

## OILS, ESSENTIAL

The volatile etherial fraction obtained from a plant or plant part by a physical separation method is called an essential oil. The physical method involves either distillation (including water, steam, water and steam, or dry) or expression (pressing). For the most part, essential oils represent the odorous part of the plant material, and therefore these oils have traditionally been associated with the fragrance and flavor industry (see Perfumes). Since essential oils frequently occur as a very small percentage by weight of the original plant material, the processing of large quantities is often required to obtain usable amounts of oil. As a result, expression of an essential oil is only employed in those cases where both the form of the natural plant material, such as a citrus peel, and the quantity of oil present make the process feasible.

It has frequently been observed that the aroma of an essential oil is substantially different from that of the plant before processing. Because this phenomenon is largely the result of the treatment of the plant material with heat or hot water, various other methods have evolved over the years in an attempt to obtain a concentrate of the volatiles which more truly represents the aroma of the original. With the exception of the method of expression, almost all of these involve treatment of the plant material with one or more organic solvents (or mixtures thereof) followed by concentration of the extracted solute. Solvent extraction frequently yields, in addition to the volatile oil, various quantities of semi- or nonvolatile organic material such as waxes (qv), fats, fixed oils, high molecular weight acids, pigments, and even alkaloidal material. However, because solvent extraction often results in a product with superior and more representative odor properties to that of a distilled oil, many natural products critically important to the flavor and fragrance industry are available as various extracts in addition to an essential oil.

Some of the commonly used botanical extracts include the following.

### 1. Absolute

This is concentrated extract obtained by treatment of a concrete or other hydrocarbon-type extract of a plant or plant part with ethanol. It is usually liquid and should be totally soluble in alcohol. By this method, waxes, hydrocarbons (including terpenoid), as well as most of the odorless material of the concrete are removed from the extract.

#### 1.1. Absolute Oil

This is the steam distillable portion of an absolute. Frequently, the absolute oil possesses superior odor properties to that of the corresponding essential oil.

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### **1.2. Aroma Distillate**

Used by the flavor industry, aroma distillates are the product of continuous extraction of the plant material with alcohol at temperatures between ambient and 50°C followed by steam distillation, and, lastly, concentration of the combined hydro–alcoholic mixture. On cooling, terpenes often separate from the aroma distillate and are removed.

### **1.3. Concrete**

Hydrocarbon extracts of plant tissue, concretes are usually solid to semisolid waxy masses often containing higher fatty acids such as lauric, myristic, palmitic, and stearic as well as many of the nonvolatiles present in absolutes.

### **1.4. Infusion**

Infusion botanical extracts are tinctures that have been concentrated by either total or partial removal of the alcohol by distillation.

### **1.5. Oleoresin**

Natural oleoresins are exudates from plants, whereas prepared oleoresins are solvent extracts of botanicals, which contain oil (both volatile and, sometimes, fixed), and the resinous matter of the plant. Natural oleoresins are usually clear, viscous, and light-colored liquids, whereas prepared oleoresins are heterogeneous masses of dark color.

### **1.6. Pommade**

These are botanical extracts prepared by the enfleurage method wherein flower petals are placed on a layer of fat which extracts the essential oil. This method is applied to low odored flowers, which do not yield appreciable oil on steam or water distillation, or flowers of valuable but delicate odor (such as jasmin), which are destroyed on such treatment. Pommades, as such, are seldom used by the industry at present (ca 1995), but are further processed to provide more concentrated extracts such as absolutes. Absolutes, being alcohol-soluble, are much more convenient forms for the perfumer.

### **1.7. Resin and Resinoid**

Natural resins are plant exudates formed by the oxidation of terpenes. Many are acids or acid anhydrides. Prepared resins are made from oleoresins from which the essential oil has been removed. A resinoid is prepared by hydrocarbon extraction of a natural resin.

### **1.8. Tincture**

This is prepared by aqueous alcoholic extraction of the raw plant material. Since the extract is not further concentrated, the plant extract is not exposed to heat.

Essential oils are isolated from various plant parts, such as leaves (patchouli), fruit (mandarin), bark (cinnamon), root (ginger), grass (citronella), wood (amyris), heartwood (cedar), gum (myrrh oil), balsam (tolu balsam oil), berries (pimento), seeds (dill), flowers (rose), twigs and leaves (thuja oil), and buds (cloves).

Exceptions to the simple definition of an essential oil are, for example, garlic oil, onion oil, mustard oil, or sweet birch oils, each of which requires enzymatic release of the volatile components before steam distillation.

In addition, the physical process of expression, applied mostly to citrus fruits such as orange, lemon, and lime, yields oils that contain from 2–15% nonvolatile material. Some flowers or resinoids obtained by solvent extraction often contain only a small portion of volatile oil, but nevertheless are called essential oils. Several oils are dry-distilled and also contain a limited amount of volatiles; nonetheless they also are labeled essential oils, eg, labdanum oil and balsam oil Peru. The yield of essential oils from plants varies widely. For example, nutmegs yield 10–12 wt % of oil, whereas onions yield less than 0.1% after enzymatic development.

The function of the essential oil in the plant is not fully understood. Microscopic examination of plant parts that contain the oil sacs readily shows their presence. The odors of flowers are said to act as attractants for insects involved in pollination and thus may aid in preservation and natural selection. Essential oils are almost always bacteriostats and often bacteriocides. Many components of essential oils are chemically active and thus could participate readily in metabolic reactions. They are sources of plant metabolic energy, although some chemists have referred to them as waste products of plant metabolism. Exudates, which contain essential oils, eg, balsams and resins, act as protective seals against disease or parasites, prevent loss of sap, and are formed readily when the tree trunks are damaged.

The cultivation of essential oil-bearing plants has kept pace with modern agricultural methods. Hybrids are grown to yield oils of specific odor, flavor, or other properties. New plants have been developed, eg, lavandin, and new essential oils are isolated and evaluated every year. Very few are commercialized. New growing areas for specific oils are opened that offer quality or economic advantages, such as soil conditions, irrigation, and the availability of labor. Most oils are prepared close to their source so as to provide access to the freshly harvested plant material and to keep processing costs low. Exceptions include the absolutes and other extracts of natural oleoresins, such as myrrh, olibanum, and labdanum, which tend to maintain their odor quality over a longer period of time. A few oils are still produced under very primitive conditions.

Rectified oils have been redistilled to improve a particular property or characteristic, such as flavor or aroma. For example, natural oil of peppermint is frequently rectified to remove dimethyl sulfide, which has a powerful and objectionable cooked vegetable note deleterious to the use of the oil in crème de menthe liqueurs. Distillation is also used to remove psoralens, which are harmful photosensitizing agents present in natural bergamot oil. Color may be removed, eg, from cassia oil, by vacuum steam distillation. A desirable component, such as 1,8-cineole (eucalyptol) 85% in eucalyptus oil, may be concentrated further by distillation to remove a forerun (topping).

Concentrated or folded oils are processed by various physical means to remove wholly or partly undesirable or nonflavor components, such as terpenes or sesquiterpenes, which have poor alcohol and water solubility, very low flavor value, and poor stability. Although this group, for the most part, comprises citrus oils with high terpene contents which cause clouding in drink applications, other oils such as spearmint are included. The processing methods include fractional distillation, topping, solvent extraction, countercurrent extraction, supercritical extraction, thin-film evaporation, and molecular distillation. In some cases, both distillation and solvent extraction are needed for complete removal of terpenes. Thus, such oils as tangerine-terpeneless, lemon-sesquiterpeneless, or orange-80% terpeneless are processed oils. Some oils, particularly citrus, are folded or concentrated to reduce the terpene content to a designated level, ie, when half of the volatile constituents of the oil are removed, their removal is said to double the concentration and the oil is then called twofold. Although termed concentration, this process is, nevertheless, not merely a concentration in the ordinary sense, since the flavor body of the concentrate is always weaker than that of the complete essential oil, demonstrating that valuable products are lost in the course of removing the terpenes. In the past, a distinction was made between terpeneless and sesquiterpeneless oils, but this distinction has been abandoned since it is only fractional distillation which can practically remove monoterpenes without removing sesquiterpenes at the same time.

Aroma chemicals are isolates, or chemically treated oils or components of oils. Some components are removed physically, others chemically. In most cases, they are further purified by distillation. For example, Bois de Rose (rosewood) oil may be distilled to isolate linalool, which may be then further treated chemically to yield derivatives such as linalyl acetate, an important fragrance ingredient and a primary component in its

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own right of lavender and lavandin oils. Vetiver oil Haiti, although containing only 70% alcohols, is treated with acetic anhydride, then carefully distilled to include valuable odor components in the distillate, even though they may not be esters.

A number of other valuable aroma chemicals can be isolated from essential oils, eg, eugenol from clove leaf oil, which can also, on treatment with strong caustic, be isomerized to isoeugenol, which on further chemical treatment can be converted to vanillin (qv). Sometimes the naturally occurring component does not require prior isolation or concentration, as in the case of cinnamaldehyde in cassia oil which, on direct treatment of the oil by a retro-aldol reaction, yields natural benzaldehyde (qv). This product is purified by physical means.

## 2. Economic Aspects

Essential oils are used as flavoring and fragrance agents in every possible application. Combinations have raised greatly the total sales volume; eg, mint and cinnamon are used in toothpaste, mouthwash, or lozenges. Combinations can be found in every fragranced product, such as fine fragrances, soaps, detergents, room fresheners, paper, printing ink, paint, candles, condiments, floor polishes, etc. Convenience foods and frozen foods are flavored best by essential oils or oleoresins. Although citronella oil was used as such as an insect repellent, synthetic repellents have, for the most part, taken their place. Flavor essential oils are encountered in baked goods, snack foods, soft drinks, liqueurs, tobacco, sauces, gravies, salad dressings, and other food products.

In 1993, the United States imported nearly  $22 \times 10^6$  kg of essential oils at a total value of almost  $\$190 \times 10^6$ , an increase over 1992 of ca  $2.3 \times 10^6$  kg and  $\$935,000$ . Table 1 lists the quantities and values of 35 imported essential oils. The United States exports seven principal essential oils: orange, lemon, peppermint, spearmint, cedarwood, clove, and nutmeg. The latter two are not grown in the United States but are imported as dried spice, processed for oil, and then exported.

## 3. Composition

The volatile components of essential oils, for the most part, are made up of relatively low molecular weight ( $\geq \sim 300 - 350$ ) organic molecules of carbon, hydrogen, and oxygen, and occasionally nitrogen and sulfur. Less frequently, chlorine and bromine are found, eg, in seaweed volatiles. By far the largest class of natural volatiles of plants is the terpenes, which consist of head-to-tail condensation products of unsaturated five-carbon isoprene units. The simplest terpenes are monoterpenes with 10 carbon atoms. They may be aliphatic, alicyclic, or bi- or tricyclic, with varying degrees of unsaturation up to three double bonds. Sesquiterpenes contain three isoprene units, diterpenes four, triterpenes six, etc. Diterpenes (C-20) or larger units are rarely found in volatile oils, but may be extracted from the botanical. Oxygenated terpenes (terpenoids) usually accompany terpenes in essential oils, but are often present in a lower total percentage (see Terpenoids).

Other commonly occurring chemical groups in essential oils include aromatics such as  $\beta$ -phenethyl alcohol, eugenol, vanillin, benzaldehyde, cinnamaldehyde, etc; heterocyclics such as indole (qv), pyrazines, thiazoles, etc; hydrocarbons (linear, branched, saturated, or unsaturated); oxygenated compounds such as alcohols, acids, aldehydes, ketones, ethers; and macrocyclic compounds such as the macrocyclic musks, which can be both saturated and unsaturated.

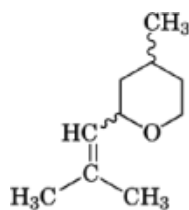
An essential oil may contain  $>200$  components, and often the trace substances ( $\geq$  ppm) are essential to the odor and flavor of the oil. The absence or decreased presence of even one component may be cause for odor or flavor rejection of the oil. The same species of plant grown in different parts of the world usually contains the same chemical components, but the relative percentages may be different. Climatic and topographical conditions affect plant chemistry and can alter the essential oil content both qualitatively and quantitatively.

**Table 1. U.S. Imports of Specified Essential Oils, 1993<sup>a</sup>**

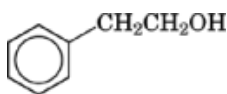
Essential oils	CAS Registry Number	Amount, kg	Value, <sup>b</sup> $\times 10^3$ \$
anise oil	[8007-70-3]	49,455	400.8
bergamot oil	[8007-75-8]	37,821	2,362.9
caraway oil	[8000-42-8]	10,878	411.8
cassia oil	[8007-80-5]	385,158	16,477.1
cedarwood oil	[8000-27-9]	338,179	1,693.6
citronella oil	[8000-29-1]	885,843	3,955.2
citrus oils, other		358,230	2,866.6
clove oils		462,770	1,486.7
cornmint		248,841	1,157.7
eucalyptus oil	[8000-48-4]	454,152	1,859.2
geranium oil	[8000-46-2]	64,251	2,924.9
grapefruit oil	[8016-40-4]	178,501	1,331.4
jasmin oil	[8022-96-6]	10,716	1,967.8
lavender oil (including spike <sup>c</sup> )	[8000-28-0]	417,518	6,253.5
lemon oil	[8008-56-8]	1,406,479	23,028.6
lemongrass oil		67,796	479.4
Bois de Rose oil		30,088	700.6
lime oil	[8008-26-2]	756,724	13,267.9
mint oil, other varieties		79,498	859.6
nutmeg oil	[8008-45-5]	109,520	935.6
onion and garlic oils		73,563	5,219.6
orange oil	[8008-57-9]	11,908,627	16,205.6
orris oil	[8002-73-1]	3,387	2,752.7
patchouli oil	[8014-09-3]	390,100	7,398.6
peppermint oil	[8006-90-4]	146,739	2,558.1
petitgrain oils		76,507	2,010.1
pine oil	[8002-09-3]	2,117	12.3
rose oil (Attar of Roses)	[8007-01-0]	2,504	6,666.0
rosemary oil	[8000-25-7]	63,894	717.5
sandalwood oil	[8006-87-9]	31,052	3,280.9
sassafras oil		250,880	1,027.0
spearmint oil	[8008-79-5]	318,487	3,019.5
vetiver oil	[8016-96-4]	48,434	2,795.3
ylang ylang oil (cananga <sup>d</sup> )	[8006-87-3]	45,105	2,865.4
other essential oils		2,214,041	46,671.7
<i>Total</i>		<i>21,927,855</i>	<i>187,621.2</i>

<sup>a</sup>Ref. 1.<sup>b</sup>All values are fob country of origin.<sup>c</sup>CAS Registry Number [8016-78-2].)<sup>d</sup>CAS Registry Number [68606-83-7].

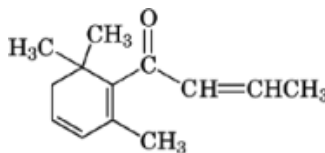
For example, Bulgaria and Turkey both grow *Rosa damascena* Mill. for the production of rose oil. Each contains the same constituents, but the relative percentages are somewhat different although not sufficiently so to cause rejection of one over the other. Synthetic versions of several of the key aroma ingredients of rose oil, such as *cis*- and *trans*-rose oxides (**1**),  $\beta$ -phenethyl alcohol [60-12-8], (**2**), and *trans*- $\beta$ -damascenone [23726-93-4] (**3**), are available commercially.



(1)



(2)



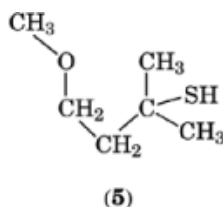
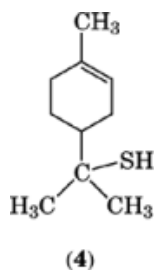
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#### 4. Analytical Methods

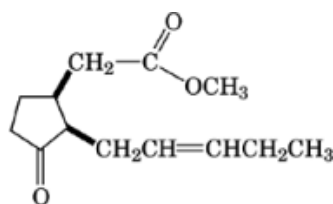
Early methods for the determination of the quality of an essential oil involved such subjective techniques as odor and color comparison with respect to a standard retention sample. Gradually, analytical techniques evolved to include specific gravity, refractive index, distillation range, and iodine number determination, and gas-liquid chromatography (glc) analysis of essential oils provided quick and routine determination of qualitative and quantitative profiles of the volatile constituents of an oil. It became obvious that many essential oils were much more complex than originally believed. Many structures, both simple and complicated, were worked out by natural products chemists before the availability of chromatography. Some of the early structures needed revision as purer isolates became available and as more sophisticated tools for structure elucidation were developed, including ir and uv spectroscopy, mass spectrometry (ms), and  $^1\text{H}$ - and  $^{13}\text{C}$ -nmr. With the advent of capillary glc, the more sensitive flame ionization detection (FID), and the marriage of this separation technique with the total ion current detector of the mass spectrometer (ms/gc), baseline separation of most volatile components of an oil was achieved. Not only can trace constituents present at levels below 1% in the oil be readily identified, but new, previously undetected components have become evident. To aid in their structure elucidation, new, more powerful, and selective characterization tools such as Fourier-transform gc/ir, high resolution ms/gc (by means of which an empirical formula may be obtained), chemical ionization ms/gc (which can provide the molecular weight of a molecule), and ftnmr and cryogenic nmr with much improved sensitivity have been developed and are being routinely used.

A component with critical odor properties may be present in an oil at ultratrace levels for which a discreet glc peak cannot be readily assigned. This is often the case with molecules containing heteroatoms such as nitrogen and, particularly, sulfur. In this case, the use of olfactory detection involving glc sniff runs is required to pinpoint the elution time of the trace constituent. Thus equipped, the natural product "detective" can zero in on the compound and, through preconcentration methods or the use of ultrasensitive spectroscopy tools, sufficient information can frequently be obtained for a preliminary postulation of structure, which must then

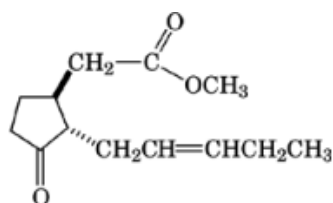
be confirmed through synthesis. Through these methods, such powerfully odored and important new aroma and flavor molecules as *p*-menthene-8-thiol [71159-90-5] (4) in grapefruit (2) and 4-methoxy-2-methyl-2-butanethiol [94087-83-9] (5) in black currant bud oil (3) have been made available to the flavorist and perfumer.



Along with the refinement in separation and characterization methodology, an increasing awareness has evolved on the part of fragrance chemists of the role played by chirality in the odor properties of certain organic molecules. With the ability to separate, synthesize in high optical purity, and assign absolute configurations to enantiomers, the relative odor contributions of individual optical isomers can frequently be determined. The results are often surprising, as in the case of “methyl jasmonate” from jasmin oil, lemon peel, boronia, etc. Following the isolation and characterization of methyl *epi*-jasmonate from the pheromone glands of the male oriental fruit moth (4) and the disclosure that this is the only epimer occurring in ripe lemon peels (5), the odor thresholds of the stereoisomers of methyl jasmonate [91905-97-4] were determined (6). It was found that ( $\pm$ )-methyl *epi*-jasmonate [53369-26-9] (6) is more than 400 times stronger than ( $\pm$ )-methyl jasmonate [20073-13-6] (7), the principal ingredient in both commercial synthetic methyl jasmonate and in jasmin absolute. Also, (+)-methyl *epi*-jasmonate [42536-97-0] is more than four times stronger than ( $\pm$ )-methyl *epi*-jasmonate (6). It was, therefore, concluded that the (–)-methyl jasmonate [1211-29-6] and (+)-methyl jasmonate [78609-06-0] contribute almost nothing to the odor of the commercial mixture (7). It is apparent that it is the small amount of methyl *epi*-jasmonate which occurs both in commercial methyl jasmonate and in various natural oils and extracts which is the main contributor to the typical lemony-jasmin odor of these materials. Moreover, since it has been demonstrated (5) that methyl *epi*-jasmonate is the thermodynamically less stable form, its predominance in the living plant and its conversion to the more stable methyl jasmonate during harvesting and processing cannot be excluded. Indeed, it has been found that methyl *epi*-jasmonate occurs in high concentration in the volatiles of living *Cymbidium kanran* orchid but is transformed to methyl jasmonate on picking (8).



(6)



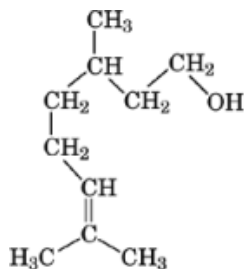
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## 5. Commercial Essential Oils

The information given for the commercial oils represents data critically selected from published reliable sources or, in some cases, analyses performed in the authors' laboratories on authentic oil samples. These data are provided as a general guide to composition only and are not meant to be exclusive of analytical results obtained by other researchers on similar oils. Where the literature provides ranges of composition, these have, in several cases, been included. Many variables affect the composition of essential oils.

### 5.1. Rose

Of all the natural oils, rose is probably the most desired material used in the fine fragrance industry. For years chemists have tried to unravel the mystery of the odor-donating components of this high priced natural material. Simple glc analysis shows that nine components constitute nearly 89% of the total volatiles of rose otto (9) (see Table 2).



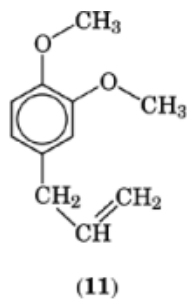
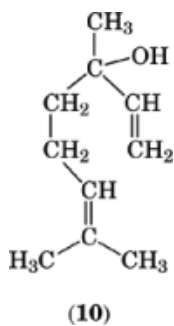
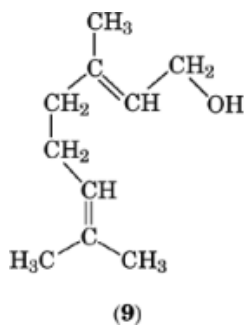
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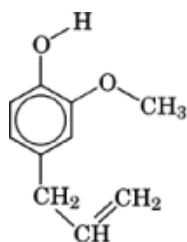
**Table 2. Constituents of Otto of Rose Bulgarian**

Component	CAS Registry Number	Structure number	Percent
citronellol	[106-22-9]	(8)	36
paraffin hydrocarbons <sup>a</sup>			25
geraniol	[624-15-7]	(9)	17
$\beta$ -phenethyl alcohol	[60-12-8]	(2)	3
linalool	[78-70-6]	(10)	2
ethanol	[64-17-5]		2
eugenol methyl ether	[93-15-2]	(11, R = CH <sub>3</sub> )	1.5
eugenol	[97-53-0]	(11, R = H)	1.3
geranial <sup>b</sup>	[141-27-5]		1
Total			88.8

<sup>a</sup>Nonadecane [629-92-5], 1-nonadecene [18435-45-5], heneicosane [629-94-7], heneicosene [27400-79-9], eicosane [112-95-8], and eicosene [27400-78-8].

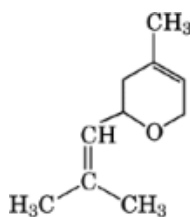
<sup>b</sup>3,7-Dimethyl-*trans*-2,6-octadienal; see also geraniol (9).



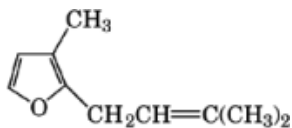


(11)

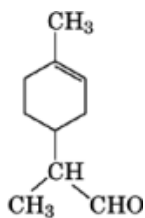
Of all these, probably  $\beta$ -phenethyl alcohol (**2**) comes closest to the odor of fresh rose petals; however, mixing all these components does not reproduce the total fine character of the natural oil. It has been determined that a number of trace constituents representing less than 1% of the volatiles are critical to the development of the complete rose fragrance (10). These include *cis*- and *trans*-rose oxide (**1**), nerol oxide (**12**), rose furan (**13**), *para*-menth-1-en-9-al (**14**),  $\beta$ -ionone (**15**),  $\beta$ -damascone (**16**), and  $\beta$ -damascenone (**3**).



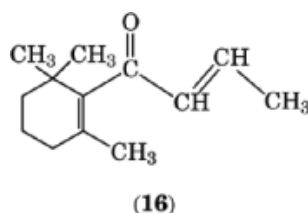
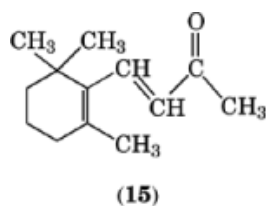
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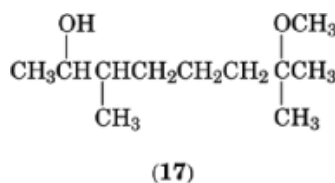
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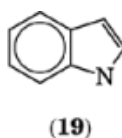
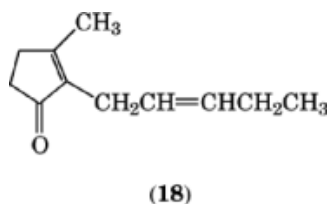


Sometimes a skilled perfumer detects a sandalwood-musky note in authentic Bulgarian otto of rose. This note has been identified (11) as the trace ingredient, 7-methoxy-3,7-dimethyl-2-octanol [41890-92-0] (17), which has been commercially available for some time as Ossyrol (trademark of Bush, Boake, Allen Inc). This compound had never before been identified in nature, but demonstrates how, sometimes, synthetic fragrance chemists can anticipate nature.



