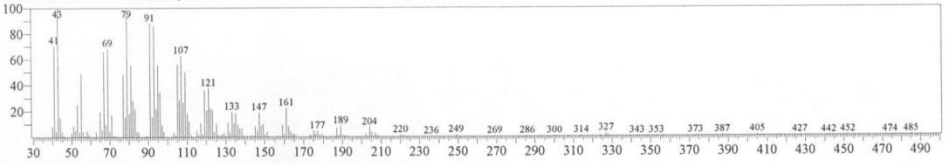


Spectrum3 #Calculation Result#
MassPeaks:309 BasePeak:105.10(2353)

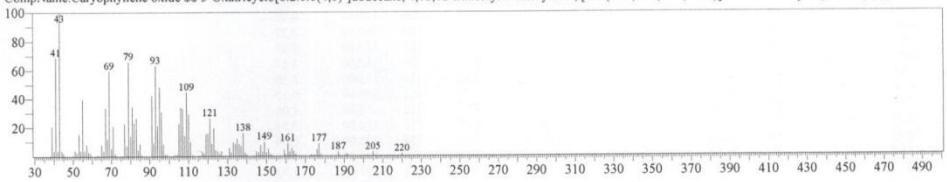


Spectrum Comparison

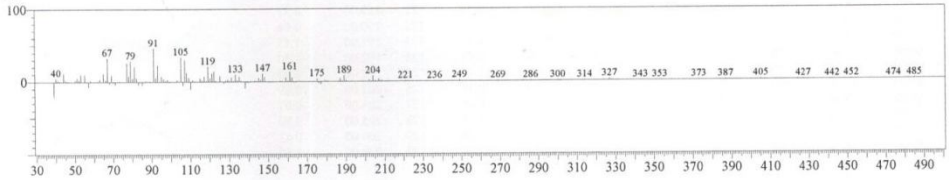
Spectrum1 #Data# Limon Oil.QGD R.Time:17.980(Scan#:2997)
MassPeaks:301
RawMode:Averaged 17.975-17.985(2996-2998) BasePeak:43.00(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11s.lib Entry:20008 Formula:C15H24O CAS:1139-30-6 MolWeight:220
MassPeaks:130 BasePeak:43.00(10000)
CompName:Caryophyllene oxide $$ 5-Oxatricyclo[8.2.0.0(4,6)-]dodecane, 4,12,12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- $$ 5-Oxatricyclo(8.2.0.0(4,6))dodecane

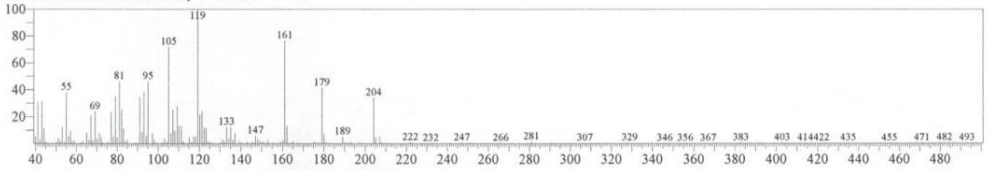


Spectrum3 #Calculation Result#
MassPeaks:305 BasePeak:91.05(4603)

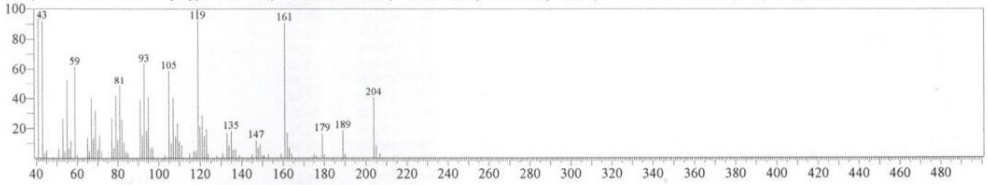


Spectrum Comparison

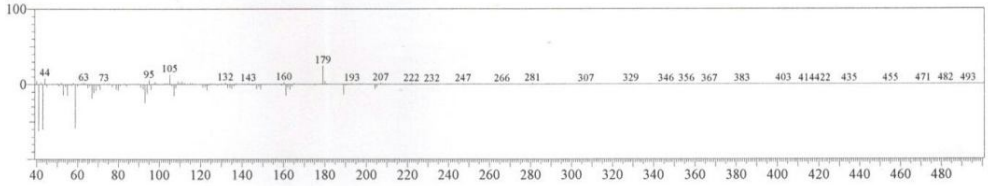
Spectrum1 #Data# Limon Oil.QGD R.Time:18.495(Scan#:3100)
MassPeaks:275
RawMode:Averaged 18.490-18.500(3099-3101) BasePeak:119.15(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:59424 Formula:C15H26O CAS:21284-22-0 MolWeight:222
MassPeaks:82 BasePeak:119.00(10000)
CompName:Cubenol $$ 1-Isopropyl-4,7-dimethyl-1,3,4,5,6,8a-hexahydro-4a(2H)-naphthalenol-, [1S-(1.alpha.,4.beta.,4a.beta.,8a.alpha.)]- $$ (-)-Cubenol $$ 10.beta.H-Cadin-4-

