Chapter 3

Basic Plant Taxonomy, Basic Essential Oil Chemistry, Extraction, Biosynthesis, and Analysis

"A weed is a flower in the wrong place, a flower is a weed in the right place, if you were a weed in the right place you would be a flower; but seeing as you're a weed in the wrong place you're only a weed—it's high time someone pulled you out."

Ian Emberson

CHAPTER ASSETS

BASIC PLANT TAXONOMY

Learning how and why a plant manufactures an essential oil is relevant to understanding aromatherapy. The way plants make essential oils gives some insight into their complexity. Traditionally, biochemists have studied primary metabolism and organic chemists have studied secondary metabolism. In aromatherapy, it is useful to have an overall picture of both metabolic processes. Why some plants make essential oils is the subject of ongoing scientific debate and is relevant to the therapeutic potential of using essential oils in healthcare.

The process of extraction clarifies the need for unadulterated essential oils. Unadulterated essential oils are required for clinical use to prevent possible side effects from solvents or residues. The process of steam distillation or expression produces an essential oil with no residue. CO_2 extraction (supercritical carbon dioxide) does not produce a residue but it does produce a different extract. Steam-distilled German chamomile *(Matricaria recutita)* is dark blue due to the high content of chamazulene. CO_2 extract is green—no chamazulene.

The Latin names of plants can seem a bit intimidating initially, but they are the best way of being sure you have the correct essential oil. Carl Linnaeus (1707–1778) established the basis for naming plants in Latin (Stearn 1998). Today, botanical (Latin) names are recognized globally by gardeners, botanists, herbalists, and aromatherapists. A plant may have many common names, but it only has one Latin name and the common names may mean completely different plants. For example, in aromatherapy, bergamot means the essential oil extracted from the peel of the citrus fruit *Citrus bergamia.* To a gardener, bergamot means the plant *Monarda didyma*. In aromatherapy, *geranium* means *Pelargonium* "Graveolens" [the plant cultivated today is actually a cultivar group involving hybrids of *P. capitatum*, *P. radens*, and *P. graveolens* (Tucker 2014)]. To a gardener, *geranium* means the plant *Pelargonium* sp., although a medicinal plant person might assume geranium means *Geranium maculatum.*

Plant taxonomy, by its simplest definition, includes (1) naming and describing, (2) identifying, and (3) classifying of plants. The botanical name for each plant is composed of two words. The first word is the name of the genus. The second word is the name of the species. All plants can be grouped into categories. For plants to be properly identified they are divided into division, class, order, family, genus, and species. This process takes into account the number, shape and position of leaves on the stem; the shape and position of the flowers; the number and shape of the petals; whether the plant is hairy, prickly, or smooth; whether the stem is ridged; and so on.

EXAMPLES OF WHY THE BOTANICAL NAME IS IMPORTANT

Lavender

Lavender belongs to a plant family called Lamiaceae (previously Labiatae): the mint family. This family includes many species and some are used in aromatherapy. Plants in this family usually have five united petals with two lobes on the top and three on the bottom forming lips (labia). The leaves are usually directly opposite each other on the stem and often the stem is square. The Latin name for the lavender genus is *Lavandula,* so all lavenders begin with *Lavandula.* (See Table 3-1.) Two of the most commonly used "lavenders" are *Lavandula angustifolia* and *Lavandula latifolia.*

Lavandula angustifolia is sometimes called *L. vera* or *L. officinalis,* although the correct name is *L. angustifolia* (Lawrence 1989). This plant also has several common names: English lavender, French lavender, and true lavender.

Lavandula latifolia is sometimes called *L. spica,* and its common name is spike lavender or spike. Spike is completely different from spikenard *(Nardostachys jatamansi),* which is closely related to valerian and belongs to the family Valerianaceae.

Lavandula angustifolia and *Lavandula latifolia* were both listed in the *British Pharmacopoeia* and supplied to hospitals in vats labeled simply "lavender." However, the two plants have very different therapeutic properties. *L. angustifolia* is a sedative, relaxant, and hypotensor. *L. latifolia* is a stimulant and expectorant.