## 5.2. Jasmin

“If the rose is the queen of flowers, the jasmin is the fairest and prettiest princess. The two together reign supreme in the world of flowers as well as in the world of perfume” (12). As in the case of rose, jasmin has been the subject of many investigations, and more than 95 compounds have been identified to date in extracts of *Jasminum officinale* L. var. *grandiflorum*, the source of commercial jasmin oil, concrete, and absolute. The principal components are shown in Table 3 (13).



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**Table 3. Constituents in *Jasminum officinale*<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent
phytol <sup>b</sup>	[150-86-7]		
isophytol <sup>c</sup>	[505-32-8]		27
benzyl benzoate	[120-51-4]		16
benzyl acetate	[140-11-4]		15
benzyl alcohol	[100-51-6]		6
linalool		(10)	6
geranyl linalool <sup>d</sup>	[1113-21-9]		4
<i>cis</i> -jasmone	[488-10-8]	(18)	4
methyl jasmonate			3
eugenol			2
indole	[120-72-9]	(19)	2
<i>cis</i> -3-hexenyl benzoate	[25152-85-6]		2
methyl linolenate <sup>e</sup>	[301-00-8]		2
<i>Total</i>			89

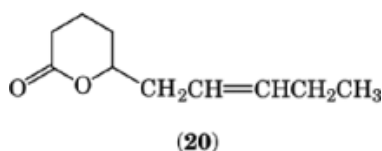
<sup>a</sup>Ref. 13.

<sup>b</sup>3,7,11,15-Tetramethyl-*trans*-2 hexadecen-1-ol.

<sup>c</sup>3,7,11,15-Tetramethyl-1-hexadecen-3-ol.

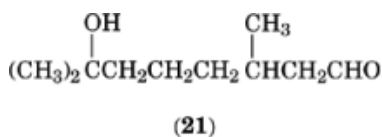
<sup>d</sup>3,7,11,15-Tetramethyl-1,6,10,14-hexadecatetraen-3-ol.

<sup>e</sup>Methyl (*Z,Z,Z*)-9,12,15-octadecatrienoate.



Of the 11 compounds which constitute approximately 86% of jasmin volatiles, only benzyl acetate, *cis*-jasmone (18), and methyl jasmonate possess the characteristic odor of jasmin. Trace components including *cis*-jasmin lactone [34686-71-0] (20) (0.9%) and methyl *epi*-jasmonate (6) (0.1%) are the key contributors to the jasmin odor.

As early as 1967, IFF chemists (11), in an in-depth study of jasmin absolute, identified an ultratrace amount of one of the key compounds in the entire fragrance repertoire, hydroxycitronellal [107-75-7] (21). This chemical has been used for many years in almost every “white flower” fragrance to give a very diffusive and lasting lily-of-the-valley and jasmin note, but this represents the only known identification of the compound in nature. This illustrates that the human nose can often predict the presence of a molecule well before the instrumentation becomes sufficiently sensitive to detect it.

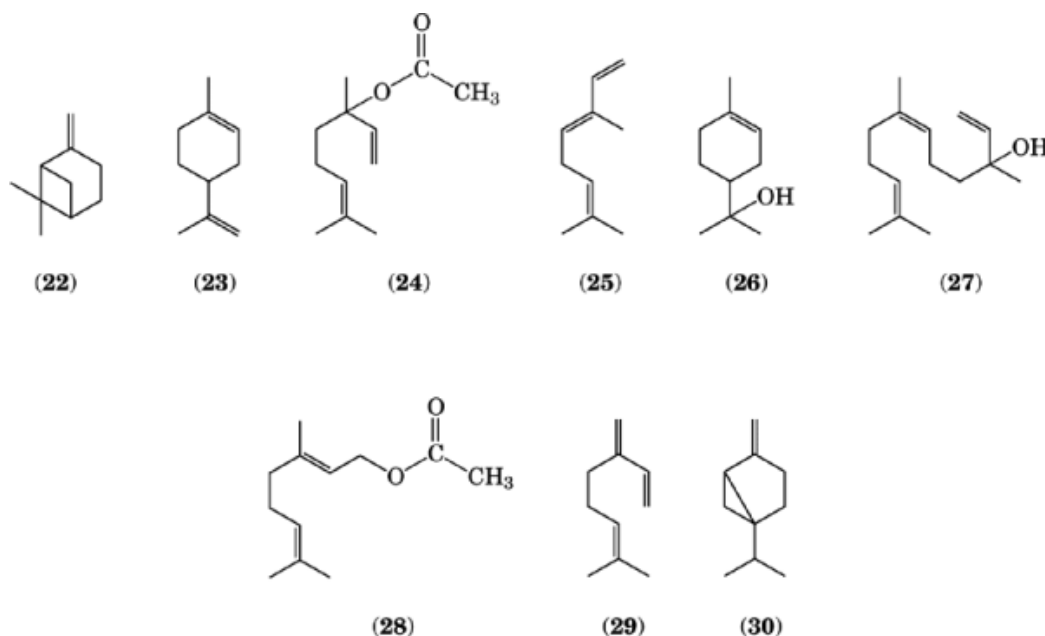


### 5.3. Orange Flower (Neroli) Oil

“The rose we call the queen of flowers, the jasmin the fairest and prettiest princess, but the orange flower is the most fragile and dainty of our royal family of flowers. If the rose stirs our memories, the jasmin our hopes, the orange flower stirs sentiments—sentiments most romantic!” (14). Commercial neroli oil [8016-38-4] is obtained

**Table 4. Components of Neroli Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent
linalool		(10)	36.0
$\beta$ -pinene	[127-91-3]	(22)	16.0
limonene	[138-86-3]	(23)	11.6
linalyl acetate	[115-95-7]	(24)	5.8
<i>trans</i> - $\beta$ -ocimene	[3779-61-1]	(25)	5.1
$\alpha$ -terpineol	[98-55-5]	(26)	4.0
<i>trans</i> -nerolidol	[7212-44-4]	(27)	3.9
geranyl acetate	[16409-44-2]	(28)	2.8
geraniol		(9)	2.4
myrcene	[123-35-3]	(29)	1.8
sabinene	[3387-41-5]	(30)	1.2
Total			90.6

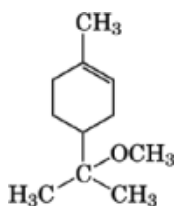
<sup>a</sup>Ref. 15.**Fig. 1.** Structures of some components of neroli oil.

by steam distillation of the freshly picked blossoms of the bitter orange *Citrus aurantium* L. subspecies *amara*, which is cultivated in Mediterranean countries as well as in Haiti and several other tropical countries. More than 125 components have been identified in the oil; the principal ones are shown in Table 4 and Figure 1.

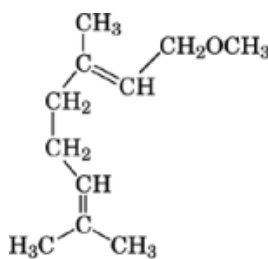
Of the 10 constituents which represent nearly half the oil of neroli, only linalool (10) can be said to contribute directly to the characteristic aroma of orange flower oil. In 1977, IFF chemists performed an in-depth analysis of this oil and identified three simple terpenic compounds, each present at less than 0.01%,  $\alpha$ -terpenyl methyl ether [1457-68-0] (31), geranyl methyl ether [2565-82-4] (32), and linalyl methyl ether [60763-44-2] (33) (11). The latter two compounds possess green floral-citrus aromas and have been known to

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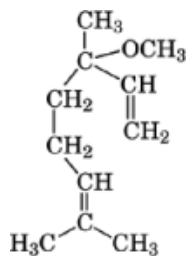
perfumery for some time;  $\alpha$ -terpenyl methyl ether (**31**) has been called the orange flower ether by IFF chemists owing to its characteristic odor.



(31)



(32)



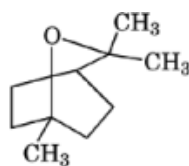
(33)

### 5.4. Lavender and Lavandin

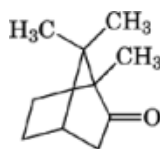
Lavender and lavandin [8022-15-9] are considered together both because of their somewhat similar odors and because they are botanically related. Lavender oil is obtained by steam distillation of the flowering plant *L. angustifolia* Mill., the so-called English Lavender, whereas lavandin comes from the corresponding parts of *L. hybrida* Reverchon, a cross between true lavender and spike lavender *L. latifolia* Med. Both plants are cultivated for their oil around the Mediterranean region. Each species exists in a large number of varieties and cultivars. Ranges for the principal constituents of a number of varieties of lavender and lavandin are provided in Table 5 (16).

Table 5. Comparison of Constituents of Oils of Lavender and Lavandin<sup>a</sup>

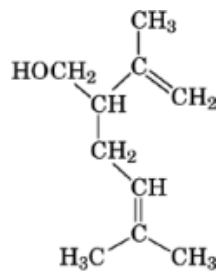
Component	CAS Registry Number	Structure number	Percent in lavender <sup>b</sup>	Percent in lavandin
3-octanone	[106-68-3]		nd-2	nd- < 1
eucalyptol	[470-82-3]	(34)	trace-5	6-22
limonene		(23)	trace-1	< 1 - 2
<i>cis</i> - and <i>trans</i> - $\beta$ -ocimenes <sup>c</sup> and $\gamma$ -terpinene <sup>d</sup>			< 1 - 11	1-6
linalool		(10)	6-51	34-41
camphor	[76-22-2]	(35)	nd-trace	< 1 - 8
lavandulol	[498-16-8]	(36)	trace-8	< 1 - 1
terpinen-4-ol and lavandulyl acetate	[562-74-3]	(37)	< 1 - 30	2-7
linalyl acetate	[25905-14-0]	(24)	7-57	2-31
borneol <sup>e</sup>	[507-70-0]		< 1	1-2
$\alpha$ -terpineol		(26)		

<sup>a</sup>Ref. 16.<sup>b</sup>nd = not detected.<sup>c</sup>*trans*- $\beta$ -Ocimene [3779-61-1] (25) = 3, 7-dimethyl-(*E*)-1, 3, 6-octatriene; *cis*- $\beta$ -ocimene [3338-55-4] = 3, 7-dimethyl-(*Z*)-1, 3, 6-octatriene.<sup>d</sup> $\gamma$ -Terpinene [99-85-4] = 1-methyl-4-isopropyl-1, 4-cyclohexadiene.<sup>e</sup>The reduction product of camphor (35), ie, *endo*-1,7,7-trimethyl bicycloheptane[2.2.1]-2-ol.

(34)



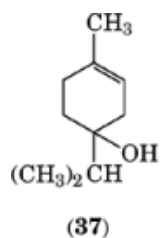
(35)



(36)

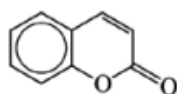
Table 6. Provisional AFNOR Specifications for Lavender and Lavandin Oils

Component	CAS Registry Number	Lavender, %	cv. <i>abrialis</i>	cv. <i>grosso</i>
3-octanone	[106-68-3]	2 max	<i>a</i>	<i>a</i>
eucalyptol <sup>b</sup>	[470-82-3]	1.5 max	6–11	4–7
limonene	[138-86-3]	0.5 max	<i>a</i>	<i>a</i>
<i>cis</i> - $\beta$ -ocimene	[3338-55-4]	4–10	1.5–4	<i>a</i>
<i>trans</i> - $\beta$ -ocimene	[3779-61-1]	2–6	3–7	<i>a</i>
linalool	[78-70-6]	25–38	30–38	25–35
camphor <sup>c</sup>	[76-22-2]	< 0.6	7–11	6–8
lavandulol	[498-16-8]	0.3 min	0.5–1.5	0.3–0.5
terpinen-4-ol	[562-74-3]	2–6	< 1	2–4
$\alpha$ -terpineol	[98-55-5]	1 max	<i>a</i>	<i>a</i>
linalyl acetate	[115-95-7]	25–45	20–30	28–38
lavandulyl acetate	[25905-14-0]	2 min	1–2	1.5–3

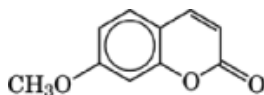
<sup>a</sup>No specifications.<sup>b</sup>1,8-Cineole [470-82-3].<sup>c</sup>The reduction product of camphor (**35**), ie, *endo*-1,7,7-trimethyl bicycloheptane[2.2.1]-2-ol.

Generally speaking, lavandin oil is characterized by a lower quantity of esters, the most critical of which for odor quality is linalyl acetate (**24**). The French specification organization (AFNOR) has fixed provisional standards for both oils (17) (Table 6).

Because it has been long recognized that trace components play an important role in determining the quality of these oils, a large number of detailed investigations of the trace constituents of both oils have been undertaken. Some of the compounds that have been determined to contribute important notes include coumarin [91-64-5] (**38**); unbelliferone methyl ether [531-39-9] (hernerin) (**39**); 4-vinyl-4-methyl- $\gamma$ -butyrolactone [1073-11-6] (**40**); methyl *cis*- and *trans*-3-methyl-2-(3'-methyl-2-butenyl)-3-cyclohexenyl ketone [73019-21-3] (Diels-Alder adducts of ocimene and methyl vinyl ketone); as well as a series of compounds related to the last named (11).



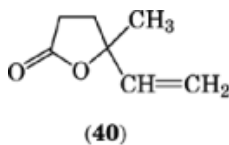
(38)



(39)

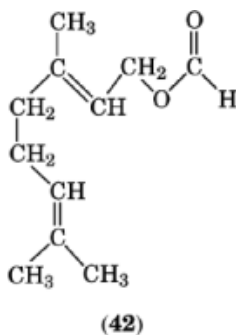
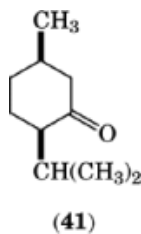
**Table 7. Components of Geranium Bourbon Oil<sup>a</sup>**

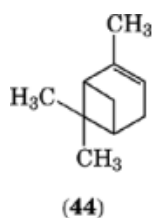
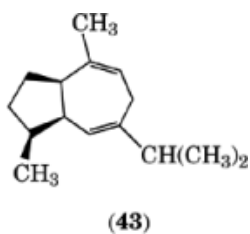
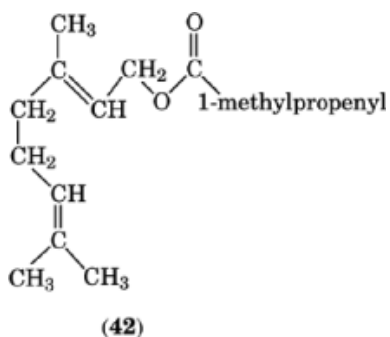
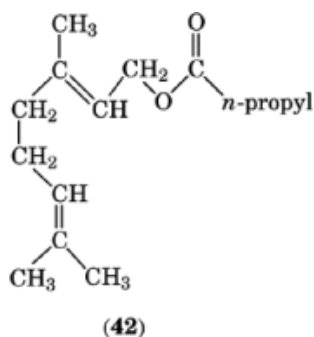
Component	CAS Registry Number	Structure number	Percent
citronellol		(8)	21
geraniol		(9)	18
linalool		(10)	11
isomenthone	[491-07-6]	(41)	8
citronellyl formate	[105-85-1]		8
geranyl formate	[61759-63-5]	(42), R = H	7
6,9-guaiadiene	[37839-64-8]	(43)	5
geranyl butyrate	[106-29-6]	(42), R = <i>n</i> -propyl	2
geranyl tiglate	[7785-33-3]	(42), R = 1-methylpropenyl	1
$\alpha$ -pinene	[80-56-8]	(44)	1
<i>Total</i>			82

<sup>a</sup>Ref. 18.

### 5.5. Geranium Oil

This oil is produced in China, Egypt, India, Réunion Island, Morocco, and Algeria by steam distillation of the leaves and branches of *Pelargonium* sp. Geranium oil Réunion is also called Geranium Bourbon from the old name for the island (Ile de Bourbon). Because the importance of geranium oil in perfumery cannot be overemphasized, it has been the subject of numerous investigations. The relative percentages of the principal constituents of geranium oil vary appreciably depending on species, source, and growth conditions, but a representative profile of a typical Geranium Bourbon is shown in Table 7 (18).



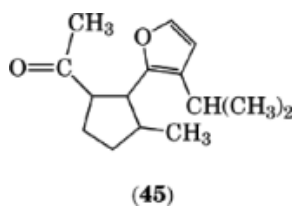


In 1961, chemists (19) isolated a minor component of geranium oil, characterized it as rose oxide (**1**), and reported that this compound contributed to the characteristic geranium odor. Rose oxide (**1**) is manufactured by the photooxidation of citronellol (**8**).

Part of the characteristic odor of geranium oil is described as peppery. In 1964, another trace constituent of the oil, furopelargone [1143-45-9, 1143-46-0] (**45**), was characterized and found to possess the typical peppery note (20). It has been demonstrated that furopelargone (**45**) can be made through the photooxidation of 6,9-guaiadiene (**43**), a component of geranium oil (11).

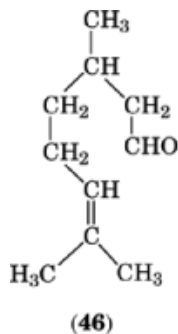
Table 8. Comparison of the Ingredients of Citronella Oils<sup>a</sup>

Component	CAS Registry Number	Structure number	<i>C. nardus</i> , %	<i>C. winterianus</i> , %
geraniol		(9)	21	23
citronellol		(8)	6	11
citronellal	[106-23-0]	(46)	6	35
<i>cis</i> -methyl isoeugenol <sup>b</sup> and <i>trans</i> -methyl isoeugenol <sup>c</sup>	[6380-24-1][6379-72-2]		10	
limonene		(23)	9	3
camphene	[79-92-5]	(47)	7	<sup>d</sup>
borneol			5	<sup>d</sup>
geranyl acetate		(28)	2	5
$\beta$ -cubebene	[13744-15-5]	(48)	4	2
elemol	[639-99-6]	(49)	1	3
eugenol		(11)		3
citronellyl acetate	[150-84-5]		1	2
Total			72	87

<sup>a</sup>Ref. 21.<sup>b</sup>1,2-Dimethoxy-4(*Z*-1-propenyl)benzene [6380-24-1].<sup>c</sup>1,2-Dimethoxy-4(*E*-1-propenyl)benzene [6379-72-2].<sup>d</sup>Trace amounts.

## 5.6. Citronella Oil

This is commercially produced by steam distillation of either of two related species of *Cymbopogon* grasses, *C. nardus* for the Ceylon type and *C. winterianus* for the Java type, which is also cultivated in Taiwan, Guatemala, Honduras, and Haiti. The oil finds significant usage in industrial fragrancng and as a source of citronellal (46), geraniol (9), and citronellol (8) for use in their own right or as raw materials for chemical conversions, including the manufacture of the critical fragrance compound, hydroxycitronellal (21). The comparative composition of the principal ingredients of typical samples of the two oils is given in Table 8 (21).

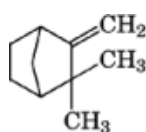


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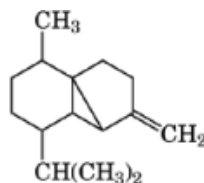
**Table 9. Components of a Typical 1988 Calabrian Bergamot Oil<sup>a</sup>**

Component	Structure number	Percent
limonene	(23)	42
linalyl acetate	(24)	27
$\gamma$ -terpinene		8
linalool	(10)	7
sabinene	(30)	1
myrcene	(29)	1
$\alpha$ -pinene	(44)	1
Total		87

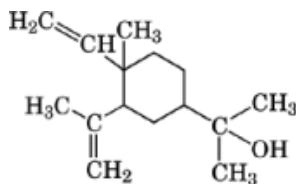
<sup>a</sup>Ref. 22.



(47)



(48)



(49)

From a perfumery point of view, trace ingredients again play an important role in the typical aroma of citronella oil. In 1980, IFF chemists isolated and characterized two nonterpenic compounds, melonol (2,6-dimethyl-5-hepten-1-ol [4234-93-9]) and melonal (2,6-dimethyl-5-heptenal [106-72-9]), with interesting green-melon odors (10). Although neither of these had previously been reported in nature, melonal has been a product of commerce for a number of years.

### 5.7. Bergamot Oil

Obtained by expression from the rind of the inedible fruit *Citrus bergamia* Risso, bergamot oil is a high volume fragrance material. The trees are primarily cultivated for their oil in the Calabria region of Italy. Increasingly, however, quality oil from northwestern Africa is becoming available. The composition of the principal components of a typical Calabrian oil from the 1988 season is shown in Table 9 (22).

Table 10. Components of Typical Commercial Lime Oils<sup>a</sup>

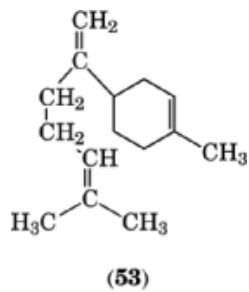
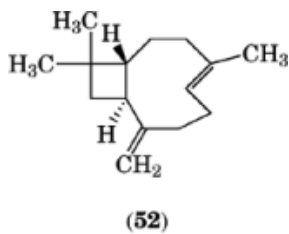
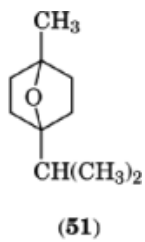
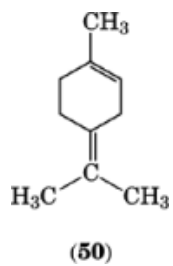
Component	CAS Registry Number	Structure number	Distilled oil, %	Terpeneless oil, %
limonene		(23)	45	
$\gamma$ -terpinene			11	
terpinolene	[586-62-9]	(50)	9	
$\alpha$ -terpineol		(26)	9	46
eucalyptol		(34)	5	
1,4-cineole	[470-67-7]	(51)	3	
$\alpha$ -farnesene <sup>b</sup>	[21499-64-9]		2	
<i>para</i> -cymene <sup>c</sup>	[99-87-6]		2	
$\alpha$ -pinene		(44)	1	
$\beta$ -pinene		(22)	1	
myrcene		(29)	1	
borneol			1	4
terpinen-4-ol		(37)	1	5
decanal	[112-31-2]		1	
$\beta$ -caryophyllene	[13877-93-5]	(52)	1	
$\beta$ -bisabolene	[495-61-4]	(53)	1	
$\gamma$ -terpineol	[586-81-2]	(54)		7
terpinen-1-ol	[586-82-3]	(55)		5
<i>trans</i> - $\beta$ -terpineol	[7299-40-3]	(56)		4
$\alpha$ -bergamotene	[17699-05-7]	(57)		4
$\alpha$ -fenchyl alcohol	[512-13-0]	(58)		3
<i>cis</i> - $\beta$ -terpineol	[7299-41-4]	(59)		1
linalool		(10)		1
geranial				0.4
Totals			94	80.4

<sup>a</sup>Refs. 25 and 26.<sup>b</sup>3,7,11-Trimethyl-(*E,E*)-1,3,6,10-dodecatetraene.<sup>c</sup>*p*-Isopropyltoluene.

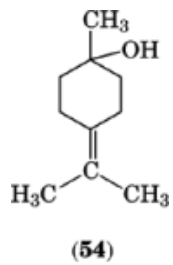
Bergamot oil has undergone a large number of investigations with regard to its trace components. In 1964, Firmenich chemists (23) claimed that *cis*-jasnone (**18**) and *cis*-5-oceten-2-one [19093-20-0] were important to the bergamot odor. In 1969, a series of novel trace bifunctional monoterpenoid molecules were characterized (24). Of these, two esters had very interesting citrus odors; they are the *cis*- and *trans*-1-acetates [64777-00-0, 64777-01-1] of 2,6-dimethyl-2,7-octadiene-1,6-diol.

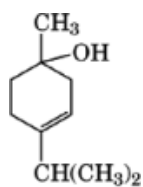
### 5.8. Lime Oil

This oil is obtained from the fruit *Citrus aurantifolia* Swingle; the Key, Mexican, or West Indian lime; or *C. latifolia* Tanaka, the Persian lime, either by steam distillation or expression. Either the entire crushed fruit or only the peel may be used, depending on the specific properties desired. A typical commercial distilled lime oil contains the constituents shown in Table 10 (25).

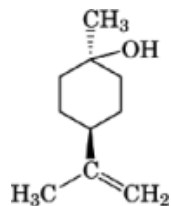


Because of its more interesting odor and flavor properties, many perfumers and flavorists prefer to use a terpeneless lime oil. A typical analysis is shown in Table 10 (26).