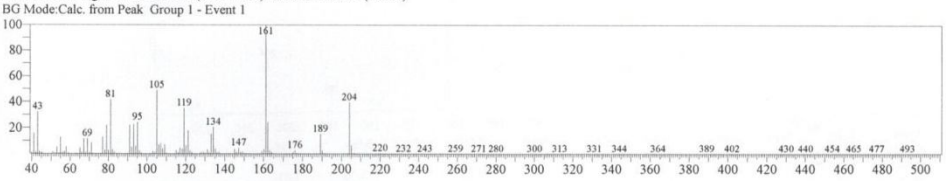


Spectrum3 #Calculation Result#
MassPeaks:276 BasePeak:179.15(2453)

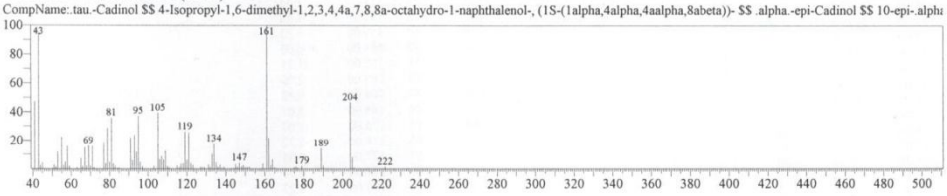


Spectrum Comparison

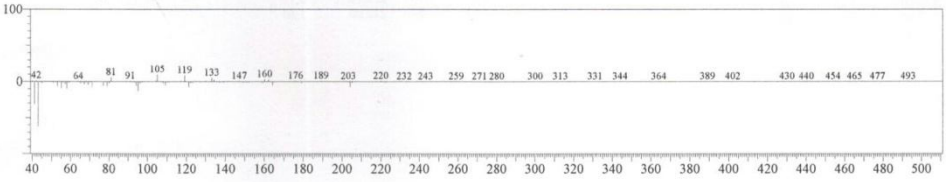
Spectrum1 #Data# Limon Oil.QGD R.Time:18.920(Scan#:3185)
MassPeaks:300
RawMode:Averaged 18.915-18.925(3184-3186) BasePeak:161.15(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:59439 Formula:C15H26O CAS:5937-11-1 MolWeight:222
MassPeaks:94 BasePeak:161.00(10000)
CompName:.tau.-Cadinol $$ 4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7,8,8a-octahydro-1-naphthalenol-, (1S-(1alpha,4alpha,4aalpha,8abeta))- $$ .alpha.-epi-Cadinol $$ 10-epi-.alph

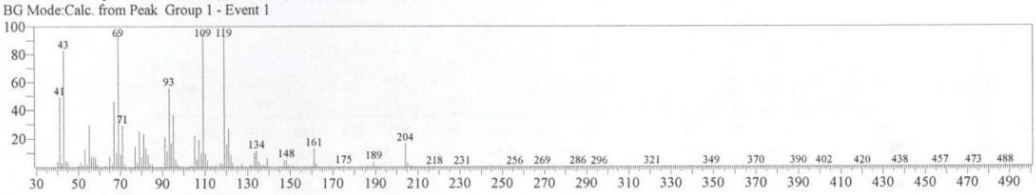


Spectrum3 #Calculation Result#
MassPeaks:266 BasePeak:105.10(969)