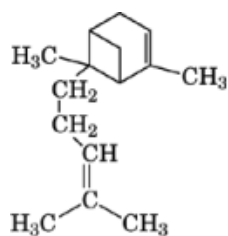




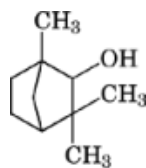
(55)



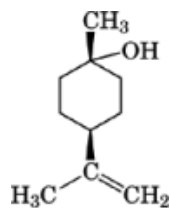
(56)



(57)



(58)



(59)

From West Indian lime oil, a trace low boiling constituent, 1-methyl-1,3-(or 1,5 [1489-57-2])-cyclohexadiene has been characterized (27). This compound, which possesses an intense and characteristic lime aroma, was later confirmed to be the 1,3-isomer [1489-56-1] (11). This compound can easily be made in

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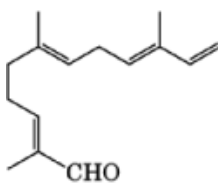
a biomimetic way through the reaction of citral [5392-40-5] (3,7-dimethyl-2,6-octadienal) with citric acid (28, 29).

### 5.9. Orange Oil

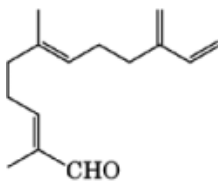
Orange oil, sweet, in terms of the quantity produced, ranks number one among the citrus oils. It is primarily obtained by expression from the peel of *Citrus sinensis* (L.) Osbeck. The United States, Cyprus, Guinea, Israel, and Brazil are the principal producers; specialty orange oils are produced in many other countries. A typical cold-pressed Valencia orange oil has the gross composition shown by the following (30). Neral [106-26-3] has the systematic name (*Z*)-5,7-dimethyl-3,6-heptadienal.

Component	Structure number	Percent
limonene	(23)	95
myrcene + noctanal	(29)	2
$\alpha$ -pinene	(44)	0.4
linalool	(10)	0.3
decanal		0.3
sabinene	(30)	0.2
geranial		0.1
neral		0.1
dodecanal		0.1
Total		98.5

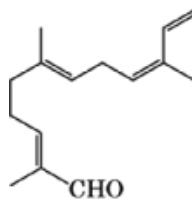
Decanal, a well-known fragrance and flavor item, gives, in dilution, the characteristic odor impression of sweet orange. In 1965, the trace constituents,  $\alpha$ - and  $\beta$ -sinensal (**60,61**), were isolated from orange oil (31). According to one authority, “(*E,E,E*) $\alpha$ -sinensal [17909-77-2] (**60**) has an orangelike note, whereas (*E,E*) $\beta$ -sinensal [3779-62-2] (**61**) is dominated by a strong metallic-fishy undertone and at high concentrations, causes an unpleasant odor sensation. (*E,E,Z*) $\alpha$ -Sinensal [61432-64-2] (**62**) (*E,E,Z*-2,6,10-trimethyl-2,6,9,11-dodecatetraenal) has the same odor character as (*E,E,E*) but is the weakest of the three aroma compounds (32). Many elegant syntheses of the sinensals have been reported in the chemical literature; however, none is practical.



(60)



(61)



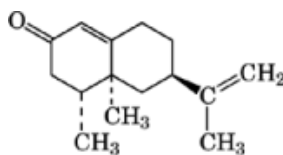
(62)

### 5.10. Grapefruit Oil

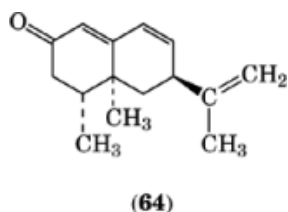
The grapefruit is a relatively recent arrival on the citrus scene, having presumably evolved from an earlier species, possibly the West Indian shaddock. The fruit is still undergoing refinement, and commercial grapefruit oil, obtained by expression of the peel of *Citrus paradisi* Macfayden, is much milder and sweeter than that available in the marketplace only a few years ago. Primary producers of grapefruit oil include the United States, Israel, Brazil, the West Indies, and Nigeria. A typical Israeli oil has the following composition (33):

Component	Structure number	Percent
limonene	(23)	93
myrcene	(29)	2
$\alpha$ -pinene	(44)	1
sabinene	(30)	0.4
octanal		0.3
$\beta$ -pinene	(22)	0.2
decanal		0.2
<i>trans</i> - $\beta$ -ocimene	(25)	0.1
$\gamma$ -terpinene		0.1
Total		97.3

In 1964, the presence of nootkatone [4674-50-4] (**63**), a known molecule, was confirmed in grapefruit oil (34). Some have considered nootkatone responsible for the characteristic aroma of grapefruit oil, but highly purified (+)-nootkatone (**63**) actually displays very weak odor properties. This was also observed in 1983 in a report that grapefruit oil contains a series of nootkatone analogues, one of which, (+)-8,9-didehydronootkatone [5090-63-1] (**64**), displays a particularly valuable grapefruit aroma similar to, but definitely stronger than, that of (+)-nootkatone (**63**) itself (35). Just prior to this work, investigators characterized the true character-donating component of grapefruit oil and juice as *p*-menthene-8-thiol (**4**). This compound is present in fresh grapefruit juice (in which it naturally occurs at or below the ppb level) (36).



(63)



### 5.11. Sandalwood Oil, East Indian

The use of sandalwood oil for its perfumery value is ancient, probably extending back some 4000 years. Oil from the powdered wood and roots of the tree *Santalum album* L. is produced primarily in India, under government control. Good quality oil is a pale yellow to yellow viscous liquid characterized by an extremely soft, sweet-woody, almost animal-balsamic odor. The extreme tenacity of the aroma makes it an ideal blender-fixative for woody-Oriental-floral fragrance bases. It also finds extensive use for the codistillation of other essential oils, such as rose, especially in India. There the so-called attars are made with sandalwood oil distilled over the flowers or by distillation of these flowers into sandalwood oil. The principal constituents of sandalwood oil are shown in Table 11 (37) and Figure 2.

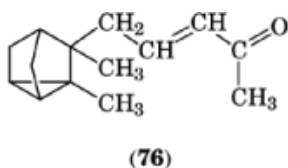
**Table 11. Constituents of Sandalwood Oil, East Indian<sup>a, b</sup>**

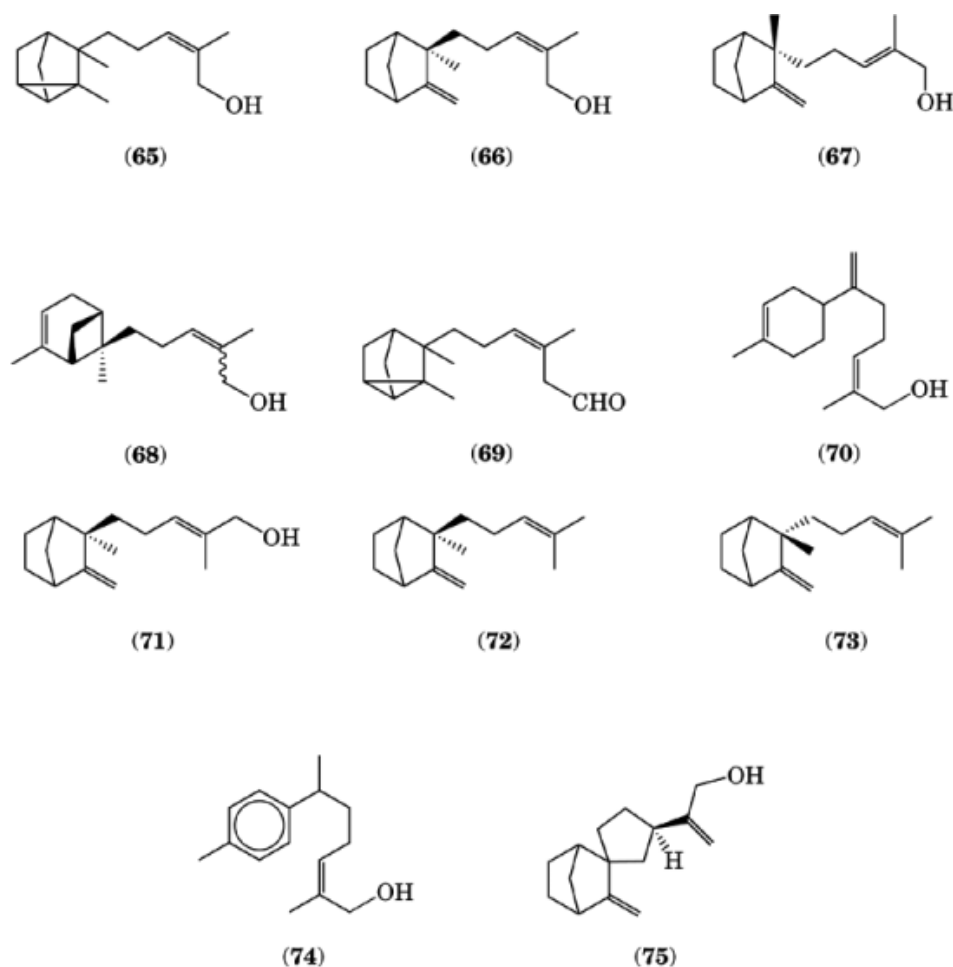
Component	CAS Registry Number	Structure Number	Percent
<i>cis</i> - $\alpha$ -santalol	[115-71-9]	(65)	50
<i>cis</i> - $\beta$ -santalol	[77-42-9]	(66)	21
<i>epi</i> - $\beta$ -santalol	[42495-69-2]	(67)	4
$\alpha$ -bergamotol	[88034-74-6]	(68)	4
$\alpha$ -santalal	[13827-97-9]	(69)	3
<i>cis</i> -lanceol	[10067-28-4]	(70)	2
<i>trans</i> - $\beta$ -santalol	[37172-32-0]	(71)	2
$\beta$ -santalene	[511-59-1]	(72)	1
<i>epi</i> - $\beta$ -santalene	[25532-78-9]	(73)	1
<i>cis</i> -nuciferol	[78339-53-4]	(74)	1
spirosantalol	[117020-19-6]	(75)	1
Total			90

<sup>a</sup>Ref. 37.

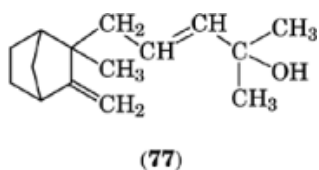
<sup>b</sup>See Fig. 2.

The principal component, *cis*- $\alpha$ -santalol (65), has controversial odor properties; *cis*- $\beta$ -santalol (66) contributes most to the odor of sandalwood. A number of trace constituents have been characterized, two of which (76) [59300-43-5] and (77) [63569-02-8] are worthy of mention for their very clean sandalwood notes (38).





**Fig. 2.** Constituents of East India sandalwood oil. See Table 11.



### 5.12. Patchouli Oil

This oil is obtained by the steam distillation of the dried leaves of a small plant *Pogostemon cablin* Benth. which is cultivated primarily in Southeast Asia, Indonesia, and the Philippines. It is of particular interest to the fragrance industry because of its unique woody, herbaceous, earthy aroma. Oil which is produced locally generally has substantially different odor properties from that made from exported leaves. However, whether the oil is the product of native or European-American distillation, the odor of the oil improves significantly upon aging. A full yield of oil is only obtained if the walls of the oil glands are first ruptured, preferably by means

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of a controlled fermentation achieved by stacking or baling of the dried leaves. The principal constituents of a commercial Javan oil are shown in Table 12 (39) and Figure 3.

**Table 12. Constituents of a Commercial Javan Patchouli Oil<sup>a, b</sup>**

Component	CAS Registry Number	Structure number	Percent
patchouli alcohol	[5986-55-0]	(78)	30
$\alpha$ -bulnesene	[3691-11-0]	(79)	17
$\alpha$ -guaiene	[3691-12-1]	(80)	14
seychellene	[20085-93-2]	(81)	9
$\alpha$ -patchoulene	[560-32-7]	(82)	5
$\beta$ -caryophyllene		(52)	4
$\beta$ -patchoulene	[514-51-2]	(83)	2
$\delta$ -cadinene	[483-76-1]	(84)	2
pogostol	[21698-41-9]	(85)	2
nor-patchoulenol	[41429-52-1]	(86)	1
caryophyllene oxide	[13877-94-6]	(87)	1
nortetrapatchoulol		(88) <sup>c</sup>	
Total			87

<sup>a</sup>Ref. 38.

<sup>b</sup>See Fig. 3.

<sup>c</sup>Only 0.00% by weight.

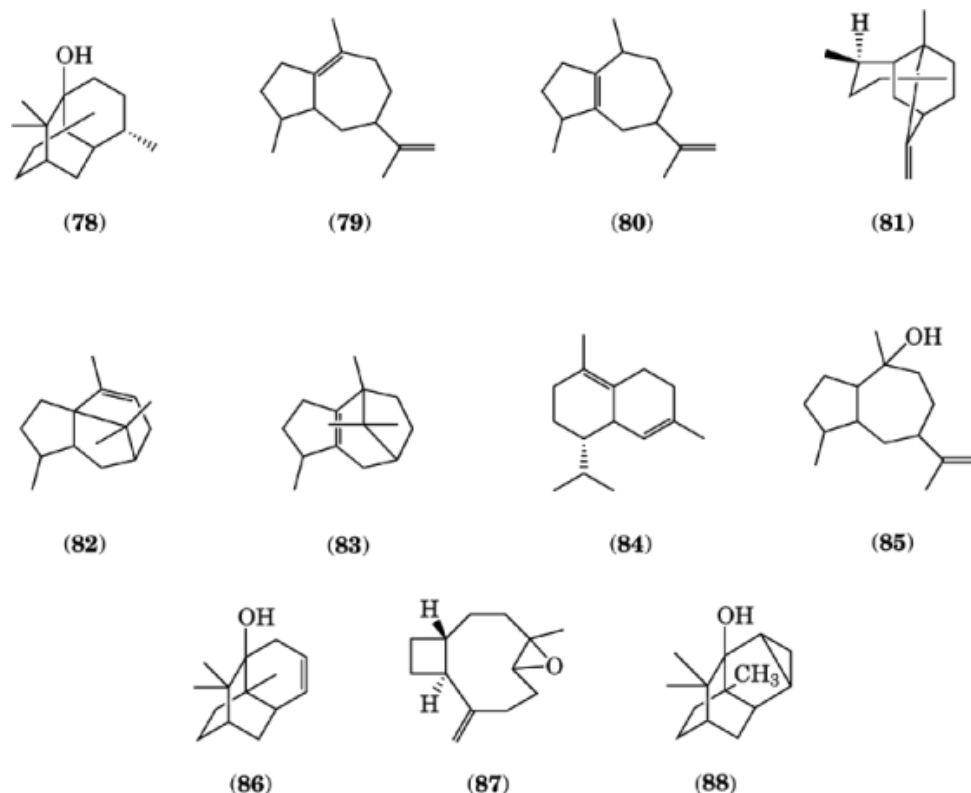
Patchouli oil is one of a class of unique essential oils consisting mostly of sesquiterpenoid material, of which patchouli alcohol constitutes 30%. It has been reported (40) that patchouli alcohol (78) is totally odorless. However, patchouli alcohol has been synthesized, proving that this compound indeed possesses the basic odor of patchouli oil (41). Moreover, as early as 1966, an in-depth analysis of patchouli oil derived from both dried and green leaves was performed and identified two novel character-donating components, norpatchoulenol (86) and nortetrapatchoulol (88) (41). The latter compound (88), present in the oil to the extent of only 0.001% by weight, is the strongest-odored of all. It has been reported elsewhere that norpatchoulenol (86) is the true carrier of the odor of patchouli oil (40).

### 5.13. Vetiver Oil

This oil is also a high volume fragrance material, prized for its precious woody note. Like patchouli, vetiver, obtained by steam distillation of the dried root of the grass *Vetiveria zizanoides* Staph., consists almost entirely of sesquiterpenic (C-13–C-15) compounds. The grass, a tall perennial which is native to India, Indonesia, and Sri Lanka and grows wild throughout southeast Asia, is cultivated for its oil in southern India, Indonesia (Java), Malaysia, the Philippines, Japan, Réunion, Africa, Haiti, the Dominican Republic, South America, the West Indies, and Mauritius. For the most part, distillation takes place in the field. Réunion and Haiti are the largest producers of vetiver oil. It is an amber to dark-brown viscous liquid with a sweet, very heavy, woody–earthy odor, reminiscent of roots and wet soil, with a rich, precious-woody undertone. Vetiver oil is used extensively in perfumery for fougère, chypre, oriental, moss, and woody notes. The oil is also used for the manufacture of a commercial product, vetiver acetate [52771-09-2], an acetylated vetiver oil possessing a faint, fresh-sweet, slightly woody odor. Some of the principal constituents of a Haitian vetiver oil have been reported (42) and are shown in Table 13 and Figure 4.

### 5.14. Galbanum Oil

This material is a natural oleoresin collected from several species of *Ferula* which grow wild in Iran and countries of Asia Minor such as Lebanon. Although both a hard and a soft galbanum are offered commercially,



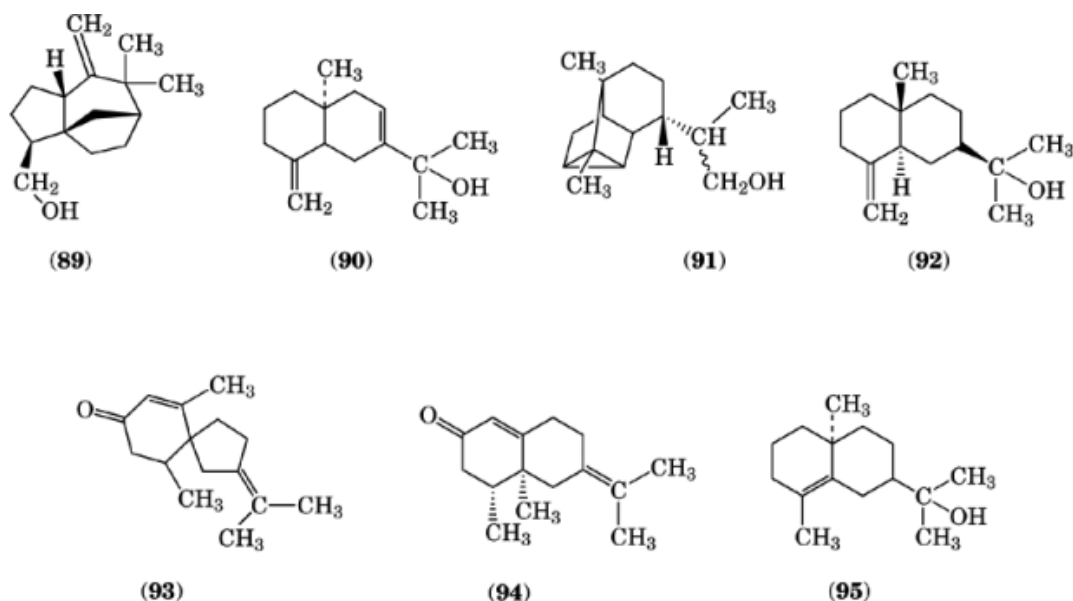
**Fig. 3.** Constituents of a commercial Javan oil.

**Table 13.** Some Components of a Haitian Vetiver Oil<sup>a</sup>

Component	CAS Registry Number	Structure number	Percent
zizanol	[28102-79-6]	(89)	13.4
vetiselinenol	[28102-68-3]	(90)	11.2
cyclocopacamphenol	[30810-34-5]	(91)	6.6
$\beta$ -eudesmol	[95529-67-2]	(92)	5.5
$\beta$ -vetivone	[18444-79-6]	(93)	5.2
$\alpha$ -vetivone	[15764-04-2]	(94)	3.2
elemol		(49)	2.3
10- <i>epi</i> - $\gamma$ eudesmol	[1209-71-8]	(95)	2.2
<i>Total</i>			57.6

<sup>a</sup>See Fig. 4.

only the soft variety is of interest to perfumery. Soft galbanum is a dark amber-colored to yellowish grayish olive brown viscous liquid with a powerful green-woody, almost balsamic–resinous odor. The oil is obtained by steam or steam–water distillation of the oleoresin in either Europe or the United States and is a colorless to pale olive-yellow mobile liquid with an intensely green fresh-leafy odor which dries to a woody, balsamic, bark-like aroma with musk-like undertones. The pine-like topnote is frequently removed by topping to enrich the soft, tenacious green-woody note so important to perfumery. The principal components of untopped galbanum oil [8023-91-4] shown in Table 14 are, not surprisingly, terpene hydrocarbons (43). Galbanum oil contains a wide



**Fig. 4.** Some of the principal constituents of a Haitian vetiver oil. See Table 13.

variety of compounds, including terpenoids (qv), nonterpenoids, olefins, and even sulfur-containing molecules. Of all of these, only a few contribute to the typical galbanum character.

**Table 14. Components of Untopped Galbanum Oil**

Component	Structure number	Percent
$\beta$ -pinene	(22)	60
$\alpha$ -pinene	(44)	14
$\Delta^3$ -carene		4
limonene	(23)	4
myrcene	(29)	3
$\alpha$ -thujene		1
sabinene	(30)	1
<i>para</i> -cymene		1
<i>cis</i> - $\beta$ -ocimene		1
Total		89

The presence in galbanum oil of the isomeric 1,3,5-undecatrienes was almost simultaneously announced by three groups of investigators (44–46), although one group (45) claims to have isolated and characterized the compounds as early as 1963. Of the four possible geometrical isomers, 1,3-*trans*,5-*cis*-undecatriene [51447-08-6] and 1,3-*trans*,5-*trans*-undecatriene [19883-29-5], have been identified in galbanum oil. Of these, the 1,3-*trans*,5-*trans*-isomer possesses the intense green galbanum odor, whereas the 1,3-*trans*,5-*cis*-isomer has a fatty galbanum note (11).

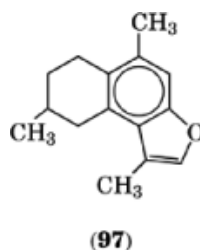
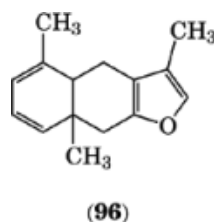
A second compound which was identified as important in the aroma of galbanum oil was 2-isopropyl-4-methylanisole [31574-44-4]. This compound also possesses a powerful green galbanum odor (47).

Another commercially available compound which is important to the galbanum aroma is 2-methoxy-3-isobutylpyrazine [24683-00-9] (48), which possesses an intense green pepper odor.

In 1969,  $\alpha$ -methylcyclopentadecanolide [4459-57-8] was isolated from galbanum (49). In 1978, three additional  $\alpha$ -methyl macrolides,  $\alpha$ -methylcyclododecanolide [71736-24-8],  $\alpha$ -methylcyclotridecanolide [27198-63-6], and  $\alpha$ -methylcyclotetradecanolide [32539-85-8], were characterized as galbanum constituents (50). These four undoubtedly contribute to the musky undertone of galbanum.

### 5.15. Myrrh

This is a typical natural oleo-gum-resin consisting of two-thirds water-soluble gum and one-third alcohol-soluble resin. It occurs naturally in the trunks of small trees of various *Comiphora* species which grow in eastern Africa north of the equator and in southwestern Arabia. It is processed either to an absolute or to an essential oil by various manufacturers in Europe or the United States. Myrrh [8016-37-3] has been prized since ancient times for its rich, sweet, warm, balsamic, incense-like fragrance. Until recently, the chemical composition of myrrh has been little studied, and early investigators alluded to the complex sesquiterpenoid nature of the volatile portion without providing further detail. The important aroma components are furanosesquiterpenoids which can be related to elemol (49) and  $\beta$ -eudesmol (92). These include the novel furanocadinane [115526-32-4] (96) (12% in volatiles), which possesses a deep rich leathery, sweet, warm, balsamic incensey aroma characteristic of myrrh, and the dihydropyrocurzerenone [52557-06-9] (97) (>1% in volatiles), which was described as having a rich, heavy, resinous, sweet incense note characteristic of myrrh (51).



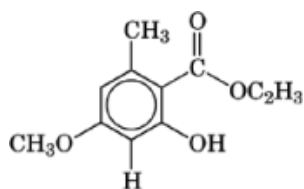
### 5.16. Oakmoss

Extracts of oakmoss are extensively used in perfumery to furnish parts of the notes of the fougère or chypre type. The first step in the preparation of an oakmoss extract is treatment of the lichen *Evernia prunastri* (L.) Ach., collected from oak trees mainly in southern and central Europe, with a hydrocarbon solvent to obtain a concrete. The concrete is then further processed by solvent extraction or distillation to more usable products, of which absolutes are the most versatile for perfumery use. A definitive analysis of oakmoss volatiles was performed in 1975 (52). The principal constituents of a Yugoslav oakmoss are shown in Table 15 (53). A number of phenolic compounds are responsible for the total odor impression. Of these, methyl  $\beta$ -orcinol carboxylate is the most characteristic of oakmoss.

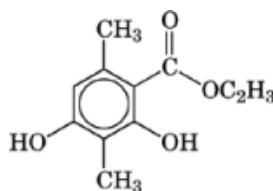
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Table 15. Components of a Yugoslav Oakmoss<sup>a</sup>

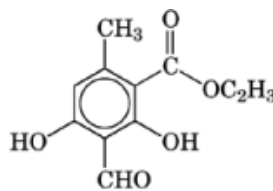
Component	CAS Registry Number	Structure number	Percent
ethyl everninate	[6110-36-7]	(98, R = CH <sub>3</sub> ; R' = H)	18
methyl $\beta$ -orcinol carboxylate	[4707-47-5]	(98, R = H; R' = CH <sub>3</sub> )	16
orcinol monomethyl ether	[3209-13-0]	(99, R = CH <sub>3</sub> )	16
orcinol	[504-15-4]	(99, R = H)	13
ethyl hemmatomate	[39503-14-5]	(98, R = H; R' = CHO)	5
ethyl orsellinate	[2524-37-0]	(98, R = R' = H)	4
atranol	[526-37-4]	(100; R = H)	3
chloroatrinol	[57074-21-2]	(100; R = Cl)	1
<i>Total</i>			76

<sup>a</sup>Ref. 53.

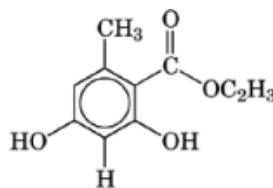
(98)



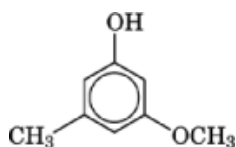
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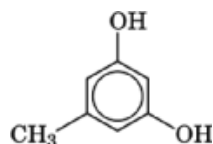
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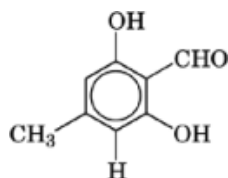
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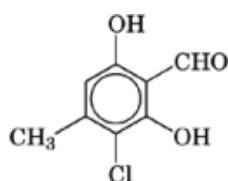
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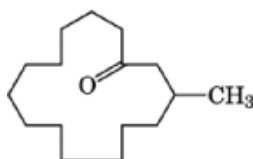
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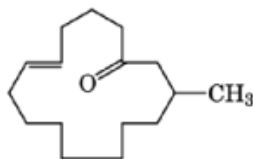
(100)

### 5.17. Tonquin Musk

This particular natural musk is obtained from the scent glands of the male musk deer, *Moschus moschiferus*, which is native to the Himalayas region and southern China. Because of its characteristic animal, civety, musky odor, it is a highly prized perfumery ingredient which has been used since ancient times. As it is still common practice to kill the animal in order to remove the gland, more than 70,000 deer are slaughtered annually to produce 0.5–1.5 t of musk. As a result of this, the possession or use of natural Tonquin musk or its extracts is forbidden in many parts of the world, including the United States. Therefore, there has been intense interest in the identification of the chemicals responsible for the characteristic odor of Tonquin musk. Investigation of musk began in 1906 with the isolation (54) followed by the characterization (55) of the principal odor constituent of Tonquin musk as muscone (**101**) ( $\beta$ -methylcyclopentadecanone [541-91-3]).



(101)



(102)

Since muscone (**101**), by itself, does not reproduce the total odor impression of this musk, IFF chemists (56) as early as 1971 in an analysis of tincture of Tonquin musk, reported a series of macrocyclic ketones (Table 16) which play a key role in creating the characteristic odor of this musk (11). The introduction of a double bond into a macrocyclic ketone (eg, **102**) changes the odor from flowery musk to animal musk.

**Table 16. Macrocyclic Ketones of Tonquin Musk**

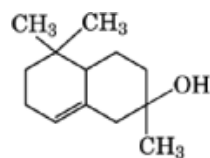
Component	CAS Registry Number	Odor description
muscone <sup>a</sup>	[541-91-3]	powerful soft, sweet animal musk
$\beta$ -methylcyclotridecanone	[61415-11-0]	strong floral musk with an animal character
cyclotetradecanone	[3603-99-4]	angelica-like musk
5-cyclopentadecen-1-one	[35720-58-2]	very animal, sweet, ambrette musk
14-methyl-5-cyclopentadecen-1-one <sup>b</sup>		strong musky, civet notes

<sup>a</sup>Structure (**101**).

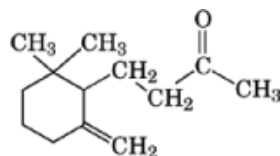
<sup>b</sup>Structure (**102**)

### 5.18. Ambergris

Known from antiquity, ambergris [8038-65-1], a substance of animal origin formed in the stomach or intestine of the sperm whale (*Physeter macrocephalus* L.) has been prized both as a perfume and as a drug. In modern usage, it has been employed only in perfumery, but this is no longer possible owing to laws forbidding the importation of gray ambergris or any other whale product. Few reports exist on the constituents of ambergris; however, it has been reported (57) that the compounds shown in Table 17 play a key role in the total odor impression of ambergris. Of these, Ambrox (**106**), which is commercially available, has the finest ambergris odor.



(103)



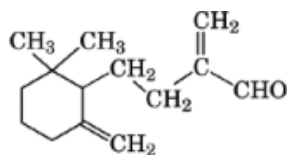
(104)

**Table 17. Aroma Constituents of Ambergris**

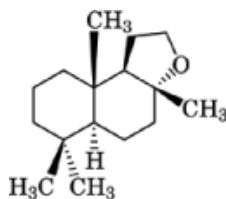
Component	CAS Registry Number	Structure number	Odor description
$\gamma$ -homocyclo geranyl chloride <sup>a</sup>	[72892-58-1]		ozony-seawater
$\alpha$ -ambrinol	[41199-19-3]	(103)	moldy-animal-fecal
$\gamma$ -dihydroionone	[13720-12-2]	(104)	weak tobacco
$\gamma$ -ambronal	[72892-63-8]	(105)	seawater
Ambrox <sup>b</sup>	[3738-00-9]	(106)	moist, creamy, soft, persistent amber odor with velvety effect

<sup>a</sup> 1,1-Dimethyl-2-(2-chloroethyl)-3-methylene cyclohexane.

<sup>b</sup> Ambrox is the registered trademark of Firmenich SA, Switzerland.



(105)



(106)

## 5.19. Tobacco

Among all the natural products of interest to the fragrance and flavor industry, tobacco oil [8037-19-2] probably enjoys the largest volume of usage throughout the world by the general population. Whereas the greatest part is directly consumed as smoking products, tobacco extracts find limited use in fragrance and flavor formulations owing to their ability to supply interesting and unique aromatic, sweet, floral, pungent, or hay-like notes. As a result of tobacco's position in the flavor industry, interest has been generated in elucidating the chemical nature of the components present in the various tobacco types, but not until recently has the flavor contribution of the key tobacco constituents been definitively reported. IFF chemists (58) performed a comparative analysis of the four tobacco types, ie, Virginia, burley, Turkish, and black, and evaluated the contribution to tobacco smoke flavor of a large number of the volatile constituents. They reported that, although many of the components were compatible with tobacco flavor and aroma to varying degrees, probably the key chemicals are those shown in Table 18:

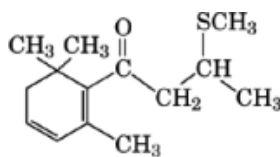
Table 18. Tobacco Constituents

Constituent	CAS Registry Number	Structure number	Odor description
methylthiodamascone <sup>a</sup>	[68697-67-6]	(107)	rich sweet tobacco aromatics, smooth harshness
methylthiodamascenone	[68697-66-5]		
solanone <sup>b</sup>	[40286-47-3]		hay-tea aromatics, body and mouth-coating effects
norsolanadione <sup>c</sup>	[35953-21-0]	(108)	burley, cocoa aromatics
megastigmatrienone (isomer mix)	[13215-88-8]		rich, pungent tobacco aromatics, fullness, and body

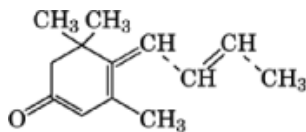
<sup>a</sup>See structure (107). This 4,5-position is saturated.

<sup>b</sup>5-Isopropyl-8-methyl-6,8-nonadien-2-one.

<sup>c</sup>5-Isopropyl-3-nonene-2,8-dione.



(107)



(108)

Of these, the megastigmatrienone isomer mix (108) possesses the truest tobacco aroma and taste; solanone is equally important for its hay-tea aromatics and its body and mouth-coating effect.

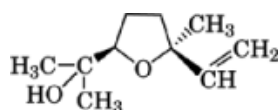
5.20. *Osmanthus*

The tiny, powerfully fragrant, creamy yellow to orange flowers of *Osmanthus fragrans* (Thunb.) Lour, a tree native to the Himalayas, China, and southern Japan, also known as sweet or fragrant olive, are employed for the production of a concrete, absolute, pommade, or infusion, the use of which is, however, traditionally limited to the local area. An interesting comparison of the volatile concentrates of two different colors of osmanthus, light-cream and golden-orange, was reported in 1986 (59). The principal constituents of each are shown in Table 19.

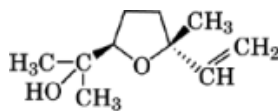
**Table 19. Comparative Composition of Components of the Volatile Concentrates of Two Different *Osmanthus* Flowers**

Component	CAS Registry Number	Structure number	In creamy, %	In golden-orange, %
<i>cis</i> -linalool oxide (furanosyl)	[5989-33-3]	(109)	2.4	21.1
<i>trans</i> -linalool oxide (furanosyl)	[34995-77-2]	(110)	3.5	14.6
$\gamma$ -decalactone	[706-14-9]		5.3	11.7
1-decanol	[112-30-1]		0.6	9.2
farnesol <sup>a</sup>	[4602-84-0]		6.0	0.2
$\beta$ -ionone	[79-77-6]	(15)	1.2	5.9
eugenol			3.4	1.9
undecanoic acid	[112-37-8]		0.4	3.1
linalool		(10)	2.1	2.4
benzyl alcohol			1.2	0.2
$\alpha$ -ionone	[6901-97-9]	(111)	0.2	0.9
nonanal	[124-19-6]		0.7	0.1
<i>Total</i>			27.0	71.3

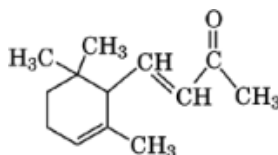
<sup>a</sup>3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol.



(109)



(110)



(111)

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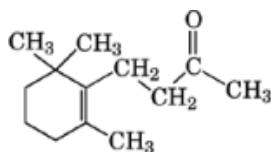
When a comparative analysis of the headspace volatiles of living and picked osmanthus flowers was performed by the dynamic headspace trapping method using Tenax GC, even more dramatic differences were observed, shown in Table 20 (60).

**Table 20. Differences Between the Volatiles of Living vs Picked Osmanthus<sup>a</sup>**

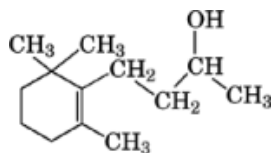
Compound	CAS Registry Number	Structure number	In living flower volatiles, %	In harvested flower volatiles, %	
				Air-purged	Nitrogen-purged
4-hydroxy-4-methyl-2-pentanone	[123-42-2]		1.3	1.3	4.7
<i>trans</i> -2-hexenal	[6728-26-3]			1.1	
<i>cis</i> -3-hexenol	[928-96-1]			1.1	
2-(2-methoxyethoxy) ethanol	[111-77-3]			1.0	
$\gamma$ -butyrolactone	[96-48-0]				4.4
<i>cis</i> -3-hexenyl acetate	[3681-71-8]		0.3	1.5	6.1
<i>para</i> -cymene <sup>b</sup>					8.5
<i>cis</i> -/ <i>trans</i> -linalool oxide (furanosyl)		(109,110)	2.0	2.5	10.0
<i>cis</i> -3-hexenyl butyrate	[16491-36-4]		0.2	1.2	4.2
geraniol		(9)	15.0	11.4	18.0
geranial			2.1	1.0	
$\beta$ -damascenone		(3)	0.1		
dihydro $\beta$ -ionone	[17283-81-7]	(112)	4.7	13.8	8.0
$\gamma$ -decalactone			7.0		
dihydro $\beta$ -ionol	[3293-47-8]	(113)	0.5		
jasmin lactone		(20)	0.2		
$\beta$ -ionone		(15)	13.2	5.7	4.0
4-keto $\beta$ -ionone	[27185-77-9]	(114)	1.9		
Total			48.5	41.5	67.9

<sup>a</sup>Ref. 20.

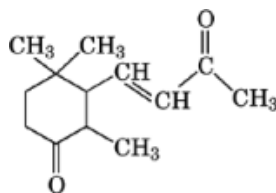
<sup>b</sup>*p*-Isopropyltoluene.



(112)



(113)



(114)

It is interesting to compare data for headspace volatiles of the living vs picked and both of these with respect to the direct analysis of the extracts shown in Table 19.

### 5.21. Olibanum

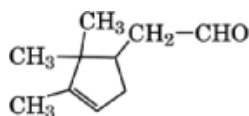
As in the case of myrrh, olibanum (frankincense) is a natural oleo gum resin. It is obtained from the bark of various species of *Boswellia*, of the family Burseraceae, native to southern Arabia, northeastern Africa, and the mountainous regions of western India. Two commercial brands of olibanum oil [8016-36-2], called Aden and Eritrean, exist. These gums usually result from two species *Boswellia carterii* Bird. (Arabia and Somalia) and *B. frereana* Bird. (Somalia). The volatiles profiles of oils from the two gums are remarkably different, as shown in Table 21 (61). Several saturated and unsaturated  $\gamma$ -butyrolactones with strong coumarinic odors which are key contributors to the characteristic aroma of olibanum have been reported (62): 3-isopropyl-2-butenyl lactone [10547-89-4],  $\gamma$ -isopropyl- $\gamma$ -butyrolactone [38624-29-2],  $\gamma$ -isopropenyl- $\gamma$ -butyrolactone [22616-89-3], and  $\alpha,\gamma,\gamma$ -trimethyl- $\gamma$ -butyrolactone [2610-96-0].

**Table 21. Volatile Components of Two Brands of Olibanum<sup>a</sup>**

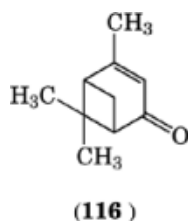
Component	CAS Registry Numbers	Structure numbers	In Aden, %	In Eritrean, %
$\alpha$ -pinene		(44)	43.0	4.6
camphene		(47)	2.0	1.1
$\beta$ -pinene		(22)	1.5	
sabinene		(30)	1.0	
hexyl acetate	[142-92-7]			1.5
<i>ortho</i> -cymene <sup>b</sup>	[527-84-4]		0.5	
limonene/eucalyptol		(23)/(34)	7.0	5.8
<i>para</i> -cymene <sup>b</sup>			7.5	
linalool		(10)		2.5
campholenic aldehyde	[4501-58-0]	(115)	1.5	
verbenone	[80-57-9]	(116)	6.5	
octyl acetate	[112-14-1]		1.5	52.0
<i>Total</i>			72.0	67.5

<sup>a</sup>Ref. 61.

<sup>b</sup>Cymene = isopropyltoluene.



(115)



### 5.22. Amyris Oil

Obtained by steam distillation of the wood of *Amyris balsamifera* L., the so-called West Indian sandalwood which is indigenous to northern South America, Central America, and the West Indies, amyris oil [8015-65-4] is a pale yellow to brownish yellow viscous oil with a slightly oily-sweet and occasionally peppery balsamic woody note. It finds use as a blender and fixative for soap fragrances. The volatile constituents, which are primarily hydrocarbon and oxygenated sesquiterpenes, are shown in Table 22 and Figure 5 (63).

**Table 22. Components of Amyris Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent
valerianol	[20489-45-6]	(117)	22
$\beta$ -eudesmol		(92)	17
10- <i>epi</i> - $\gamma$ -eudesmol		(95)	11
elemol		(49)	10
selina-3,7(11)-diene	[6813-21-4]	(118)	4
<i>epi</i> - $\alpha$ -selinene	[70560-75-7]	(119)	3
<i>ar</i> -curcumene <sup>b</sup>	[4176-06-1]		3
$\beta$ -bisabolene		(53)	2
$\alpha$ -agarofuran	[5956-12-7]	(120)	1
dihydroagarofuran <sup>c</sup>	[5956-09-2]		1
$\alpha$ -acoradiene	[24048-44-0]	(121)	1
Total			76

<sup>a</sup>Ref. 63. See Fig. 5.

<sup>b</sup>2-Methyl-6-(*p*-methylphenyl)-2-heptene.

<sup>c</sup>Saturated rings (see structure 120).

### 5.23. Anise Oil

Steam-distilled from the dried crushed fruits of *Pimpinella anisum* L., which is cultivated around the world, anise oil is a water-white to very pale yellow mobile liquid with an intensely sweet and clean odor reminiscent of the ripe crushed fruit. The principal constituent is *trans*-anethole [4180-23-8] (4-(*trans*-1-propenyl)anisole). It once found quite extensive use as an important ingredient in licorice candy, cough-drops, baked goods, pharmaceutical preparations, pipe tobacco, etc. However, for many applications, the oil has been largely replaced by synthetic anethole, frequently made from estragole [7677-68-1] (4-(2-propenyl)anisole) isolated from American pine oil. In regard to cost, the natural anise oil cannot compete with the synthetic anethole, but its flavor is still preferred by many connoisseurs for its fine and delicate sweetness, its rich body, and bouquet. The toxic *cis* isomer of anethole, 4-(*cis*-2-propenyl)anisole [140-67-0], always exists as a trace component where *trans*-anethole occurs in nature.

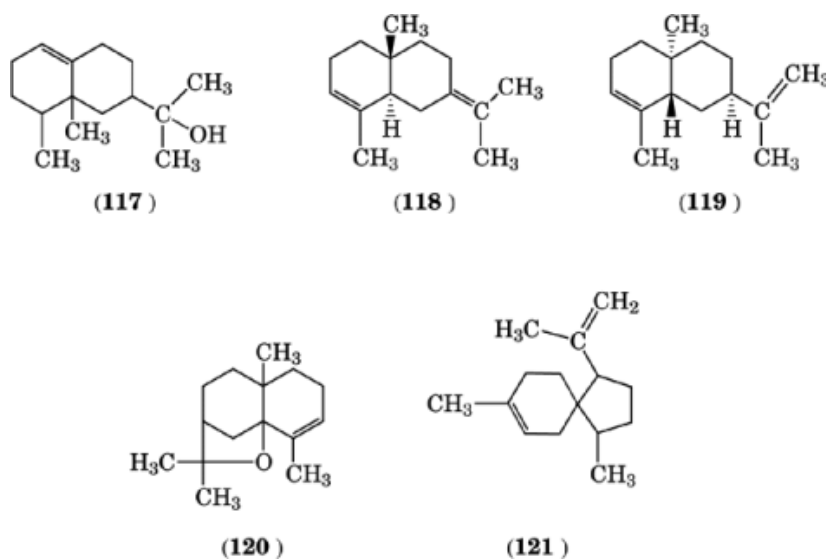


Fig. 5. Components of amyris oil.

#### 5.24. Anise Oil, Star

Steam-distilled from the fresh or partly dried whole or crushed fruits of *Illicium verum* Hook f., anise star oil [84650-59-9], was once extensively produced in regions of southeastern Asia, where it is native. Its post-World War II production has not regained its earlier levels. The oil is a pale yellow or almost water-white liquid with an intensely sweet odor. Owing to the high anethole content, it is also strongly reminiscent of true anise oil. Crude anise star oil is frequently rectified prior to distribution or use, bringing the anethole content up to 90–95%. The principal constituents of Vietnamese and Chinese crude star anise oils have been compared and are shown in Table 23 (64).

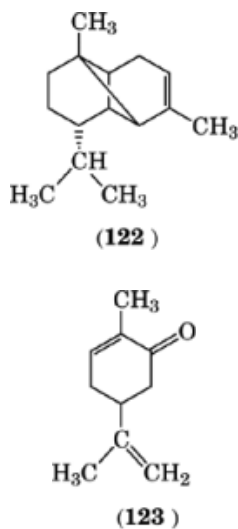
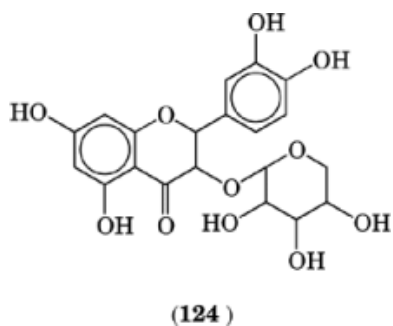


Table 23. Comparison of Ingredients of Vietnamese and Chinese Crude Anise Oils<sup>a</sup>

Component	CAS Registry Number	Structure number	In Vietnamese, %	In Chinese, %
terpene hydrocarbons			15.8	3.0
$\alpha$ -copaene	[3856-25-5]	(122)	0.1	0.1
linalool		(10)	1.1	0.6
$\alpha$ -bergamotene/ $\beta$ -caryophyllene		(57)/(52)	0.6	0.6
<i>cis</i> - $\beta$ -farnesene <sup>b</sup>	[28973-97-9]		0.1	0.1
estragole <sup>c</sup>			0.8	5.5
$\alpha$ -terpineol		(26)	0.4	0.2
carvone	[99-49-0]	(123)	<sup>d</sup>	<sup>d</sup>
$\beta$ -bisabolene		(53)	0.1	0.2
<i>cis</i> -anethole <sup>e</sup>			0.3	0.2
<i>trans</i> -anethole <sup>e</sup>			78.6	82.7
<i>para</i> -anisaldehyde <sup>f</sup>	[123-11-5]		0.5	1.7
methyl anisate <sup>g</sup>	[121-98-2]		<sup>d</sup>	<sup>d</sup>
<i>para</i> -methoxyphenyl-2-propanone	[122-84-9]		0.2	0.2
<i>trans</i> -methylisoeugenol				0.1
feniculine	[22255-13-6]	(124)	0.6	5.1
cinnamic alcohol	[104-54-1]		<sup>d</sup>	0.1
Total			83.4	96.3

<sup>a</sup>Ref. 64.<sup>b</sup>7,11-Dimethyl-3-methylene-(*Z*)-1,6,10-dodecatriene.<sup>c</sup>4-(2-Propenyl)anisole; anisole = methoxybenzene.<sup>d</sup>Trace.<sup>e</sup>*cis*- and *trans*-4(1-Propenyl)anisole.<sup>f</sup>*p*-Methoxybenzaldehyde.<sup>g</sup>Methyl *p*-methoxybenzoate.

### 5.25. Sweet Basil Oil

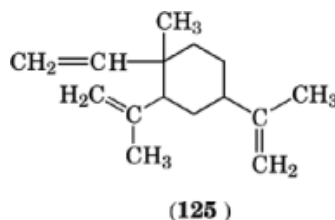
A large number of species and varieties of the herb basil are cultivated throughout the world both for their culinary use and as sources of essential oils. The true sweet basil oil, however, which is steam-distilled from the flowering tops of the species *Ocimum basilicum* L. in France and in the United States, is readily distinguishable from the many other types by its chemical content. The absence of camphoraceous notes and the presence of a perfect odor balance between linalool (10) and estragole is characteristic of the sweet basil oil [8015-73-4]. It is usually a pale yellow to almost colorless mobile liquid, with a sweet-spicy, slightly green odor, fresh with a faint balsamic woody undertone and a lasting sweetness. Although the low production volume makes this a relatively expensive oil, its great strength makes it very useful and generally applicable in fine perfumery and

flavor work. The principal components of sweet basil oil, as well as, for comparison, the volatiles profile in the headspace over living sweet basil plant, are shown in Table 24 (65).

**Table 24. Components of Sweet Basil Oil and Headspace of Living Sweet Basil<sup>a</sup>**

Component	CAS Registry Number	Structure number	In distilled oil, %	In headspace, %
estragole	[7677-68-1]		82	45
limonene/1,8-cineole		(23)/(34)	4	1
linalool	[78-70-6]	(10)	3	27
<i>trans</i> - $\beta$ -ocimene	[3779-61-1]	(25)	1	2
$\alpha$ -bergamotene	[17699-05-7]	(57)	1	2
$\beta$ -pinene	[127-91-3]	(22)	1	
eugenol	[97-53-0]		1	
eugenol methyl ether	[93-15-2]	(11)	1	
myrcene	[123-35-3]	(29)		4
$\beta$ -elemene	[515-13-9]	(125)		2
1-octen-3-ol	[3391-86-4]			1
<i>Totals</i>			94	84

<sup>a</sup>Ref. 65.



## 5.26. Bay Oil

Steam distillation of the leaves of the tree *Pimenta racemosa* (Mill) which is indigenous to certain islands of the West Indies, particularly Dominica and Puerto Rico, is called bay or bay leaf oil. The same source was used in the past to produce Bay Rum in which rum was distilled over the leaves. Bay oil [8006-78-8] is a yellowish to dark brown mobile liquid with a fresh-spicy, sometimes medicinal odor with a lasting sweet-balsamic undertone. The oil finds extensive use in hair tonics, after-shave lotions as well as other men's-type fragrances. There is little or no use by the flavor industry. The range of components for a number of bay leaf oils is shown in Table 25 (66).