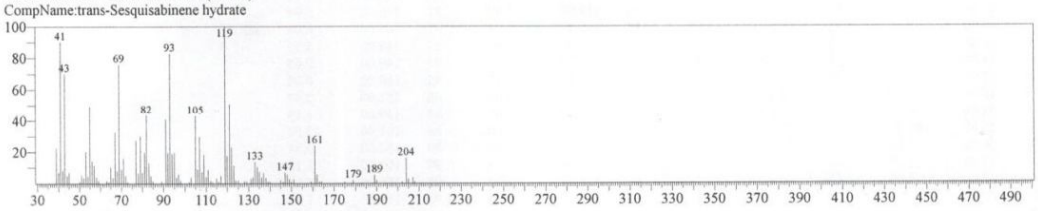


Spectrum Comparison

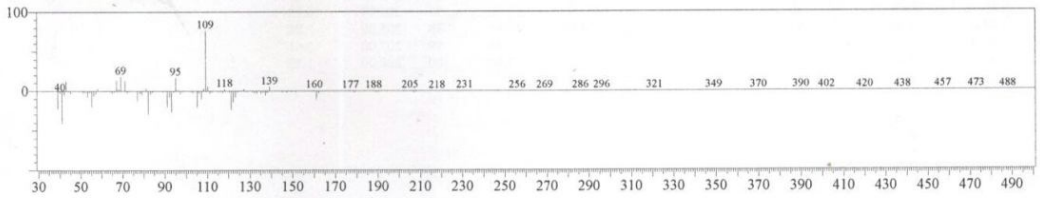
Spectrum1 #Data# Limon Oil.QGD R.Time:19.580(Scan#:3317)
MassPeaks:274
RawMode:Averaged 19.575-19.585(3316-3318) BasePeak:119.15(10000)
BG Mode:Calc. from Peak Group 1 - Event 1



Spectrum2 #Library# NIST11.lib Entry:59425 Formula:C15H26O CAS:0-00-0 MolWeight:222
MassPeaks:100 BasePeak:119.00(10000)
CompName:trans-Sesquisabinene hydrate

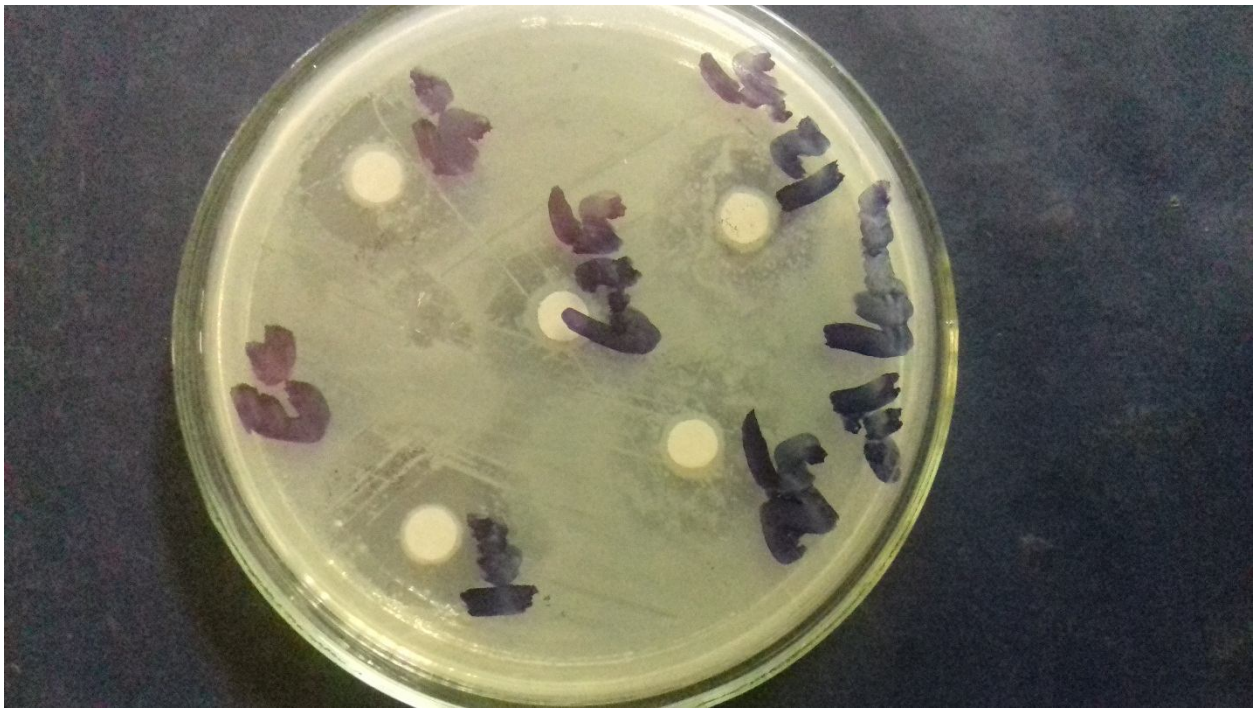


Spectrum3 #Calculation Result#
MassPeaks:276 BasePeak:109.15(7620)