## 5.27. Bitter Orange Oil

The cold-expressed oil from the peel of the nearly ripe fruit of *Citrus aurantium* L. subsp. *amara* is called bitter orange oil [68916-04-1]. Although it is related botanically to bergamot, there are substantial odor and flavor differences between the two. The tree is cultivated primarily in Spain, Guinea, and the West Indies, and the odor and flavor vary considerably from region to region. Cold-pressed bitter orange oil is a pale yellow to dark yellow or pale brown mobile liquid with a peculiar rich, fresh, dry aroma with a lasting sweet-floral undertone. The oil is the main ingredient of the orange or triple-sec liqueur flavors and as an intensifier for sweet orange-flavored drinks. In perfumery it finds extensive use in colognes and fine fragrances of the chypres, fougère, and fresh aldehydic citrus type. A comparison of the volatiles of Spanish and Italian oils of the same season has been performed and the principal ingredients are shown in Table 26 (67).

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**Table 25. Components of Bay Leaf Oil<sup>a</sup>**

Component	Structure number	Percent
eugenol		38–75
chavicol <sup>b</sup>		11–21
myrcene	(29)	14–32
1,8-cineole	(34)	0.2–2
<i>trans</i> - $\beta$ -ocimene	(25)	0.4–2
3-octanone		1
limonene	(23)	1
1-octen-3-ol		1
$\beta$ -caryophyllene	(52)	1
$\alpha$ -terpineol	(26)	1
geranyl acetate	(28)	1

<sup>a</sup>Ref. 66.

<sup>b</sup>4-(2-Propenyl)phenol [501-92-8].

**Table 26. Comparison of Components of Spanish and Italian Bitter Orange Oils<sup>a</sup>**

Component	Structure number	In Spanish, %	In Italian, %
limonene	(23)	94.34	92.43
myrcene	(29)	1.81	2.07
$\alpha$ -terpineol	(26)	0.57	0.06
$\alpha$ -pinene	(44)	0.45	0.59
$\beta$ -pinene	(22)	0.30	0.90
linalyl acetate	(24)	0.28	0.78
octanol		0.18	0.17
linalool	(10)	0.15	0.37
decanal		0.14	0.19
octanal		0.13	0.24
geranyl acetate	(28)	0.13	0.09
nootkatone	(63)	0.08	0.03
<i>Total</i>		98.56	97.92

<sup>a</sup>Ref. 67.

### 5.28. Black Pepper

Black pepper oil [8006-82-4] is obtained by steam distillation of the dried ripe fruit of a vine-like plant *Piper nigrum* L. native to southern and southeastern India and possibly the Sunda islands. Primary centers for cultivation are Indonesia, India, Malaya, and Indochina. Little if any pepper oil is distilled in the local areas of production. The bulk of the black pepper grown is utilized as a condiment. The oil is an almost water-white to greenish gray mobile liquid which becomes more viscous on aging. Its odor, which is described as fresh, dry-woody, and warm-spicy, is quite reminiscent of the dried fruit. However, as the pungent principles of black pepper are not steam-distillable, the flavor is totally lacking in this quality. Two grades of pepper oil, light and heavy, are distinguished by the pepper trade. The former consisting of distillation foreruns has the typical flavor of freshly ground peppercorns but without tenacity and deteriorates rapidly. The latter, containing the higher boiling components, although inferior with respect to the naturalness of the aroma, possesses superior stability and tenacity. Components of black pepper oil are shown in Table 27 (68). An oleoresin and concrete, which contain not only the oil but the pungent principles as well, are also produced.

**Table 27. Principal Components of Black Pepper Oil<sup>a</sup>**

Component	Structure number	Percent
sabinene	(30)	19
limonene	(23)	18
$\beta$ -caryophyllene	(52)	15
$\beta$ -pinene	(22)	10
$\alpha$ -pinene	(44)	9
$\Delta^3$ -carene		5
$\beta$ -phellandrene <sup>b</sup> /1,8-cineole		4
myrcene	(29)	2
$\alpha$ -phellandrene <sup>c</sup>		2
<i>para</i> -cymene		1
terpinen-4-ol	(37)	1
<i>trans</i> - $\beta$ -farnesene <sup>d</sup>		1
piperitone <sup>e</sup>		1
<i>Total</i>		88

<sup>a</sup>Ref. 68.<sup>b</sup>3-Methylene-6-isopropylcyclohexene [555-10-2].<sup>c</sup>2-Methyl-5-isopropyl-1,3-cyclohexadiene [99-83-2].<sup>d</sup>7,11-Dimethyl-3-methylene-(*E*)-1,6,10-dodecatriene [18794-81-6].<sup>e</sup>3-Methyl-6-isopropyl-2-cyclohexen-1-one [89-81-6].**5.29. Bois de Rose Oil**

Although early Essential Oil Association standards (1959, 1963) gave several possible botanical sources for Bois de Rose (or rosewood) oil, it was later concluded that this oil is obtained from wood of the evergreen tree *Aniba rosaeodora* var. *amazonica* Ducke, which grows wild in the Amazon basin of Brazil and Peru (69). It is steam-distilled locally to yield a colorless-to-pale yellow liquid with a refreshing sweet-woody, floral-spicy odor. The topnote varies widely with source and quality, but is usually described as camphoraceous-peppery, reminiscent of nutmeg and cineole-eucalyptus terpenes. The oil is used either in its original form in flavors and perfumery or rectified to enrich the principal component, linalool (10), which finds extensive use in perfumery. A typical commercial Bois de Rose oil [8015-77-8] made in 1988 contains the components shown in Table 28 (70).

**Table 28. Components of Bois de Rose Oil<sup>a</sup>**

Component	Structure number	Percent
linalool	(10)	78
$\alpha$ -terpineol	(26)	6
geraniol	(9)	2
linonene/1,8-cineole	(23)/(34)	2
<i>cis</i> -linalool oxide	(109)	1
<i>trans</i> -linalool oxide	(110)	1
geranial		1
$\beta$ -pinene	(22)	1
$\alpha$ -pinene	(44)	1
neral		1
<i>Total</i>		94

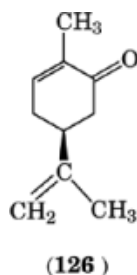
<sup>a</sup>Ref. 70.

## 5.30. Cananga Oil

The flowers of *Cananga odorata* Hook. f. et Thomson are used for the production of both cananga oil [68606-83-7] and ylang-ylang oil. In the case of cananga oil, a small quantity (10–30%) of leaves and twigs are also usually added to the still to facilitate even transfer of steam throughout the otherwise glutinous mass. It has been determined that a botanical difference does exist between trees used for each oil: forma *macrophylla* for cananga oil and forma *genuina* in the case of ylang. The oils may be differentiated in other ways: cananga oil is produced only in the northern and western parts of the island of Java in Indonesia from wild-growing trees using primitive stills, whereas ylang is obtained primarily from cultivated trees grown in the Comoro islands and Madagascar, with smaller amounts coming from Haiti, Réunion, and some of the French South Pacific islands. Cananga is a so-called total or complete essential oil in that, during the water distillation of the flowers, no fractions or cuts are taken; a total oil is removed. The yield and general odor quality of cananga oil is inferior to that of ylang. This is primarily a function of the distillation process, in which the flowers are packed tightly in the still. The flowers of *C. odorata* are delicate and easily lose their fragrance when damaged. Also, generally speaking, less care is taken in the choice of blossoms for the cananga oil still than for ylang. Java cananga oil is a yellow to orange-yellow or greenish yellow, somewhat viscous liquid possessing a sweet-floral, balsamic, and tenacious odor. The initial impression is woody-leathery, followed by a fresh-floral undertone. Cananga gives a much heavier odor impression than does ylang. It is generally assumed that most of the compounds found in ylang are also present in cananga, but in different proportions. Cananga generally contains more sesquiterpenes and sesquiterpene alcohols and a smaller quantity of esters than does ylang. Very few in-depth studies of cananga oil have been performed. Cananga finds use in soap and fine perfumery.

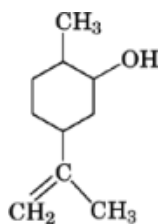
## 5.31. Caraway Oil

Produced by steam distillation of the crushed ripe seeds of *Carum carvi* L., caraway oil finds extensive use in food flavors, alcoholic liqueurs, and cheeses. The small herb, which grows wild in many regions of the world, is extensively cultivated in the Netherlands, Poland, Denmark, and parts of the former USSR. The Netherlands is the largest producer of the oil, which is offered commercially in two grades: crude or natural, and double-rectified or redistilled. The former is the direct distillate obtained from the fruits and is a pale yellow-to-brownish mobile liquid with a strong odor reminiscent of the fruit but with fatty-harsh undertones. It has a burning, warm, biting taste. The redistilled oil is colorless to pale yellow with a stronger and less fatty odor. The flavor is less sweet and more biting than the crude. Although (+)-carvone (**126**) is recognized as the odor-impact molecule of caraway, many lesser constituents play an important role in the total aroma and taste effect. The principal components of a Dutch oil are shown in Table 29 (71).

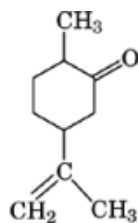


**Table 29. Components of a Dutch Caraway Oil<sup>a</sup>**

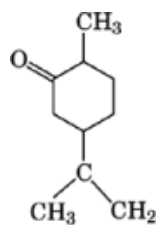
Component	CAS Registry Number	Structure number	Percent
(+)-carvone	[2244-16-8]	(126)	50
limonene		(23)	47
dihydrocarveol	[619-01-2]	(127)	0.6
<i>cis</i> -dihydrocarvone	[3792-53-8]	(128)	0.5
myrcene		(29)	0.4
<i>trans</i> <sup>b</sup> -carveol	[1197-07-5]	(129)	0.3
<i>trans</i> -dihydrocarvone	[69424-02-8]	(128)	0.2
<i>cis</i> <sup>b</sup> -carveol	[2102-59-2]	(129)	0.1
perillaldehyde	[2111-75-3]	(130)	0.1
linalool		(10)	0.1
sabinene		(30)	0.1
<i>cis-trans</i> -1,2-epoxylimonene	[1195-92-2]	(131)	0.2
<i>Total</i>			99.6

<sup>a</sup>Ref. 71.<sup>b</sup>The OH group is *cis* or *trans* to the propenyl group.

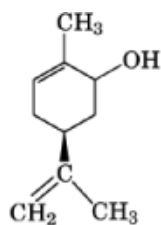
(127)



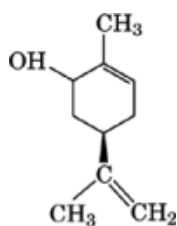
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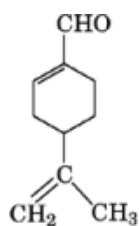
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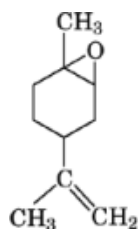
(129)



(129)



(130)



(131)

The oil possesses moderate antibacterial and strong antifungal properties. Thus the application of the oil to the crust of cheese could serve to prevent the formation of mycotoxin in the cheese. The optical purity of the carvone in caraway has been determined using a chiral gc column (72). It was found to be (*R*)(+) = 97.64% and (*S*)(-) = 2.36%.

### 5.32. Cardamom Oil

One of the oldest essential oils known, cardamom oil [8000-66-6] is steam-distilled from the seeds of *Elettaria cardamomum* Maton, a plant of the ginger family which grows wild and also is cultivated in India, Sri Lanka, and in Central America, primarily in Guatemala. India consumes more than 50% of the cardamom spice

produced each year. The oil is an almost colorless to pale yellow to light brown mobile liquid which darkens when exposed to sunlight. The topnote of cardamom oil is warm-spicy, aromatic, at first penetrating camphoraceous-cineole-like or medicinal as in eucalyptus. The drydown becomes balsamic-woody, sweet and almost floral with extreme tenacity. A comparison of the constituents of a commercial oil and of the headspace volatiles of living ripe cardamom seed is shown in Table 30 (73).

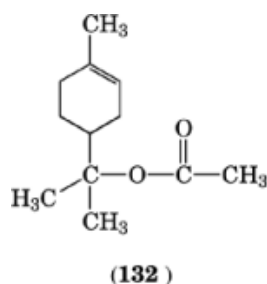
**Table 30. Comparison of Components of the Headspace of Living Ripe Cardamom Seed and Commercial Oil<sup>a</sup>**

Component	Structure number	In headspace, %	In commercial oil, %
1,8-cineole	(34)	19.7	44.7
$\alpha$ -terpinyl acetate	(132)	17.4	23.6
myrcene	(29)	12.5	0.1
geraniol	(9)	7.1	0.4
linalool	(10)	6.2	4.9
geranial		5.7	0.2
$\alpha$ -terpineol	(26)	3.2	1.2
sabinene	(30)	2.9	1.4
neral		1.7	0.4
terpinolene	(50)	1.0	
Total		77.4	76.9

<sup>a</sup>Ref. 73.

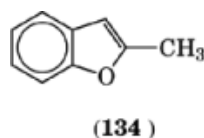
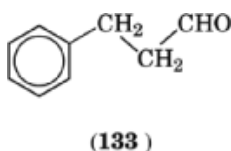
### 5.33. Cassia Oil

Also known as Chinese cinnamon oil, cassia oil is the steam distillation of the dried leaves, twigs, and bark of *Cinnamomum cassia* Blume, tall slender trees which grow in the southeastern areas of China and some parts of Vietnam and India. The bark of the trees is known throughout the world as cinnamon bark or cassia-cinnamon, not to be confused with true cinnamon bark Ceylon (Sri Lanka) which is a completely different species. The oil, which is produced in local stills by a water distillation, is a crude dark-brown liquid with a strong spicy, warm, woody-resinous aroma with an intensely sweet-balsamic undertone. It finds extensive use in the flavoring of soft drinks and as a raw material for the manufacture of natural benzaldehyde. Although some oil is purified by filtration and rectification in China, most material is shipped crude either for use as is or for cleanup or concentration by the user. Adulteration with synthetic cinnamaldehyde can still be a problem, but the use of modern analytical techniques such as isotope analysis has definitely lessened the risk of it to the user. Some companies go so far as to have representatives at the site of the distillation to oversee the process and personally seal the drums of crude oil. The headspace volatiles of living cassia leaf have been analyzed for comparison with those of picked leaf and of an authentic commercial oil (Table 31) (74).



**Table 31. Comparative Analysis of Cassia Leaf Volatiles<sup>a</sup>**

Component	CAS Registry Number	Structure number	In living, %	In picked, %	In commercial oil, %
<i>trans</i> -2-hexenal			4.0	0.8	
<i>cis</i> -3-hexenol			1.5	3.0	
<i>trans</i> -2-hexenol	[2305-21-7]		4.3	3.5	
<i>n</i> -hexanol	[25917-35-5]		1.2	1.1	
benzaldehyde	[100-52-7]		0.2	0.4	0.9
benzyl alcohol			0.4	0.1	
salicaldehyde	[90-02-8]		0.4	0.2	0.2
$\beta$ -phenethyl alcohol		(2)	2.1	0.1	0.4
hydrocinnamaldehyde	[104-53-0]	(133)			0.2
2-methyl benzofuran	[4265-25-2]	(134)			0.4
<i>cis</i> -cinnamaldehyde	[57194-69-1]		0.8	0.8	0.2
2-methoxybenzaldehyde	[135-02-4]			0.6	0.6
phenethyl acetate	[103-45-7]				0.4
<i>trans</i> -cinnamaldehyde	[14371-10-9]		47.4	68.8	72.8
cinnamic alcohol			20.6	0.3	0.3
coumarin		(38)	7.9	4.4	1.7
2-methoxy cinnamaldehyde	[1504-74-1]		1.0	1.4	11.5
4-methoxy cinnamaldehyde	[1963-36-6]		4.1	12.3	
2-methoxy cinnamyl acetate	[1504-61-6]				1.6
<i>Total</i>			95.7	98.0	91.1

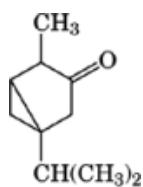
<sup>a</sup>Ref. 74.

### 5.34. Cedarleaf Oil

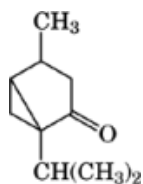
Also known commercially as thuja oil [8007-20-3], cedarleaf oil is steam-distilled almost exclusively from the leaves and twigs of the Eastern or Northern White Cedar *Thuja occidentalis* L., which grows abundantly in the northeastern United States and eastern Canada. The oil is distilled locally mostly in New York State, Vermont, and Quebec. It is a colorless to pale greenish yellow mobile liquid with an intensely sharp and quite fresh camphoraceous aroma. Although the principal constituent,  $\alpha$ -thujone, is considered to be a skin irritant and somewhat poisonous, the low level required in perfumes permits its use. It finds occasional use in fine fragrances of the chypre or fougère type and in some consumer products. The analysis of a number of cedarleaf oils has been performed, and the range for the principal constituents is shown in Table 32 (75).

**Table 32. Range of Composition for Primary Components of Thuja Oil<sup>a</sup>**

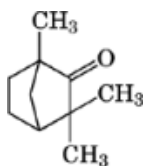
Component	CAS Registry Number	Structure number	Percent
$\alpha$ -thujone	[546-80-5]	(135)	31.2–47.1
$\beta$ -thujone	[471-15-8]	(136)	8.1–11.7
fenchone	[1195-79-5]	(137)	6.5–14.7
bornyl acetate	[76-49-3]	(138)	3.2–5.5
terpinen-4-ol	[562-74-3]	(37)	1.9–5.7
$\alpha$ -pinene	[80-56-8]	(44)	1.7–3.6
camphor	[76-22-2]	(35)	1.5–3.0
$\alpha$ -terpinyl acetate	[80-26-2]	(132)	1.3–2.5
sabinene	[3387-41-5]	(30)	1.1–2.3
limonene	[138-86-3]	(23)	1.0–3.3
$\gamma$ -terpinene	[99-85-4]		1.0–1.9

<sup>a</sup>Ref. 75.

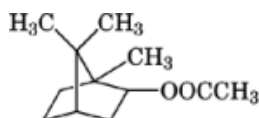
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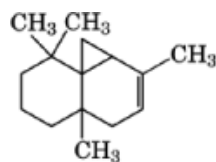
### 5.35. Cedarwood Oil

A large number of different types of cedarwood oil are produced. The largest volume oils are “Texas-type” from *Juniperus ashei* Buchh. (Texan cedarwood oils [68990-83-0]), “Virginia” from *Juniperus virginiana*, and “Chinese” from several varieties of trees of Japanese and Chinese origin. Cedarwood oils are used to provide woody fragrance notes and as fixatives for perfumes. The principal constituents of oils from *J. ashei* and *J. virginiana* are shown in Table 33 (76).

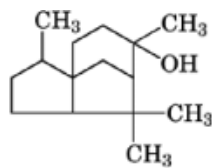
**Table 33. Constituents of Oils from *J. ashei* and *J. virginiana*<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent in <i>J. ashei</i>	Percent in <i>J. virginiana</i>
thujopsene	[470-40-6]	(139)	60.4	27.6
cedrol	[77-53-2]	(140)	19.0	15.8
$\alpha$ -copaene		(122)	2.8	6.3
$\alpha$ -cedrene	[469-61-4]	(141)	1.8	27.2
$\beta$ -cedrene	[546-28-1]	(142)	1.6	7.7
widdrol	[6892-80-4]	(143)	1.1	1.0
<i>Total</i>			86.7	85.6

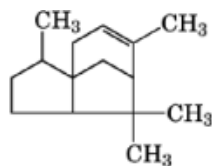
<sup>a</sup>Ref. 76.



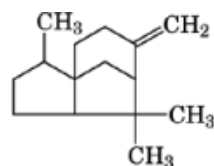
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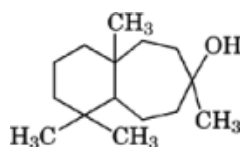
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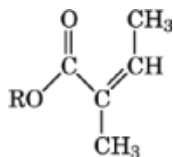
### 5.36. Roman Chamomile Oil

Steam distilled from the ligulate florets of *Chamaemelum nobile* (L.) All. (*Anthemis nobilis* L.), a member of the Dog Fennel or *Chamomile* family which is native to the Azores, northern Africa, and western Europe where it is extensively cultivated, Roman chamomile oil is a pale blue mobile liquid (when fresh but fades with aging) with a sweet herbaceous, fruity-warm, tealeaf-like aroma. The odor is extremely diffusive but with little tenacity. The pale blue color is due to the presence of a high boiling hydrocarbon, chamazulene, which only distills in trace amounts in the true essential oil. The oil has a bitter and medicinal flavor which finds some application in certain types of alcoholic beverages. However, it finds frequent but sparing use in perfumes where it contributes a warm, fresh, natural note difficult to achieve by other means. The oil, the principal constituents of which are shown in Table 34, possesses an extremely high ester value (77).

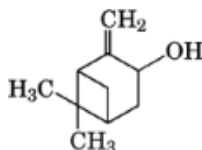
**Table 34. Components of Roman Chamomile Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent
3-methylpentyl isovalerate	[35852-41-6]		21.0
methallyl angelate	[61692-78-2]	(144)	15.8
3-methylpentyl isobutyrate	[53082-58-9]	(144)	11.9
2-methylbutyl angelate	[61692-77-1]	(144)	7.8
pinocarveol	[5947-36-4]	(145)	4.8
pinocarpone	[16812-40-1]	(146)	4.3
3-methylbutyl angelate	[10482-55-0]	(144)	4.1
isobutyl angelate	[7779-81-9]	(144)	3.4
$\alpha$ -pinene		(44)	3.0
3-methylpentyl methacrylate	[113615-00-2]		2.6
3-methylbutyl isobutyrate	[2050-01-3]		2.2
2-methylbutyl isobutyrate	[2445-69-4]		1.7
methallyl methacrylate	[816-74-0]		1.4
3-methylpentyl 2-methylbutyrate	[83783-89-5]		1.3
2-methylbutyl methacrylate	[60608-94-8]		1.2
3-methylpentyl acetate	[35897-13-3]		1.0
<i>Total</i>			87.6

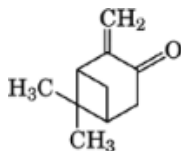
<sup>a</sup>Ref. 77.



(144 )



(145 )



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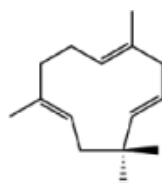
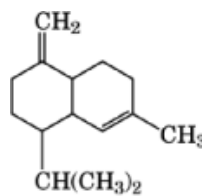
### 5.37. Cinnamon Bark Oil

True cinnamon bark oil, ie, "Ceylon," is steam-distilled (occasionally water-distilled) from the dried inner bark of the shoots of coppiced bushes of *Cinnamomum zeylanicum* Nees, primarily in Sri Lanka but also in India, Burma, Indochina, and several Indonesian islands. In each of these areas it grows wild but also is cultivated for its oil and as a spice. (Coppicing involved the felling of a mature tree and repeated harvesting of the shoots which grow from the stump.) The quality of the bark and its oil is strongly affected by climatic and soil conditions as well as the age of the coppiced trees and the handling before and during curing and processing. Although some distillation takes place locally, the best grades of oil are produced in Europe and the United States. Because an appreciable quantity of the important volatiles are soluble in the distillation waters, extraction of the dissolved volatiles after separation of the oil layer and use of skillful distillation techniques are necessary to obtain the best oils.

Ceylon cinnamon bark oil is a pale yellow-to-dark or brownish yellow liquid of extremely powerful, diffusive, warm-spicy, sweet, and tenacious odor. The best oils have a dry-powdery-dusty, but warm, uniform and lasting dry-out note. The flavor is distinctly sweet and spicy, and the best oils are five to ten times stronger in flavor than ordinary cinnamon bark oils. The oil finds extensive use in flavors for food and candy, baked goods and beverages, dental preparations, mouth rinses and gargles, and as a masking agent for pharmaceuticals with strongly unpleasant medicinal flavors. This essential oil ranks among the most powerful natural antiseptic germicides. Cinnamon bark oil is much appreciated by perfumers for its warm dry spiciness, immediate sweetness, and tremendous diffusive power, as well as its ability to blend well with woody-oriental and olibanum notes. A typical sample of Sri Lankan cinnamon bark oil has the components shown in Table 35 (78).

**Table 35. Components of Sri Lankan Cinnamon Bark Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent
<i>trans</i> -cinnamaldehyde			72.0–82.2
cinnamyl acetate	[103-54-8]		3.2–3.7
eugenol			1.1–13.3
$\beta$ -caryophyllene		(52)	1.0–2.0
linalool		(10)	0.7–1.1
cinnamyl alcohol			0.5–0.6
benzyl benzoate			0.4–1.0
$\alpha$ -terpineol/borneol			0.4–0.6
<i>ortho</i> -methoxy cinnamaldehyde			0.3–0.8
<i>para</i> -cymene			0.3–0.4
$\alpha$ -humulene	[6753-98-6]	(147)	0.2–0.6
<i>cis</i> -cinnamaldehyde			0.1–1.0

<sup>a</sup>Ref. 78.**(147)****(148)****5.38. Citronella Oil**

Citronella oil is steam-distilled from citronella grass, of which some 30 varieties exist growing both wild and cultivated throughout southern Asia, including China and Taiwan and the islands of Indonesia, as well as in northern Australia. The grasses are also grown in East Africa, South and Central America, the West Indies, Madagascar, the Comoro islands, and the Seychelles. Two types of the oil exist commercially: Java-type and Ceylon (Sri Lankan). By far, the largest-volume oil is citronella-Java, obtained from *Cymbopogon winterianus* Jowitt, the so-called Maha Pengiri grass cultivated in Taiwan, Hainan, Java, Malaysia, Guatemala, and Honduras. One advantage of the Maha Pengiri grass is that it yields up to twice as much essential oil as does the Ceylon-type which comes from *C. nardus* L. It also contains more of the components important for the production of synthetic or semisynthetic perfumery materials, eg, citronellal (**46**), which may be transformed into menthol [89-78-1] (*trans*-2-isopropyl-*cis*-5-methylcyclohexanol), or hydroxycitronellal (**21**), geraniol (**9**), and citronellol (**8**), which may be used as such, or after conversion to esters. Components of a *C. winterianus* oil are shown in Table 36 (79).

**Table 36. Components of *C. winterianus* Citronella Oil<sup>a</sup>**

Component	Structure number	Percent
citronellal	(49)	32.0
geraniol	(9)	20.0
citronellol	(8)	14.5
geranyl acetate	(28)	8.0
citronellyl acetate	(121)	5.0
limonene	(23)	4.0
elemol	(49)	2.5
2,6-dimethyl-5-heptenal		1.5
linalool	(10)	1.5
3,7-dimethyl-3,6-octadien-1-ol		1.5
neral		1.0
<i>Total</i>		81.5

<sup>a</sup>Ref. 79.**5.39. Clove Bud Oil**

Clove bud oil is water- (and sometimes steam-) distilled from the dried flower buds of a slender, medium-sized, cultivated tropical tree, *Syzygium aromaticum* L., also known as *Eugenia caryophyllata* Thunb. and *Jambosa caryophyllus* K. Spreng, which originated and still grows wild in the Moluccas island group, particularly the island of Amboyna, in the eastern Indonesian archipelago. The cultivation of clove trees is at least 2000 years old. The bud oil is the largest of the essential oils obtained from parts, including the stems as well as twigs and leaves, of the clove tree. Although most of the clove leaf and clove stem oil is distilled locally, clove bud oil is, for the most part, produced in European and U.S. distilleries. Madagascar, Zanzibar (Tanzanian), or Comoro clove buds are used for the distillation; Amboyna cloves are usually sold as the highest grade of the whole spice. During steam distillation of clove buds, eugenol acetate is hydrolyzed to eugenol. Thus, water distillation is preferred. The total eugenol content of water-distilled oil is usually greater than 90%, but more than 10% of this is in the form of the acetate, which is partly responsible for the characteristic odor of quality clove bud oil. For some time it was believed in the industry that sesquiterpenes such as  $\beta$ -caryophyllene (52) were formed during both water- and steam-distillation of clove buds. By means of the dynamic headspace analysis of authentic clovebuds it has now been unequivocally shown that  $\beta$ -caryophyllene is present as such in the untreated clove bud (79). A comparison of the headspace constituents of both whole and crushed clove buds with a commercial oil is shown in Table 37 (80).

Clove bud oil is frequently used in perfumery for its natural sweet-spicy note but the greatest application is in the flavor area in a large variety of food products, including spice blends, seasonings, pickles, canned meats, baked goods, ready-made mixes, etc. As in the case of cinnamon bark oil, its well-known antiseptic properties make it ideal for application in mouth washes, gargles, dentifrices, and pharmaceutical and dental preparations. Candy, particularly chewing gum, is also flavored with clove bud oil in combination with other essential oils.

**5.40. Coriander Oil**

Crushed fully ripe fruits (seeds) of *Coriandrum sativum* L., a small herb native to southeastern Europe, yield a colorless to pale yellow steam-distilled oil with a delightfully sweet, peppery-woody aromatic odor with a floral-balsamic undertone. The herb grows not only wild but is cultivated throughout the world, and distillation takes place mainly in Europe. A tremendous quantity of fruit is grown in areas such as India for use as in curry flavors. The flavor of coriander oil [8008-52-4] is mild, sweet, and spicy-aromatic but also warm and slightly burning. It is used extensively in flavors for alcoholic beverages, candy, tobacco, pickles, meat sauces,

**Table 37. Comparison of the Headspace Components of Whole and Crushed Clove Bud with a Commercial Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	In headspace of whole buds, %	In headspace of crushed buds, %	In oil, %
eugenol <sup>b</sup>		(11, R = H)	85.1	51.3	86.8
$\beta$ -caryophyllene		(52)	6.4	29.0	2.6
<i>trans</i> - $\beta$ -farnesene <sup>c</sup>			1.0		
vanillin <sup>d</sup>	[121-33-5]		0.9	0.8	
eugenyl acetate	[93-28-7]		0.6	0.4	9.7
benzyl acetate			0.5	0.2	
isoeugenol <sup>e</sup>	[97-54-1]		0.2		
furfural	[98-01-1]		0.2	0.3	<i>f</i>
5-methyl-2-hexyl acetate	[145119-71-7]		0.2	1.0	<i>f</i>
2-nonanone	[821-55-6]		0.2	0.3	
carvone		(123)	0.2		
$\gamma$ -cadinene	[1460-97-5]	(148)	0.1	0.3	
benzyl alcohol			0.1		
benzaldehyde			0.1	0.1	
Total			95.8	83.7	99.1

<sup>a</sup>Ref. 80.<sup>b</sup>2-Methoxy-4-(2-propenyl)phenol.<sup>c</sup>7,11-Dimethyl-3-methoxybenzaldehyde.<sup>d</sup>4-Hydroxy-3-methoxybenzaldehyde.<sup>e</sup>2-Methoxy-4-(1-propenyl)phenol.<sup>f</sup>Trace amounts.

seasonings, etc. In perfumery, its warm and sweet notes are useful in oriental and “white-flower” fragrances. A comparison of the components of an authentic coriander seed oil with the headspace volatiles over freshly crushed ripe coriander seeds has been made and is shown in Table 38 (81).

**Table 38. Comparison of Components of Authentic Coriander Seed Oil and Headspace Volatiles over Freshly Crushed Ripe Coriander Seeds<sup>a</sup>**

Component	Structure number	In oil, %	In freshly crushed ripe coriander seeds, %
linalool	(10)	73.3	63.2
$\gamma$ -terpinene		5.4	0.8
$\alpha$ -pinene	(44)	5.0	0.3
camphor	(35)	4.8	
limonene	(23)	2.5	0.9
geranyl acetate	(28)	2.2	15.6
citronellal	(46)		1.3
<i>para</i> -cymene		1.6	1.3
citronellyl acetate			1.2
<i>trans</i> - $\beta$ -ocimene	(25)	<i>b</i>	1.0
camphene	(47)	1.0	
myrcene	(29)	0.6	3.2
terpinolene	(50)	0.5	0.2
Total		96.9	86.0

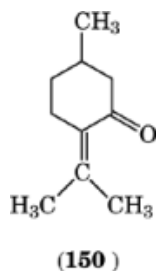
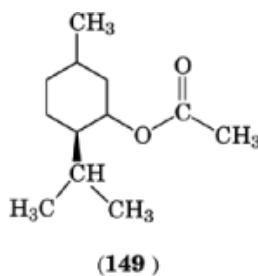
<sup>a</sup>Ref. 81.<sup>b</sup>Trace amounts.

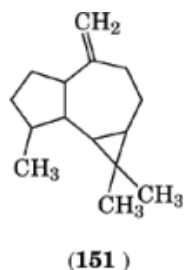
## 5.41. Cornmint Oil

The steam-distilled oil of different varieties of *Mentha arvensis* L., a native of China and Japan, is known as cornmint or Japanese mint in the United States. In the rest of the world, it is erroneously called peppermint oil and, indeed, it has a history of use in the adulteration of true peppermint oil. It is extensively cultivated in regions of China, Japan, Brazil, Taiwan, Australia, Africa, and India. The principal ingredient of the oil is menthol (70–75%), a large proportion of which can be easily recovered simply by cooling the oil and filtering. So-called dementholized cornmint oil is an item of commerce, and a typical analysis of a Japanese version is shown in Table 39 (82).

**Table 39. Components of a Dementholized Japanese Cornmint Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	Percent
menthol (isomers)			38.0
menthone <sup>b</sup>	[89-8-5]		26.3
isomenthone <sup>c</sup>	[491-07-6]		7.3
limonene		(23)	7.1
piperitone <sup>d</sup>	[89-81-6]		3.8
menthyl acetate	[89-48-5]	(149)	3.4
$\alpha$ -pinene		(44)	2.0
$\beta$ -pinene		(22)	2.0
$\beta$ -caryophyllene		(52)	1.3
pulegone	[89-82-7]	(150)	1.3
Total			91.5

<sup>a</sup>Ref. 82.<sup>b</sup>*trans*-2-Isopropyl-5-methylcyclohexanone.<sup>c</sup>*cis*-2-Isopropyl-5-methylcyclohexanone.<sup>d</sup>3-Methyl-6-isopropyl-2-cyclohexen-1-one.



#### 5.42. Eucalyptus Oil (Cineole-Rich)

More than 700 species of the genus *Eucalyptus* are known, with the large number of varieties and cultivars making this an enormous class of botanicals. Australia is considered the home of the eucalyptus, although little cultivation of trees for their commercial oils is undertaken there. Vast plantations of various species of eucalyptus, frequently grown for their timber as well as the oil, exist in Brazil, Africa, Central America, and other regions such as Spain. From a pharmacological perspective, the so-called 1,8-cineole- or eucalyptol-rich oils, obtained by steam distillation of the fresh or partly dried leaves, are of greatest commercial importance. Varieties of this type include *E. globulus* Labill., the “blue gum” or Tasmanian eucalyptus; *E. smithii* R. T. Baker, the “gully gum” tree; *E. dives* Schauer. var. C, the “broadleaf peppermint;” *E. leucoxylon* F. J. Muell.; and the “white” eucalyptus. The oils are colorless and mobile, and they are frequently rectified immediately following distillation to improve their keeping qualities and to remove unwanted low boiling aldehydes. The main use of these type oils is in pharmaceutical preparations, cough drops, vaporizers, gargles, toothpastes, and as germicides. A pharmaceutical-grade eucalyptus oil must meet the following specifications: as eucalyptol minimum 70%, it must be free of phellandrene and soluble in five volumes of 70% ethanol. A typical commercial Spanish *E. globulus* oil has the components shown in Table 40 (83).

**Table 40. Components of Spanish *E. globulus* Oil<sup>a</sup>**

Component	Structure number	Percent
1,8-cineole	(34)	71.3
$\alpha$ -pinene	(44)	14.4
limonene	(23)	2.7
<i>trans</i> -pinocarveol	(145)	2.6
<i>para</i> -cymene		1.8
aromadendrene	(151)	1.1
$\alpha$ -fenchyl alcohol/pinocarvone	(58)/(146)	1.0
Total		96.9

<sup>a</sup>Ref. 83.

Some of the other eucalyptus oils of commercial importance include the Chinese eucalyptus, a camphor/cineole-type oil; *E. citriodora* Hook., a citronellal-type oil; *E. staigeriana* F.v. Muel., a citral-type oil; and *E. macarthurii* H. Deane & Maiden, a geranyl acetate-type oil.

#### 5.43. Ginger Oil

The product of the steam distillation of the dried, unpeeled, freshly ground rhizomes of *Zingiber officinale* Roscoe, a native of the tropical coastal regions of India, ginger oil [8007-08-7] is a pale yellow to light amber-colored mobile liquid which noticeably resinifies on aging. Ginger is cultivated in most tropical and subtropical regions; for the production of essential oil, the Nigerian and Jamaican gingers are preferred. The rhizomes are

shipped to Europe and the United States for distillation. Although the odor of the oil is considerably dependent on geographical source, generally it is described as having a warm, fresh-woody-spicy and somewhat lemony topnote with a heavy and tenacious, sweet, rich, balsamic-floral undertone. The exceptional pungent quality of the fresh or dried ginger spice is not a characteristic of the essential oil, but is retained in the oleoresin, which is also a product of commerce. The oil finds use both in perfumery and flavor work. In the former, it adds a spicy-sweetness in oriental and some floral fragrances and is finding increasing use for the spicy-trend in men's fragrances. The most important flavor area is for baked goods such as cookies and spice cakes. A comparison of the headspace volatiles of fresh ginger rhizome and a commercial oil has been performed, and differences are shown in Table 41 (84). The relatively high percentage of citral (geranial/neral) in the headspace accounts for the pronounced lemony odor of the freshly cut rhizome.

**Table 41. Comparison of the Differences Between the Headspace Volatiles of Fresh Ginger Rhizome and a Commercial Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	In headspace, %	In oil, %
$\alpha$ -zingiberene	[7785-34-3]	<b>(152)</b>	15.2	34.4
$\alpha$ -farnesene <sup>b</sup>			13.7	6.0
geranial			11.7	0.7
<i>ar</i> -curcumene <sup>c</sup>			11.3	4.8
$\beta$ -sesquiphellandrene	[20307-83-9]	<b>(153)</b>	8.0	11.8
$\beta$ -phellandrene <sup>d</sup>			4.1	8.0
$\beta$ -bisabolene			3.8	6.2
neral	[112-12-9]	<b>(53)</b>	3.6	0.5
2-undecanone			3.4	0.8
myrcene			2.3	0.7
2-nonanone			1.8	0.3
2-nonanol	[628-99-9]	<b>(29)</b>	1.2	0.5
camphene			<sup>e</sup>	5.8
$\alpha$ -pinene				1.9
<i>Total</i>		<b>(44)</b>	91.1	82.4

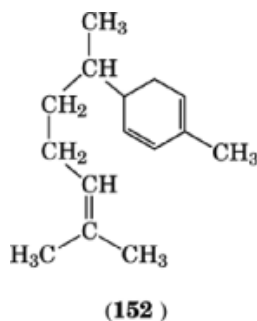
<sup>a</sup>Ref. 84.

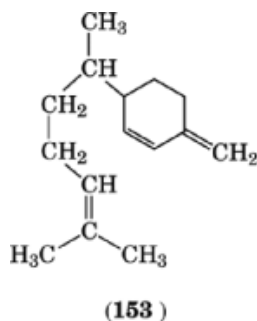
<sup>b</sup>3,7,11-Trimethyl-(*E,E*)-1,3,6,10-dodecatriene.

<sup>c</sup>2-Methyl-6-(*p*-methylphenyl)-2-heptene.

<sup>d</sup>3-Methylene-6-isopropylcyclohexene.

<sup>e</sup>Trace amounts.





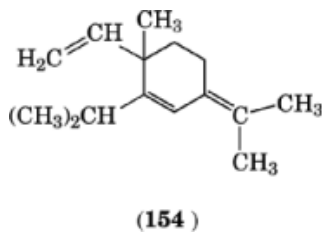
#### 5.44. Juniper Oil

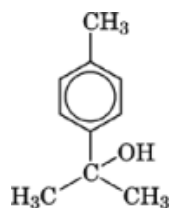
The best juniper oil [8012-91-7] is obtained from the steam distillation of the ripe crushed, dried berries of *Juniperus communis* L., a shrub which grows wild in many regions of Europe, Asia, Africa, and North America. However, most commercial juniperberry oil comes from the fermented fruits as a by-product of flavors for alcoholic beverages such as gin, brandy, liquors, cordials, and sloe-gin. This represents the actual commercial juniperberry oil, since very little true juniperberry oil is produced. A comparison of the headspace volatiles of ripe juniperberries (85) with an authentic, freshly prepared juniperberry oil (86) is shown in Table 42.

**Table 42. Comparison of Headspace Volatiles of Ripe Juniperberries with an Authentic Juniperberry Oil**

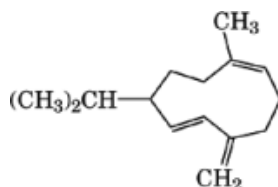
Component	CAS Registry Number	Structure number	In headspace, %	In oil, %
limonene		(23)	65.0	8.7
myrcene		(29)	13.7	8.5
sabinene		(30)	4.3	1.7
<i>cis</i> -3-hexenol			2.9	
$\beta$ -caryophyllene		(52)	2.1	7.2
$\alpha$ -elemene	[5951-67-7]	(154)	1.6	
terpinolene		(50)	1.4	0.4
8- <i>para</i> -cymenol	[68279-51-6]	(155)	1.1	
$\alpha$ -pinene		(44)	1.0	20.0
$\beta$ -elemene		(125)	0.8	
methyl salicylate <sup>a</sup>	[119-36-8]		0.8	
borneol				8.0
germacrene D	[23986-74-5]	(156)		7.0
$\alpha$ -humulene		(147)	0.5	3.9
<i>Total</i>			95.1	65.4

<sup>a</sup>Methyl 2-hydroxybenzoate.





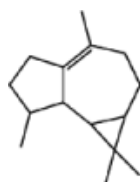
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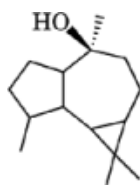
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#### 5.45. Labdanum Oil

Labdanum is the natural oleoresin obtained from various species of *Cistus* including particularly *C. ladanifer* L., commonly called laudanum, native to the Mediterranean region from Portugal to France and northwestern Africa. Various extracts and oils derived from labdanum are commercially available. These include absolutes, concretes, resinoids, and oils. The oils, called cistus oils, are of two types: the so-called cistus oil which is either steam-distilled directly from the crude gum or obtained by mixed solvent extraction, and true cistus oil obtained by steam distillation of the entire herb, including leaves, stems, and flowering tops. So-called cistus oil is an amber-colored, viscous liquid with a powerful and tenacious warm, sweet, animalic odor. True cistus oil is a pale orange liquid with a peculiar, warm, herbaceous, ambery odor and much lower tenacity than the so-called cistus oil. However, it has immense power in its topnote. Only limited quantities of the true cistus oil are produced. Both oils find specialty uses in perfumery. The principal components of a so-called cistus oil are shown in Table 43 (87).



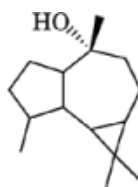
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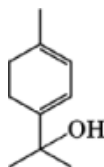
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**Table 43. Components of Cistus Oil<sup>a</sup>**

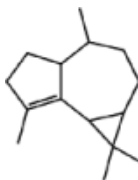
Component	CAS Registry Number	Structure number	Percent
$\alpha$ -pinene		(44)	10.8
viridiflorene	[21747-46-6]	(157)	8.4
viridiflorol	[552-02-3]	(158)	6.3
<i>trans</i> -pinocarveol		(145)	3.4
ledol	[577-27-5]	(159)	3.3
bornyl acetate		(138)	2.1
$\alpha$ -phellandren-8-ol	[1686-20-0]	(160)	1.9
$\alpha$ -gurjunene	[489-40-7]	(161)	1.7
$\alpha$ - <i>para</i> -dimethylstyrene <sup>b</sup>	[1195-32-0]		1.6
terpinen-4-ol		(37)	1.5
$\beta$ -phellandren-8-ol	[65293-09-6]	(162)	1.5
<i>para</i> -cymene			1.5
alloaromadendrene	[25246-27-9]	(163)	1.4
pinol	[2437-97-0]	(164)	1.4
eugenol			1.3
acetophenone	[98-86-2]		1.4
limonene/eucalyptol		(23)/(34)	1.3
camphene		(47)	1.0
<i>Total</i>			51.8

<sup>a</sup>So-called cistus oil. Ref. 87.<sup>b</sup>*p*-Isopropenyltoluene.

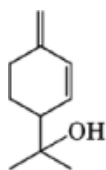
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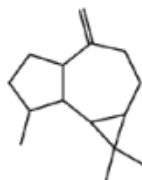
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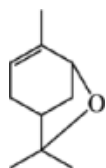
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#### 5.46. Lavender Oil Spike

Also known as spike oil, lavender oil spike is obtained by steam distillation of the flowering tops of *Lavandula latifolia* Vill., which grows wild and is also cultivated throughout the Mediterranean region, with most production in Spain and France. There was a time when spike oil, particularly Spanish lavender oil [8016-78-2], found extensive use in soap perfumery; however, with the introduction of the less expensive lavandin oil, a hybrid of true lavender (*L. angustifolia*) and *L. latifolia*, utilization of spike oil in perfumery has been reduced appreciably. French spike oil, a more delicate version, still finds considerable use in functional and industrial perfumery. A comparison of the volatiles of a commercial Spanish oil and a lab-distilled version of the same has been made and components are shown in Table 44 (88).

#### 5.47. Lemon Oil

The cold-pressed oil of the lemon (*Citrus limon* L.) is, after orange oil, the most important citrus oil. Although it is most likely native to the East India–Burma region, lemon cultivation rapidly spread throughout the tropical and subtropical world to the point that, at present, the largest lemon (and lemon oil) industry is in California; main production centers are Cyprus, Italy, Guinea, Brazil, Tunisia, Mexico, Israel, India, Pakistan, Spain, Jamaica, China, Australia, and South Africa. Expressed lemon oil is a pale yellow to greenish yellow mobile liquid with a light, fresh, sweet odor of varying tenacity, depending on the method of expression. The oil usually requires stabilization against oxidation, although Cyprus oil possesses remarkable keeping qualities. Lemon oil finds wide application in both fine and functional perfumery, for its refreshing sweet-fruity note, and flavors, where a concentrated or sesquiterpeneless lemon oil is preferred. Lemon oils have been extensively analyzed. A comparison of some components of a Sicilian and a California oil is shown in Table 45 (89).

**Table 44. Components of a Lab-Distilled and Commercial Lavender Spike Oil<sup>a</sup>**

Component	Structure number	In lab-distilled oil, %	In commercial oil, %
1,8-cineole	(34)	36.3	34.9
linalool	(10)	30.3	18.9
camphor	(35)	8.0	15.0
borneol		2.8	1.4
$\alpha$ -terpineol	(26)	2.6	1.1
coumarin	(38)	2.4	0.6
caryophyllene oxide	(87)	2.4	1.9
limonene	(23)	1.0	1.2
8- <i>para</i> -cymenol	(155)	1.0	<sup>b</sup>
<i>cis</i> -/ <i>trans</i> -linalool oxide (furanosyl)	(109)/(110)	0.5	12.7
<i>Total</i>		87.3	87.7

<sup>a</sup>Ref. 88.<sup>b</sup>Trace amounts.**Table 45. Comparison of Components of Sicilian and California Expressed Lemon Oils<sup>a</sup>**

Component	Structure number	In Sicilian oil, %	In California oil, %
limonene/eucalyptol/ <i>cis</i> - $\beta$ -ocimene	(23)/(34)	65.2	65.7
$\beta$ -pinene	(22)	10.5	11.1
$\gamma$ -terpinene		8.9	8.3
geranial		2.1	1.2
$\alpha$ -pinene	(44)	1.8	1.8
sabinene	(30)	1.8	1.9
myrcene	(29)	1.6	1.6
neral		1.3	0.7
<i>Total</i>		93.2	92.3

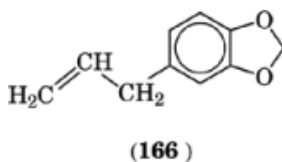
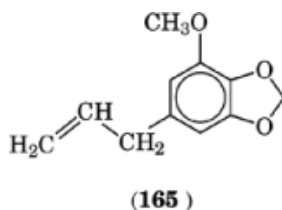
<sup>a</sup>Ref. 89.

### 5.48. Nutmeg Oil

The nutmeg, the fruit of the tree *Myristica fragrans* Hoult., which originated in the East Indies, represents another plant product with significant use in the dried natural state as a spice and a much lesser use as an oil or extract. Considerable acreage in Indonesia and, more recently, in the West Indies has been devoted to the cultivation of nutmeg. In both areas, nutmeg oil is distilled locally, although large quantities of the oil are also produced in Europe and the United States. The oil finds extensive use in both perfumery, in the modern "spicy" perfumes and in men's fragrances, and in flavor work, although a terpeneless oil is generally preferred in the latter case. As such, nutmeg oil is a significant spice additive in tomato ketchup. It is produced by steam or steam-water distillation of the freshly chopped fruits. Mace, the dried outer husk of the fruits, may be included. Some distillers prefer to remove a substantial portion of the fixed oil by hydraulic pressing prior to distillation. Nutmeg essential oil is a water-white to pale yellow mobile oil with a light, fresh, warm-spicy, and aromatic odor with a terpeny topnote and a woody, warm-sweet dryout. Nutmeg oil has been extensively analyzed, and a comparison of the components of several oils is shown in Table 46 (90).