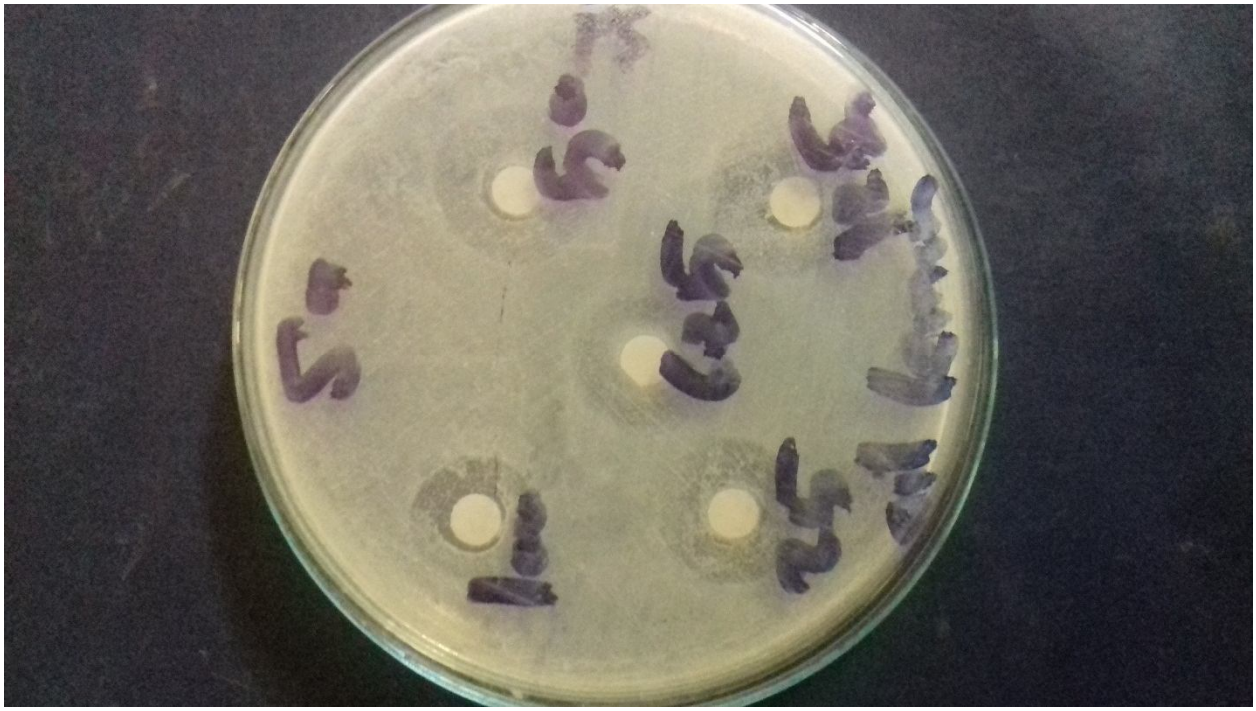
Appendix 4

Indibition Zones

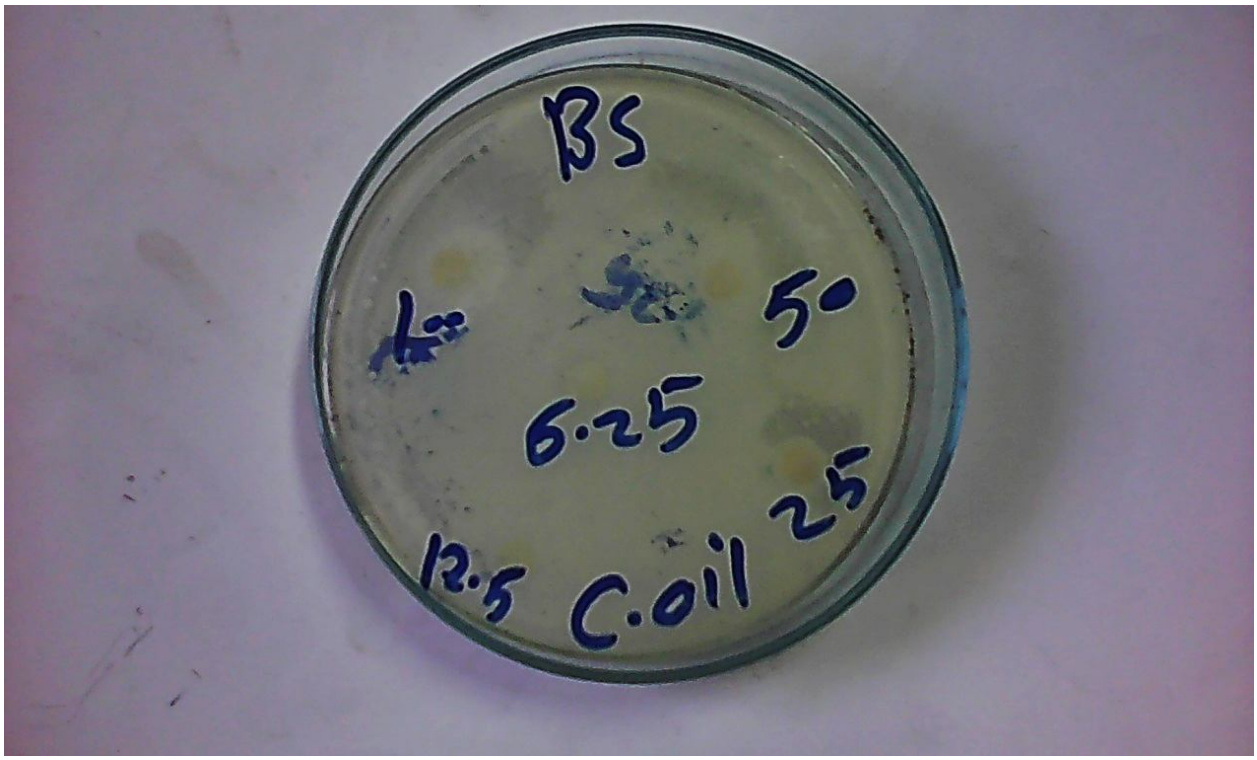


Inhibition zones of the peel oil extract against Escherichia coli

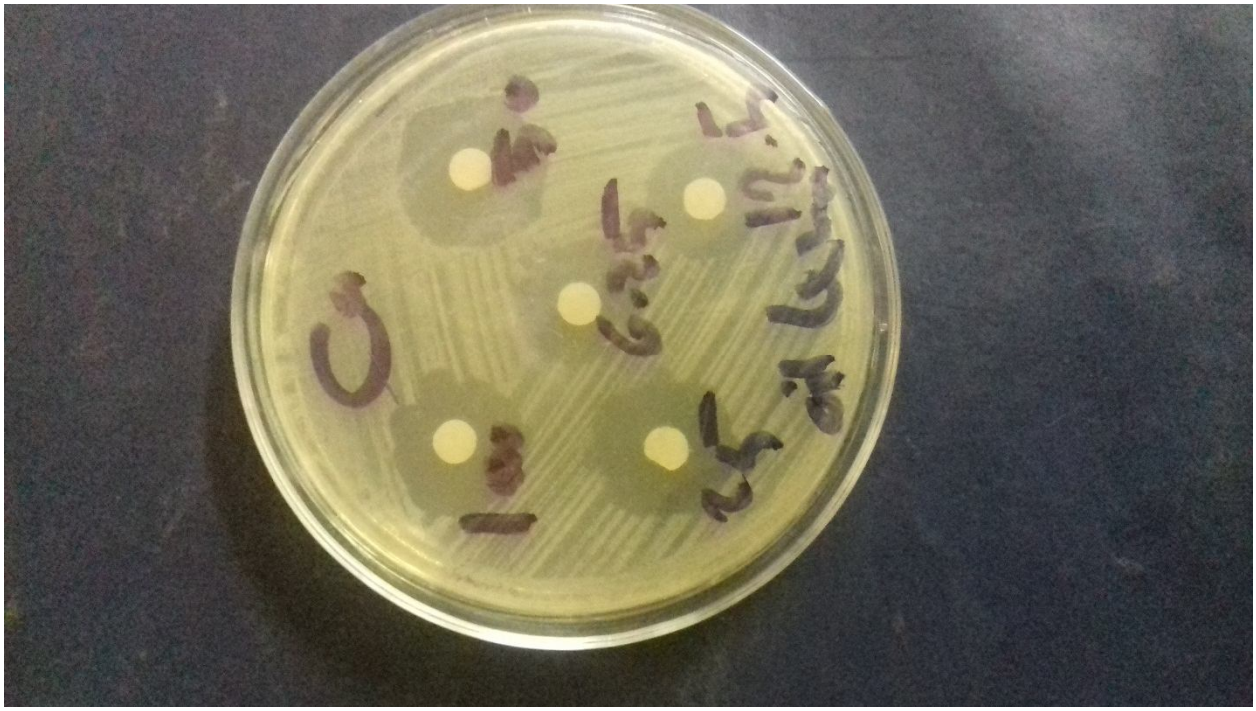
Inhibition zones of the peel oil extract against Pseudomonas aeruginosa



Inhibition zones of the peel oil extract against staphylococcus aureus



Inhibition zones of the peel oil extract against Bacillus subtilis



Inhibition zones of the peel oil extract against Candida albicans