Table 46. Comparative Analysis of the Components of Various Nutmeg Oils<sup>a</sup>

Component	CAS Registry Number	Structure number	In Sri Lankan (water-distilled), %	In Indonesian (steam-distilled), %
sabinene		(30)	28.0	16.5
$\alpha$ -pinene		(44)	13.9	21.7
terpinen-4-ol		(37)	8.9	5.9
$\beta$ -pinene		(22)	8.7	14.5
myristicin	[607-91-0]	(165)	3.3	5.5
$\alpha$ -thujene			2.5	2.7
myrcene		(29)	2.1	2.0
linalool		(10)	2.1	0.6
limonene		(23)		5.8
$\gamma$ -terpinene				5.2
safrrole	[94-59-7]	(166)		1.6
$\alpha$ -terpineol		(26)		1.1
eugenol				0.7
citronellol		(8)		0.2
Total			69.7	86.0

<sup>a</sup>Ref. 90.

#### 5.49. Oregano Oil Spanish

Steam-distilled from the dried flowering herb *Thymus capitatus* (L.) Hoffmanns & Link (also known as *Coridothymus capitatus* (L.) Reichb. f.), which grows wild in the Mediterranean region, Spanish oregano (or origanum oil [8007-11-2]) oil is one of the largest-volume oregano oils of commerce. This oil is distilled locally and is a dark brownish red to purple to orange-colored mobile liquid with a strong tar-like, herbaceous, and refreshing odor. The topnote is slightly green-camphoraceous, herbaceous, and the body is rich, dry-woody, and phenolic. On dryout, the aroma remains dry-woody and phenolic. The flavor is somewhat burning, warm-phenolic, and herbaceous; it is pleasant only in high dilution. Fine perfumery uses oregano oil for its powerfully refreshing notes and its spicy-herbaceous effect. Soap perfumery utilizes the medicinal note of its principal phenolic component, carvacrol [499-75-2] (2-methyl-5-isopropylphenol). For flavor work, the milder oregano oils such as marjoram or thyme are usually preferred. The composition of an oregano oil of Spanish origin has been analyzed, and components are shown in Table 47 (91).

**Table 47. Components of Spanish Oregano Oil<sup>a</sup>**

Component	Structure number	Percent
carvacrol		80.2
$\gamma$ -terpinene		4.0
<i>para</i> -cymene		3.9
$\beta$ -caryophyllene	(52)	3.5
$\alpha$ -thujene		2.2
myrcene	(29)	1.3
$\alpha$ -phellandrene		1.0
<i>Total</i>		96.1

<sup>a</sup>Ref. 91.**5.50. Orris**

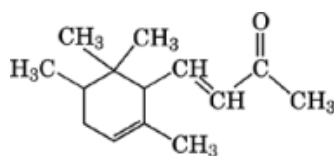
Steam-distillation of the aged (3-yr) peeled, dried, pulverized rhizomes of the decorative garden perennial *Iris pallida* Lam. yields a waxy, cream-colored mass known as orris butter or orris concrète. Fresh rhizomes are practically odorless. This material melts at body temperature and possesses a woody, fatty-oily, violet-like odor with a sweet, floral, warm, and fruity undertone. The wax, which accounts for 85–90% of the concrete, is myristic acid which, because it can cause problems in perfumery and handling, is usually removed by alkali washing in an alcoholic solution. This process yields the highly desirable, from a perfumery standpoint, but very expensive, orris absolute. Although most of the cultivation and curing of the plant material takes place in Italy, the bulk of the processing occurs in France. Most of the absolute is used in fine perfumery, although traces are effective in fruit and rum flavors. The volatiles composition of a commercial orris absolute is shown in Table 48 (92).

**Table 48. Volatiles Composition of Orris Absolute<sup>a</sup>**

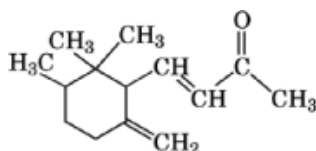
Component	CAS Registry Number	Structure number	Percent
$\alpha$ -irone (two isomers)	[79-69-6]	(167)	60.7
$\gamma$ -irone	[79-68-5]	(168)	14.9
methyl myristate <sup>b</sup>	[124-10-7]		10.0
ethyl myristate <sup>b</sup>	[124-06-1]		4.0
$\beta$ -irone	[472-46-8]	(169)	2.1
ethyl laurate <sup>c</sup>	[106-33-2]		1.6
<i>Total</i>			93.3

<sup>a</sup>Ref. 92.<sup>b</sup>Myristic acid = tetradecanoic acid.<sup>c</sup>Ethyl dodecanoate.

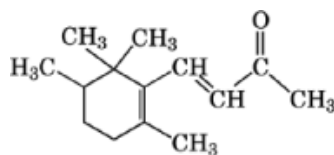
The irones (**167,168,169**), which constitute slightly more than 75% of the volatiles, are primarily responsible for the fine odor of the natural material. For this reason and because of the high cost of orris absolute, synthetic versions of the irones have been commercialized. Of the possible irone structures, the  $\gamma$ -isomer (**168**) possesses the best fragrance properties.



(167)



(168)



(169)

### 5.51. Palmarosa Oil

The grass *Cymbopogon martini* Staph., which grows wild in India from Bombay to the Himalayas, yields, on steam or water distillation, an essential oil with a pale yellow-to-olive color possessing a sweet floral-rosy odor. This oil is the best natural source of geraniol (**9**) which can be isolated either for use as is or for the preparation of other fragrance and flavor molecules. Apart from its use as a geraniol source, palmarosa oil (East Indian geranium oil [8014-19-5]) is used in many perfumes, particularly soap fragrances where its greater tenacity is a highly desirable quality. Components of palmarosa oils of various regions is shown in Table 49 (90).

**Table 49. Components of Palmarosa Oil of Different Origins<sup>a</sup>**

Component	Structure number	Percent in			
		Brazilian oil	Guatemalan oil	Indian oil	Madagascan oil
geraniol	(9)	80.9	60.0	76.2	84.0
nerol <sup>b</sup>			14.8	1.5	0.2
geranyl acetate	(28)	12.4	17.3	9.1	8.0
linalool	(10)	2.2	0.8	3.9	3.0
$\gamma$ -terpinene		1.4		0.9	1.7
elemol	(49)	0.4		1.5	0.3
limonene	(23)	0.1		1.7	0.1
myrcene	(29)	44		0.1	0.2
Total		97.9	92.9	94.9	97.5

<sup>a</sup>Ref. 90.

<sup>b</sup>3,7-Dimethyl-2,6-octadien-1-ol [106-25-2].

### 5.52. Peppermint Oil

True peppermint oil is steam-distilled from the partially dried herb of various cultivars of *Mentha X piperita*, a nonfertile hybrid of *M. aquatica* L., known as watermint, and spearmint, *M. spicata* L., which are native to southern Europe. During the nineteenth century, cuttings of *M. piperita* were brought to the United States, which is the world's largest producer of peppermint oil. Production areas include Indiana, Michigan, Ohio, Wisconsin, Oregon, and Washington state. It is important to harvest the peppermint plant at the early blooming stage so as to minimize the content of menthofuran, a characteristic but undesirable ingredient which lends a kerosene-like aroma to the oil. The essential oil must be rectified to remove water and all unpleasant-smelling or -tasting fractions, including bitter, sulfury-weedy foreruns and resinous-oily residues. Natural peppermint oil (unrectified) is a pale yellow to olive liquid possessing a strong, fresh, grassy-minty odor and a deep sweet-balsamic undertone with a clean dryout. Even the odor smells "cool." Rectified oils are water-white and free from weedy topnotes and any harsh-resinous aftertaste. Peppermint oil finds occasional use in perfumery to provide lift and freshness, but the principal use is in the flavor area for candies, chewing gums, liqueurs, oral hygiene products, etc. In 1988, the comparative analysis of the volatiles of the headspace of living peppermint, partially dried picked peppermint, and commercial peppermint oil were reported, and differences are shown in Table 50 (93).

**Table 50. Comparative Analysis of Peppermint Volatiles<sup>a</sup>**

Component	CAS Registry Number	Structure number	In living plant, %	In picked plant, %	In commercial oil, %
hexanal	[66-25-1]			0.1	
<i>cis</i> -3-hexenal	[6789-80-6]			0.5	
<i>trans</i> -2-hexenal				0.8	
<i>trans</i> -2-hexenol	[2305-21-7]			1.4	
<i>cis</i> -3-hexenol				1.4	
hexanol	[25917-35-5]			0.5	
2,4-hexadienal	[142-83-6]			0.1	
1-octen-3-ol				2.0	
eucalyptol		(34)			5.7
menthone <sup>b</sup>			0.2	12.7	18.1
isomenthone <sup>c</sup>			9.6	7.7	2.3
menthofuran	[494-90-6]		49.7	26.3	5.2
menthol (isomers)			<sup>d</sup>	4.7	48.0
pulegone		(150)	1.6	24.5	1.7
1,3,5-undecatriene (isomers)			0.6		
Total			61.6	81.6	81

<sup>a</sup>Ref. 93

<sup>b</sup>*trans*-2-Isopropyl-5-methylcyclohexanone.

<sup>c</sup>*cis*-3-Isopropyl-5-methylcyclohexanone.

<sup>d</sup>Trace amounts.

The isomers of 1,3,5-undecatriene in living plant volatiles are partly responsible for the unique, fresh natural-green character of the living herb.

### 5.53. Petitgrain Bigarade Oil

Orange flower water [8030-28-2], obtained by steam distillation of the leaves, stems, and twigs of the tree *Citrus aurantium* subsp. *amara*, is called petitgrain bigarade oil. The tree is cultivated in almost all of the mild-temperate, semitropical, and tropical regions of the world; the best-quality oil comes from trees grown and processed in the south of France. Petitgrain bigarade oil is a pale yellow to amber-colored mobile liquid with

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a pleasant, fresh-floral, sweet odor reminiscent of orange flowers with a slightly woody-herbaceous undertone and faint sweet-floral dryout. It is used in perfumery mainly for its refreshing sweet-floral notes, and in fruit and honey flavors at low levels. The constituents of petitgrain bigarade oil are shown in Table 51 (94).

**Table 51. Principal Components of Petitgrain Bigarade Oil<sup>a</sup>**

Component	Structure number	Percent
linalyl acetate	(24)	44.1
linalool	(10)	11.7
<i>trans</i> -linalool oxide (furanosyl)	(110)	7.1
<i>cis</i> -linalool oxide (furanosyl)	(109)	5.4
methyl anthranilate <sup>b</sup>		3.5
geranyl acetate	(28)	1.7
$\alpha$ -humulene	(147)	1.4
$\alpha$ -terpineol	(26)	1.3
$\alpha$ -terpinyl acetate	(132)	1.1
myrcene	(29)	1.0
geraniol	(9)	1.0
Total		79.3

<sup>a</sup>Ref. 94.

<sup>b</sup>Methyl 2-aminobenzoate [134-20-3].

### 5.54. Pimento Berry Oil

The pimento or allspice tree, *Pimenta dioca* L. (syn. *P. officinalis*, Lindl.), a native of the West Indies and Central America, yields two essential oils of commercial importance: pimento berry oil and pimenta leaf oil. The leaf oil finds some use in perfumery for its resemblance to clove leaf and cinnamon leaf oils as a result of its high content of eugenol. Pimento berry oil is an item of commerce with extensive application by the flavor industry in food products such as meat sauces, sausages, and pickles, and moderate use in perfumery, where it is used primarily as a modifier in the modern spicy types of men's fragrances. The oil is steam-distilled from dried, crushed, fully grown but unripe fruits. It is a pale yellow liquid with a warm-spicy, sweet odor with a fresh, clean topnote, a tenacious, sweet-balsamic-spicy body, and a tea-like undertone. A comparative analysis of the headspace volatiles of ripe pimento berries and a commercial oil has been performed and differences are shown in Table 52 (95).

**Table 52. Comparative Analysis of the Headspace Volatiles of Ripe Pimento Berries and a Commercial Oil<sup>a</sup>**

Component	Structure number	In headspace, %	In commercial oil, %
eugenol		31.3	71.4
myrcene	(29)	27.0	0.3
<i>trans</i> - $\beta$ -ocimene	(25)	8.4	0.3
eugenyl methyl ether	(11)	7.5	8.6
$\beta$ -caryophyllene	(52)	7.4	7.9
limonene	(23)	1.8	0.2
linalool	(10)	1.5	0.1
terpinolene	(50)	1.2	0.2
Total		86.1	89.0

<sup>a</sup>Ref. 95.

### 5.55. Pine Oil

This oil is obtained by extraction and fractionation or by steam distillation of the wood of *Pinus palustris* Mill. and other species. Most of the oil is produced in the southeastern United States. The composition of the oil depends on the fractions chosen, but the chief constituents are terpene alcohols, mainly terpineol. Pine oil finds use as a germicide in disinfectants and soaps; as an ingredient in insecticides, deodorants, polishes, sweeping compounds, and cattle sprays; and as raw material for the manufacture of perfumery-grade terpineol [8000-41-7], anethole [104-46-1], fenchone (137), and camphor (35).

### 5.56. Rosemary Oil

This oil is steam-distilled from the flowers and leaves (twigs are added in Spanish distillations) of the shrub *Rosmarinus officinalis* L., which grows wild throughout the Mediterranean region. For the most part, distillation is performed locally, with the highest quality oils coming from Spain, France, and Tunisia. The oil is a pale yellow to almost water-white mobile liquid with a strong, fresh, woody, herbaceous and minty forest-like odor. The body note is clean, woody-balsamic drying out to a pleasant dry-herbaceous and tenacious bittersweet note. It finds extensive use both in fine perfumery and functional products such as room deodorants, household sprays, insecticides, and disinfectants. A comparative analysis has been performed of the headspace volatiles of both living and picked rosemary and a high quality commercial oil, and components are shown in Table 53 (96).

**Table 53. Comparative Analysis of Headspace Volatiles of Living and Picked Rosemary and a Commercial Oil<sup>a</sup>**

Component	Structure number	In living, %	In picked, %	In commercial oil, %
<i>para</i> -cymene		19.8	13.7	1.7
limonene	(23)	14.1	14.3	1.0
myrcene	(29)	9.5	11.1	1.7
verbenone	(116)	7.2	6.0	0.1
linalool	(10)	7.1	7.6	0.8
$\alpha$ -terpineol	(26)	5.0	4.6	1.4
$\beta$ -caryophyllene	(52)	5.4	4.6	2.9
terpinen-4-ol	(37)	3.3	3.2	0.5
geraniol	(9)	3.2	1.7	
$\gamma$ -terpinene		2.7	2.6	0.5
1,8-cineole	(34)	2.0	0.7	44.5
bornyl acetate	(138)	2.0	2.3	1.3
eugenyl methyl ether	(11)	2.0	1.9	
borneol		1.5	1.4	2.6
$\alpha$ -pinene	(44)	1.0	1.3	13.3
camphor	(35)	0.2		10.1
$\beta$ -pinene	(22)	0.2	0.1	7.6
camphene	(47)	0.1	0.4	5.8
<i>Total</i>		86.3	77.5	86.8

<sup>a</sup>Ref. 96.

### 5.57. Sage Oil, Dalmatian

Several sage oils are produced commercially, each from a different species of plant. Sage oil [8022-56-8], Dalmatian is steam-distilled from the dried leaves of wild *Salvia officinalis* L. growing primarily in the former Yugoslavia; sage oil, Spanish comes from steam distillation of wild growing *S. lavandulifolia* Duhl. in Spain;

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and sage (clary) oil is steam-distilled from the flowering tops and foliage of *S. sclarea* L. originally from the Mediterranean, but now cultivated in central and eastern Europe, England, Morocco, and the United States. Sage oil, Dalmatian is a pale-yellow, mobile liquid with a strong fresh warm-spicy, herbaceous, and camphoraceous odor with a pleasant, sweet-herbaceous and tenacious dryout. The oil finds extensive use as a flavor material for liqueurs, canned meats, sauces, pickles, sausages, etc. In fine perfumery, it is used for its power and tenacity in both men's and women's fragrances. A comparison of the headspace volatiles of living *Salvia officinalis* and a commercial sage oil, Dalmation has been performed, and the components are shown in Table 54 (97).

**Table 54. Comparison of Headspace Volatiles of Living *Salvia officinalis* and Commercial Sage Oil, Dalmatian<sup>a</sup>**

Component	Structure number	In headspace, %	In commercial oil, %
thujone/isothujone	(136)	27.7	30.0
cis-3-hexenyl isovalerate		12.1	
limonene	(23)	7.1	5.9
cis-3-hexenyl acetate		5.4	
para-cymene		2.4	0.8
myrcene	(29)	2.2	0.8
$\beta$ -caryophyllene	(52)	1.7	10.4
hexyl valerate		1.5	
camphor	(35)	0.8	21.9
camphene	(47)	0.1	6.9
1,8-cineole	(34)	0.2	5.3
$\alpha$ -pinene	(44)	0.5	3.3
borneol			3.0
bornyl acetate	(138)	0.5	2.1
$\beta$ -pinene	(22)	0.4	1.8
Total		62.6	92.1

<sup>a</sup>Ref. 97.

### 5.58. Sage (Clary) Oil

Also known commercially as essence sauge sclarée clary sage oil [8016-63-5] is steam-distilled from the flowering tops and foliage of *Salvia sclarea* L., which is native to the Mediterranean region but is cultivated extensively in central and eastern Europe, the Crimea and Caucasus regions, as well as in England, Morocco, and the United States. The finest oils traditionally come from France, England, and Morocco. Clary sage oil is a colorless to pale yellow to olive mobile liquid with a tenacious sweet-herbaceous odor becoming soft and somewhat reminiscent of ambra in the undertone. The dryout note has also been described as tobacco-like, balsamic, or tea-like. The oil is used in fine perfumery as a modifier for other naturals, such as bergamot, and to provide soft, ambra notes. It is particularly effective in oriental-type fragrances. It is also used in flavorings for liqueurs and wine, and in grape flavors. A comparison of the volatiles of U.S., French, and Russian oils has been performed, and components are shown in Table 55 (98).

### 5.59. Spearmint Oil (Native)

Produced by steam distillation of the flowering tops of *Mentha spicata* Huds., native spearmint oil is one of the largest-volume essential oils of the United States. The plant, a native of Europe, was introduced into the United States in the nineteenth century, and the flavor immediately became popular there and has remained so, whereas it has never been as popular in the countries of its origin. The main producing areas are the same as for true peppermint. Distillation is carried out in the fields and either sold as such or rectified to the buyer's

**Table 55. Comparative Chemical Composition of Commercial Clary Sage Oils<sup>a</sup>**

Component	Structure number	In U.S. oil, %	In French oil, %	In Russian oil, %
linalyl acetate	(24)	44.9–53.4	49.0–73.6	45.3–61.8
linalool	(10)	20.3–28.6	9.0–16.0	10.4–19.3
$\alpha$ -terpineol	(26)	3.1	0.2–0.6	1.2–2.5
germacrene D	(156)	2.6–3.6	1.6–2.0	0.7–2.0
geranyl acetate <sup>b</sup>	(28)	1.9–3.2	0.3–0.5	0.8–1.2
geraniol	(9)	1.7–3.3	0.1–0.3	0.6–1.2
myrcene	(29)	1.3–1.7	0.1–0.2	0.3–0.5
neryl acetate		1.0–1.7	0.2–0.3	0.4–0.6

<sup>a</sup>Ref. 98.<sup>b</sup>3,7-Dimethyl-3,6-octadienyl acetate.

specifications. The crude oil obtained directly from the stills is called natural spearmint oil. It is a pale olive to yellow mobile liquid with a warm, biting, spicy-herbaceous, bitter quality. Rectified oils are less bitter with a more burning-biting, sweeter-balsamic taste. The oil finds its primary use in flavors for toothpaste, chewing gum, candy, and mouthwashes, where it blends well with peppermint. There is some use of it in perfumery for its herbaceous-green effect. The principal and characteristic constituent is *l*-carvone with a completely different odor and taste from that of the *d*-isomer. Spearmint oil has been the subject of thorough analysis, and in 1990 a comparison of the headspace volatiles of living and picked spearmint with those of a commercial oil was reported (99); differences are shown in Table 56.

**Table 56. Comparison of Headspace Volatiles of Living vs Picked Spearmint and Commercial Oil<sup>a</sup>**

Component	In headspace of live plant, %	In headspace of picked plant, %	In commercial oil, %
carvone (123)	24.0	70.0	63.0
limonene (23)	17.7	1.8	21.4
dihydrocarvone <sup>b</sup>	0.7	2.6	0.1
hexanal	0.5	<sup>c</sup>	
hexanol		2.3	0.1
menthone/isomenthone			1.2
menthol			1.7
1,3,5-undecatriene (isomers)	0.5		

<sup>a</sup>Ref. 99.<sup>b</sup>2-Methyl-5-isopropenylcyclohexanone [7764-50-3].<sup>c</sup>Trace amounts.

### 5.60. Tagetes Oil

Steam distillation immediately after flowering of the above-ground parts of *Tagetes minuta* L. (syn. *T. glandulifera* Schrank.), a native of South America but abundantly growing wild in sub-Saharan Africa and also found in Australia, Europe, Asia, and the United States, yields a dark yellow to orange-yellow mobile liquid which solidifies on exposure to air, daylight, and moisture. An absolute is also made from the concrete. The oil is distilled in Africa and France. The main components of tagetes oil are 4-octenones (or dienes or trienes) (Table 57) (100).

The branched-chain polyunsaturated ketones tagetone and ocimenone, the odor impact compounds in tagettes, are unstable and presumably responsible for the resinification of the oil.

**Table 57. Components of Tagetes Oil<sup>a, b</sup>**

Common name	Systematic name	CAS Registry Number	Percent
<i>cis</i> - $\beta$ -ocimene	2,6-dimethyl- <i>cis</i> -2,5,7-octatriene		41.6
<i>trans</i> -ocimenone	2,6-dimethyl- <i>trans</i> -2,5,7-octatrien-4-one	[33746-45-1]	12.5
dihydrotagetone	2,6-dimethyl-7-octen-4-one	[1879-00-1]	10.9
tagetone	2,6-dimethyl-2,7-octadien-4-one	[6752-80-3]	7.9
<i>cis</i> -ocimenone	2,6-dimethyl-2,5,7-octatrien-4-one	[33746-71-3]	7.0
limonene	4-isopropenyl-1-methylcyclohexene		3.9
<i>Total</i>			83.8

<sup>a</sup>Ref. 100.<sup>b</sup>Structure (23).**5.61. Thyme Oil**

The water- and steam-distilled essential oil obtained from the partially dried herb of the wild-growing *Thymus vulgaris* L., *T. zygis* L., or related species is called thyme oil [8007-46-3]. Various species of thyme grow abundantly in the Mediterranean region as well as central and eastern Europe. In addition, the plant is cultivated in many parts of the world as a dried culinary herb. Spain is a primary center for distillation. Thyme oil is a brownish orange-red liquid with a rich, powerful, sweet, warm-herbaceous odor, very aromatic and spicy. The flavor is rich, warm, biting, spicy-herbaceous. In perfumery, the oil finds primary use in functional products such as soap fragrances and only trace use in fine perfumery. The principal use of thyme oil is in flavors for sauces, dressings, pickles, canned meats, etc, and in pharmaceutical preparations including mouth washes, gargles, dentifrices (qv), cough syrups, and lozenges because of its excellent germicidal properties. A comparative analysis of the headspace volatiles over living and picked *T. vulgaris* and a commercial oil was performed and differences are shown in Table 58 (101).

**Table 58. Differences Between Headspace Constituents of Living and Picked *Thymus vulgaris* and a Commercial Oil<sup>a</sup>**

Component	CAS Registry Number	Structure number	In headspace of live plant, %	In headspace of picked plant, %	In commercial oil, %
<i>para</i> -cymene			29.7	48.6	30.0
thymol <sup>b</sup>	[89-83-8]		15.2	9.0	39.7
<i>cis</i> -3-hexenyl acetate			11.2	0.1	
1-octen-3-ol			8.2	8.0	
linalool		(10)	3.3	5.2	6.8
myrcene		(29)	3.2	2.5	1.4
$\beta$ -caryophyllene		(52)	1.8	3.1	1.2
carvacrol <sup>c</sup>			1.5	0.9	1.0
hexyl acetate			1.5		
limonene		(23)	1.3	1.1	1.8
geranyl isovalerate <sup>d</sup>	[109-20-6]		1.0		
$\alpha$ -pinene			0.1		3.1
$\alpha$ -terpineol				0.6	1.3
<i>Total</i>			78.0	79.1	86.3

<sup>a</sup>Ref. 101.<sup>b</sup>2-Isopropyl-5-methylphenol.<sup>c</sup>2-Methyl-5-isopropylphenol.<sup>d</sup>3,7-Dimethyl-2,6-octadienyl-3-methylbutanoate.

### 5.62. Turpentine Oil

The world's largest-volume essential oil, turpentine [8006-64-2] is produced in many parts of the world. Various species of pines and balsamiferous woods are used, and several different methods are applied to obtain the oils. Types of turpentines include dry-distilled wood turpentine from dry distillation of the chopped woods and roots of pines; steam-distilled wood turpentine which is steam-distilled from pine wood or from solvent extracts of the wood; and sulfate turpentine, which is a by-product of the production of sulfate cellulose. From a perfumery standpoint, steam-distilled wood turpentine is the only important turpentine oil. It is rectified to yield pine oil, yellow or white as well as wood spirits of turpentine. Steam-distilled turpentine oil is a water-white mobile liquid with a refreshing warm-balsamic odor. American turpentine oil contains 25–35%  $\beta$ -pinene (**22**) and about 50%  $\alpha$ -pinene (**44**). European and East Indian turpentines are rich in  $\alpha$ -pinene (**44**) with little  $\beta$ -pinene (**22**), and thus are excellent raw materials for the production of terpineol.  $\beta$ -Pinene (**22**) is used for the production of nerol, geraniol (**9**), and linalool (**10**), as well as further derivatives of these important chemicals.

### 5.63. Wintergreen Oil

Water distillation of the leaves of *Gaultheria procumbens* L. yields an oil which consists of essentially one chemical constituent, methyl salicylate. Because of this, the oil has been almost totally replaced by the synthetic chemical. Natural oil of wintergreen [68917-75-9] is a pale yellow to pinkish colored mobile liquid of intensely sweet-aromatic odor and flavor. The oil or its synthetic replacement find extensive use in pharmaceutical preparations, candy, toothpaste, industrial products, and in rootbeer flavor. In perfumery, it is used in fougère or forest-type fragrances.

### 5.64. Ylang Ylang

The oil produced by water- or water-and-steam-distillation of freshly early morning-picked blossoms from cultivated plantings of *Cananga odorata* Hook f. et Thomson, a tree native to Indonesia and the Philippines, is called ylang-ylang. Extensive plantings of this tree exist in the Comoro islands, Madagascar, the French South Pacific, the West Indies, and Réunion. Most ylang-ylang oil comes from the Comoro islands and Madagascar (the Nossi-Bé region). Distillation is carefully performed in small stills to minimize crushing of the delicate blossoms. Several fractions (called ylang extra, first, second, third, etc) are taken over different periods of time. The time for making the cuts is frequently determined by measuring the specific gravity of the oil which has come over. Ylang-ylang extra usually represents the first 30–45% of the total distillate. It is a pale yellow oil with a powerful, floral, and intensely sweet odor and a cresylic and benzoate topnote of limited tenacity. On dryout, it becomes more pleasant, soft, sweet, slightly spicy, and balsamic-floral. This fraction is used mainly in sophisticated perfumes of the floral and heavy-oriental type. “First” and “second” cuts are in-between quality, and are rarely used as such. Ylang-ylang “third” is a yellowish oily liquid of sweet-floral and balsamic-woody odor with a tenacious and sweet-balsamic undertone. This oil finds use in soap perfumery and less expensive consumer-type fragrances. The chemical composition of first, second, third, and extra grades of ylang-ylang oil from the Comoro islands has been reported (102), and the components are shown in Table 59.

## 6. Safety and Regulatory Aspects

Essential oils possess a variety of biological properties which may result in varying responses by humans on exposure. An important factor in these effects is the dose to which one is exposed. Thus, essential oils may have both beneficial and toxic effects, depending on their dose. The potential for biological effects from essential oils is not surprising; many botanical species are known to contain substances that possess biological properties,

**Table 59. Major Components of Ylang-Ylang Oils<sup>a</sup>**

Component	CAS Registry Number	Structure number	In first, %	In second, %	In third, %	In extra, %
<i>meta</i> -cresyl acetate <sup>b</sup> / <i>para</i> -cresyl acetate	[122-46-3]/[140-39-6]		29.0	21.4	28.7	15.9
benzyl acetate/ <i>ortho</i> -cresyl acetate <sup>c</sup>	[533-18-6]		16.1	32.3	36.6	29.9
linalool		(10)	12.2	6.1	2.1	11.0
<i>para</i> -cresyl methyl ether <sup>d</sup>	[104-93-8]		6.5	2.7	0.7	8.4
benzyl benzoate			5.4	6.5	5.5	5.2
eugenol/cinnamyl alcohol			3.0	2.4	1.8	5.6
nerol			2.0	2.9	3.0	1.3
farnesyl acetate	[29548-30-9]		2.0	2.0	2.9	1.6
$\alpha$ -humulene		(147)	1.7	2.6	1.8	0.9
farnesol			1.5	1.6	1.5	2.0
benzyl salicylate	[118-58-1]		1.2	1.1	1.9	1.9
geraniol		(9)	1.1	0.9	0.8	0.7
$\gamma$ -terpinene			0.9	0.2		
cinnamaldehyde/ <i>meta</i> -cresol <sup>e</sup> / <i>para</i> -cresol <sup>e</sup>	[108-39-4]/[106-44-5]		0.9	0.1	0.7	0.9
methyl anthranilate			0.8	0.9	1.0	0.4
benzyl alcohol			0.4	0.2	0.1	0.1
<i>Total</i>			84.4	89.9	89.1	85.8

<sup>a</sup>Ref. 102.<sup>b</sup>*m*- and *p*-Methylphenyl acetate.<sup>c</sup>*o*-Methylphenyl acetate.<sup>d</sup>*p*-Methylphenyl methyl ether (*p*-methylanisole).<sup>e</sup>*m*- and *p*-Methylphenol.

and their identification has contributed significantly to knowledge of biochemistry and physiology as well as the development of therapeutic agents, eg, quinine and digitalis.

The toxicities of many essential oils have been reported in monographs published by the Research Institute for Fragrance Materials (RIFM) (Table 60). Most essential oils used by the flavor and fragrance industries are relatively nontoxic or slightly toxic on acute oral or dermal exposure, and are considered safe when used at levels present in consumer products. In general, the levels of fragrances and flavors in consumer products, and thus the levels of any essential oil ingredients, are relatively low. For example, a fragrance oil may typically be used in a soap at 0.5%. The oil may contain 5% of orange oil distilled. The final concentration of orange oil distilled in the soap therefore is 0.025%.

Because essential oils are used predominantly by the flavor and fragrance industries, these commercial oils must undergo the same scientific scrutiny as all other flavor and fragrance substances and must be in compliance with all applicable health, safety, and environmental regulations. Guidelines and regulations on the use of essential oils in fragrances differ from those applying to essential oils used in flavors.

The industry supports several key organizations which strengthen scientific criteria and develop guidelines for the safe use of essential oils as flavor or fragrance ingredients (see Flavors and spices). The Research Institute for Fragrance Materials (RIFM) is an internationally recognized scientific organization that collects, generates, and disseminates information on the safety of fragrance ingredients, including essential oils. This information may originate from published or unpublished sources, or be generated through RIFM's ongoing research program. The findings are peer reviewed by an expert panel of academicians and published in the scientific literature.

The activities of RIFM are harmonized with those of the International Fragrance Association (IFRA) and the International Organization of the Flavour Industry (IOFI). These organizations are concerned with

**Table 60. Toxicities of Some Essential Oils<sup>a</sup>**

Essential oil	LD <sub>50</sub> , g/kg <sup>b</sup>		Irritation <sup>c</sup>	Sensitization <sup>d</sup> dose, wt %	Reference
	Oral	Dermal			
anise	2.25	>5	<sup>e</sup>	2.0	104
basil, sweet	1.4	>5 <sup>f</sup>	<sup>e</sup>	4.0	105
bergamot, expressed	>10	>20 <sup>f</sup>	<sup>e</sup>	30.0	106
bergamot, rectified	>10	>20	<sup>e</sup>	30.0	107
cedarwood, Texas	>5	>5	negative	8.0	108
cinnamon leaf, Ceylon	2.65	>5	strong	10.0	109
citronella	>5	4.7	moderate	8.0	110
galbanum	>5	>5	slight	4.0	111
geranium	>5	2.5	moderate	20.0	112
lavender	>5	>5	slight	16.0	113
lemon, distilled	>5	>5	slight	15.0	114
lemon, expressed	>5	>5	moderate	10.0	115
orange, expressed	>5	>5	moderate	8.0	116
rose, Bulgarian	>5	2.5	moderate	2.0	117
sage, Spanish	>5	>5	negative	8.0	118
spearmint	≈5	>5	moderate	4.0	119
thyme, red	4.7	>5	severe	8.0	120

<sup>a</sup>Phototoxicity is negative for all oils except bergamot, expressed, for which it is severe.

<sup>b</sup>The LD<sub>50</sub> is the statistically derived dose of a substance which results in death in 50% of a population of animals. The LD<sub>50</sub> is expressed in milligrams of substance per kilogram of body weight. The species used to determine the oral and dermal LD<sub>50</sub> are the rat and rabbit, respectively.

<sup>c</sup>Irritation results are based on the substance applied full strength to a test population for a 24-h period.

<sup>d</sup>Sensitization results are based on a human maximization test (103) using a petrolatum vehicle. The effect is expressed as the number of panelists responding over the total number of panelists tested and was 0/25 except for spearmint (0/32). That is, at the dose indicated, the oils were not irritating when tested in a 48-h closed patch test in humans.

<sup>e</sup>Not reported in the monograph (103).

<sup>f</sup>LD<sub>50</sub> values expressed as milliliter of substance per kilogram of body weight (mL/kg).

all aspects of safety evaluation and regulation in the industry, into which it has introduced self-regulatory discipline. Both IFRA and IOFI have formulated and continue to update their respective “Codes of Practice” for both the fragrance and flavor industries. These Codes set forth manufacturing, safety evaluation, and usage guidelines to assure the quality, safety, and legality of flavor and fragrance ingredients, including essential oils. For example, the IFRA Code of Practice restricts essential oils containing psoralens, thereby reducing concerns about their potential dermal phototoxicity. In addition, the United States Flavor Extracts Manufacturers Association (FEMA), the U.S. Food and Drug Administration (FDA), the Council of Europe (CoE), the Food and Agricultural Organization of the United Nations (FAO), and the World Health Organization (WHO) monitor usage and evaluate the safety of essential oils when they are used in foods and flavors.

Many essential oils have been designated by the FDA or by the expert panel of FEMA as Generally Recognized As Safe (GRAS) for their intended use in foods and flavors. The use and safety of these GRAS substances are continuously being reviewed and the list of GRAS substances updated. New essential oils intended to be used as a flavor ingredient must undergo extensive safety evaluations and scrutiny by one or more of these groups of experts before they may be used in flavors.

Many countries have adopted chemical substance inventories in order to monitor use and evaluate exposure potential and consequences. In the case of essential oils used in many fragrance applications, these oils must be on many of these lists. New essential oils used in fragrances are subject to premanufacturing or pre-marketing notification (PMN). PMN requirements vary by country and predicted volume of production. They

require assessment of environmental and human health-related properties, and reporting results to designated governmental authorities.

Essential oils are also influenced by legislation that regulates specific products that may contain these oils, eg, the U.S. Food, Drug, and Cosmetic Act and the European Community Cosmetic Directive. An example of an environmental issue that affects essential oils used in fragrances is the regulatory trend to reduce atmospheric release of volatile organic chemicals (VOCs) from consumer products and other sources. Fragrances and their essential oil ingredients are recognized as unique and essential components of consumer products, and are given specific exemptions from most VOC regulations. Essential oils would not be anticipated to be of environmental concern, considering that they originate from botanical sources. Thus, natural processes exist to degrade essential oils and recycle their components effectively in the environment.

## BIBLIOGRAPHY

"Oils, Essential" in *ECT* 1st ed., Vol. 9, pp. 569–591 by E. E. Langenau, Fritzsche Brothers, Inc.; in *ECT* 2nd ed., Vol. 14, pp. 178–216, by Max Stoll, Firmenich & Cie.; in *ECT* 3rd ed., Vol. 16, pp. 307–332 by J. A. Rogers, Jr., Fritzsche, Dodge & Olcott, Inc.

### Cited Publications

1. U.S. Dept. of Commerce, Horticultural and Tropical Products Division, FAS/USDA, Washington, D.C., Apr. 1994.
2. E. Demole, P. Enggist, and G. Ohloff, *Helv. Chim. Acta* **65**(6), 1785 (1982).
3. J. Rigaud, P. Etievant, R. Henry, and A. Latrasse, *Sci. Aliments* **6**(2), 213 (1986).
4. T. C. Baker, R. Nishida, and W. L. Roelofs, *Science (Washington, D.C.)* **214**, 1359 (1981).
5. R. Nishida and T. E. Acree, *J. Agric. Food Chem.* **32**(5), 1001 (1984).
6. T. E. Acree, R. Nishida, and H. Fukami, *J. Agric. Food Chem.* **33**(3), 425 (1985).
7. *Ibid.*, p. 425.
8. B. D. Mookherjee, R. Trenkle, and R. Wilson, *Aerosol Age*, 20 (May, 1989).
9. Technical data, B. D. Mookherjee and R. Trenkle, International Flavors & Fragrances Inc., Union Beach, N.J., 1967.
10. G. Ohloff, *Perfumer Flavor* **3**, 11 (1978).
11. B. D. Mookherjee and R. A. Wilson in B. D. Mookherjee and R. A. Wilson *On Essential Oils*, Synthite Industrial Chemicals Private Ltd., Synthite Valley, Kolenchery, India, 1986, 281–329.
12. J. Jessee, *Perfume Album*, R. Krieger, Huntington, N.Y., 1974, p. 10.
13. Technical data, B. D. Mookherjee and R. W. Trenkle, International Flavors & Fragrances Inc., Union Beach, N.J., 1967.
14. Ref. 12, p. 18.
15. M. N. Boelens and A. Oporto, *Perfumer Flavor* **16**(6), 1 (1991).
16. Technical data, B. D. Mookherjee and R. W. Trenkle, International Flavors & Fragrances Inc., Union Beach, N.J., 1985.
17. B. Lalande, *Perfumer Flavor* **9**(2), 117 (1984).
18. M. Guerere and F. DeMarne, *Ann. Fals. Exp. Chim.* **78**(837), 183 (1985).
19. Y. Naves, D. Lamparsky, and P. Ochsner, *Bull. Soc. Chim. France*, 645 (1961).
20. G. Lucas, J. Ma, J. McCloskey, and R. Wolff, *Tetrahedron* **20**, 1789 (1964).
21. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1985.
22. G. Lamonica, I. Stagno D'Alcontres, M. G. Donato, and I. Merenda, *Chimicaoggi* **8**(5), 59 (1990).
23. E. Sundt, B. Willhalm, and M. Stoll, *Helv. Chim. Acta* **47**(2), 408 (1964).
24. B. D. Mookherjee, "The Identification of Bifunctional Compounds in Bergamot Oil," *the 158th National Meeting of the American Chemical Society, Sept. 7–12, 1969, New York*.
25. S. Inoma, Y. Miyagi, and T. Akieda, *Kanzei Chuo Bunsekishoho* **29**, 87 (1989).
26. A. Fleisher, G. Biza, N. Secord, and J. Dono, *Perfumer & Flavorist* **12**(2), 57 (1987).

27. E. Kovats, *Helv. Chim. Acta* **46**(7), 2705 (1963).
28. U.S. Pat. 3,988,432 (Oct. 26, 1976), R. Steltenkamp (to Colgate-Palmolive Co.).
29. Technical data, B. D. Mookherjee and R. Santangelo, International Flavors & Fragrances Inc., Union Beach, N.J., 1975.
30. J. D. Vora, R. F. Matthews, P. G. Crandall, and R. Cook, *J. Food Sci.* **48**, 1197 (1983).
31. K. Stevens, R. Lundin, and R. Teranishi, *J. Org. Chem.* **30**, 1690 (1965).
32. G. Ohloff, *Fortsch. Chem. Org. Naturst.* **35**, 473 (1983).
33. M. H. Boelens, *Perfumer Flavor.* **16**(2), 17 (1991).
34. W. D. MacLeod, Jr. and N. Buigues, *J. Food Sci.* **29**, 565 (1964).
35. E. Demole and P. Enggist, *Helv. Chim. Acta* **66**(5), 1381 (1983).
36. E. Demole, P. Enggist, and G. Ohloff, *Helv. Chim. Acta* **65**(6), 1785 (1982).
37. E. J. Brunke and F. J. Hammerschmidt, *Dragoco Rpt.* (4), 107 (1988).
38. U.S. Pat. 4,014,823 (Mar. 29, 1977), B. D. Mookherjee, V. Kamath, and E. Shuster (to International Flavors & Fragrances Inc.).
39. B. M. Lawrence, *Perfumer Flavor.* **15**(2), 77 (1990).
40. P. Teisseire, P. Maupetit, and B. Corbier, *Recherches (R.B.D.)* **19**, 8 (1974).
41. B. D. Mookherjee, K. Light, and I. Hill, in B. D. Mookherjee and C. J. Mussinan, eds., *Essential Oils*, Allured Publishing Corp., Wheaton, Ill., 1981, p. 247.
42. S. Lemberg and R. B. Hale, "Vetiver Oils of Different Geographical Origins," Paper No. 117 presented in the *VII International Congress of Essential Oils*, Oct. 7-11, 1977, Kyoto, Japan.
43. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1985.
44. Y. Chretien-Bessiere, J. Garnerio, L. Benezet, and L. Peyron, *Bull. Soc. Chim. France*, (1), 97 (1967).
45. P. Teisseire, B. Corbier, and M. Plattier, *Recherches* **16**, 5 (1967).
46. Y. R. Naves, *Bull. Soc. Chim. France*, (9), 3152 (1967).
47. Technical data, B. D. Mookherjee and R. Santangelo, International Flavors & Fragrances Inc., Union Beach, N.J., 1975.
48. A. Bramwell, J. Burrell, and G. Riezebos, *Tetrahedron Lett.* (37), 3215 (1969).
49. Y. Naves, *Parfum Cosmet. Savons*, **12**(2), 586 (1969).
50. R. Kaiser and D. Lamparsky, *Helv. Chim. Acta* **61**(7), 2671 (1978).
51. R. A. Wilson and B. D. Mookherjee, "Characterization of Aroma Donating Components of Myrrh," paper presented at the *IXth International Congress of Essential Oils*, Mar. 13-17, 1983, Singapore.
52. R. ter Heide and co-workers, *J. Agric. Food Chem.* **23**(5), 950 (1975).
53. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1984.
54. H. Walbaum, *J. Prakt. Chem.* **73**, 488 (1906).
55. L. Ruzicka, M. Stoll, and H. Schinz, *Helv. Chim. Acta* **9**, 249 (1926).
56. B. D. Mookherjee and R. W. Trenkle, "Volatile Constituents of Tincture of Tonquin Musk," paper presented at the *VIIIth International Congress of Essential Oils*, Oct. 12-17, 1980, Cannes, Grasse, France.
57. B. D. Mookherjee and R. Patel, "Isolation and Identification of Volatile Constituents of Tincture of Ambergris," paper presented at the *VIIth International Congress of Essential Oils*, Oct. 7-11, 1977, Kyoto, Japan.
58. R. A. Wilson, B. D. Mookherjee, and J. Vinals, *Tob. Rep.*, 42 (Oct. 1983).
59. V. T. Gogiya, L. G. Kharebava, R. V. Gogiya, and E. B. Gvatua, *Rastit. Resur.* **22**, 243 (1986).
60. B. D. Mookherjee, R. W. Trenkle, and R. A. Wilson, *J. Ess. Oil Res.* **2**, 85 (1989).
61. E. Klein and H. Obermann, paper presented at the *VIIth International Congress of Essential Oils*, Oct. 7-11, 1977, Kyoto, Japan.
62. B. D. Mookherjee and R. A. Wilson, *Perfumer & Flavorist* **15**(1), 27 (1990).
63. B. Corbier, C. Ehret, and P. Maupetit, paper presented at *La Chemie des Terpenes*, Apr. 24-25, 1986, Grasse, France.
64. F. De Maack, D. Brunet, J.-C. Malnati, and J. Estienne, *Ann. Fals. Expert Chim.* **75**, 357 (1982).
65. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1991.
66. L. Peyron, J. Acchiardi, D. Bignotti, and P. Pellerin, "The Berries of *Pimenta Dioca*," Paper No. 128 presented at the *VIIIth International Congress of Essential Oils*, Oct. 12-17, 1980, Cannes, France.
67. M. H. Boelens, *Perfumer Flavor.* **16**(2), 17 (1991).
68. B. M. Lawrence, *Perfumer Flavor.* **10**(2), 52 (1985).

69. B. M. Lawrence, *Perfumer Flavor*. **9**(5), 87 (1984).
70. F. Buccellato, *Perfumer Flavor*. **13**(4), 35 (1988).
71. A. M. Janssen, Ph.D. dissertation, Rijksuniversiteit, Leiden, the Netherlands, 1989.
72. W. A. König, R. Krebber, P. Evans, and G. Bruhn, *J. High Res. Chromatog.* **13**, 328 (1990).
73. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1988.
74. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1987.
75. B. M. Lawrence, *Perfumer Flavor*. **15**(6), 56 (1990).
76. R. P. Adams, *Econ. Bot.* **41**, 48 (1987).
77. N. A. Shaath, S. Dedeian-Johnson, and P. M. Griffin, *Proceedings of the 11th International Congress of Essential Oils, Fragrances, and Flavors*, Vol. **4**, Oxford and IBH Publishing Co. Pvt. Ltd., New Delhi, India, 1989, p. 207.
78. C. Vernin, G. Vernin, J. Metzger, and L. Pujol, *Parfum. Cosmet., Arôm.* (93), 85 (1990).
79. M. Manzoor-i-Khuda, M. Rahman, M. Yusaf, and J. Chowdhury, *Bangladesh J. Sci. Ind. Res.* **21**(1/4), 70 (1986).
80. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1988.
81. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1987.
82. J. A. Retamar and E. C. DeRiscala, *Rivista Ital.* **52**, 127 (1980).
83. D. Garcia-Martin and M. C. Garcia-Vallejo, in Ref. 61, p. 362.
84. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1988.
85. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1987.
86. A. Proença and O. L. R. Roque, *J. Ess. Oil Res.* **1**, 15 (Jan.-Feb., 1989).
87. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1990.
88. J. de Pascual Teresa and co-workers, *Planta Med.* **55**, 398 (1989).
89. T. S. Chamblee and co-workers, *J. Agric. Food Chem.* **39**, 162 (1991).
90. S. R. Srinivas, *Atlas of Essential Oils*, the Bronx, N.Y., 1986.
91. B. M. Lawrence, *Perfumer Flavor*. **9**(5), 41 (1984).
92. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1989.
93. B. D. Mookherjee, R. A. Wilson, R. W. Trenkle, M. J. Zampino, and K. P. Sands, in R. Teranishi, R. G. Buttery, and F. Shahidi, eds., *Flavor Chemistry: Trends and Developments*, ACS Symposium Series 388, American Chemical Society, Washington, D.C., 1989, p. 176.
94. Z.-K. Lin, Y.-F. Hua, and Y.-H. Gu, *Acta Botan. Sinica* **28**(6), 635 (1986).
95. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1991.
96. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1992.
97. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1992.
98. B. M. Lawrence, *Perfumer & Flavorist* **15**(4), 71 (1990).
99. B. D. Mookherjee, R. W. Trenkle, and R. A. Wilson, *Pure Appl. Chem.* **62**(7), 1357 (1990).
100. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1985.
101. Technical data, B. D. Mookherjee and R. A. Wilson, International Flavors & Fragrances Inc., Union Beach, N.J., 1987.
102. J. M. Derfer, *Perfumer Flavor*. **3**(1), 45 (1978).
103. A. M. Kligman, *J. Invest. Derm.* **47**, 393 (1966).
104. *J. Food Chem. Toxicol.* **11**, 865 (1973).
105. Ref. 104, p. 867.
106. Ref. 104, p. 1031.
107. Ref. 104, p. 1035.
108. *J. Food Chem. Toxicol.* **14**, 711 (1976).
109. *J. Food Chem. Toxicol.* **13**, 749 (1975).
110. Ref. 104, p. 1067.
111. *J. Food Chem. Toxicol.* **16**, 765 (1978).
112. Ref. 108, p. 451.
113. *J. Food Chem. Toxicol.* **12**, 727 (1974).
114. Ref. 113, p. 725.
115. Ref. 113, p. 733.
116. Ref. 109, p. 913.
117. Ref. 108, p. 857.

118. Ref. 111, p. 871.  
119. Ref. 113, p. 1003.

#### General Reference

120. S. Arctander, *Perfume and Flavor Materials of Natural Origin*, 1960.

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