Another commonly used "lavender" is *Lavandula* × *intermedia* (older synonym *L. hybrida*). This is a naturally occurring hybrid that was first observed in 1828 (Tucker 2014). Today, *Lavandula* × *intermedia* tends to be a manufactured cultivar with a trade name Lavandin. It is a cross (hence the multiplication sign between the genus and the species) between two *Lavandula* species: *L. angustifolia* and *L. latifolia.* Because Lavandin belongs to the *Lavandula* genus, it can legitimately be called a "lavender." This can cause confusion when people think they have true lavender (*L. angustifolia*) when in fact they have Lavandin. There is a third less-commonly used species of lavender, *L. stoechas,* that can also be used clinically.

TABLE 3-1 *Lavenders and Some of Their Properties*

Latin Name	Common Name	Properties
Lavandula angustifolia *Lavandula vera* *Lavandula officinalis*	True lavender	Calming, sedative, good for burns, analgesic, antibacterial, immune-system enhancer
Lavandula latifolia *Lavandula spica*	Spike lavender	Expectorant, mucolytic, possible stimulant
Lavandula stoechas	Stoechas	Useful against *Pseudomonas* spp., high in ketones

Chamomile

Chamomile can also cause confusion initially. There are three main types of chamomile used in aromatherapy: German, Roman, and Moroccan (Table 3-2). They are quite different and produce different-colored essential oils that have different properties, but they all belong to the same family: Asteraceae or Compositae—the daisy family.

German chamomile *(Matricaria recutita)* is a smoky smelling, dark-blue oil that contains chamazulene. The oil's color is related to the amount of chamazulene present and the method of extraction. Chamazulene is not present in the fresh flower (or in its CO_2 extract) but is produced during distillation (Lawless 1992). It is possible to obtain a green or yellow German chamomile oil that has less than 3% chamazulene, but the dark-blue variety always has more than 7%. The price of German chamomile oil is usually related to the amount of chamazulene it contains. Chamazulene is an antiinflammatory with a history of use in the treatment of skin problems (Jakovlev et al 1983), (Ramadan et al 2006). German chamomile also contains a second antiinflammatory compound called (−)-alpha-bisabolol that is a sesquiterpene alcohol (Alves Ade et al 2010). In addition, this species has antibacterial properties (Salehi et al 2005) and is effective against *Staphylococcus aureus, Streptococcus,* and *Candida albicans* (Khezri et al 2013). CO_2-extracted German chamomile is dark green, or brownish green, and semisolid at room temperature. It smells of sweet apples with an earthy undertone.

Roman chamomile (*Chamaemelum nobile* or *Anthemis nobilis*) is commonly known as English chamomile or garden chamomile, is colorless to pale blue that turns yellow with storage. Listed in the *British Herbal Pharmacopoeia,* it contains up to 80% esters. Esters have antispasmodic properties, and essential oil of Roman chamomile is traditionally used topically as an antispasmodic and inhaled as a relaxant, while the herbal extract is used as a carminative. Roman chamomile also has mild antiinflammatory properties (Franchomme & Penoel 1990). Recent research suggests it may have antitumoral properties (Guimaraes et al 2013).

Moroccan chamomile (*Ormenis multicaulis* or *O. mixta*) is a relative newcomer to the aromatherapy world. The main component in the essential oil is santolina alcohol (Zrira et al 2007). It does not contain chamazulene. However, it does have some antibacterial properties (Darriet et al 2012). Adding further confusion is Chamomile Blue Tansy—*Tanacetum annum*. This is not a true chamomile—its genus is not *Chamaemelum* or *Ormenis*—but it is blue and it does contain chamazulene.

TABLE 3-2 *Chamomiles and Some of Their Properties*

Latin Name	Common Name	Properties
Matricaria recutita	German chamomile	Dark blue, useful for skin complaints and inflammation
Chamaemelum nobile	Roman chamomile	Pale blue or yellow, sedative, useful for spasms
Ormenis mixta	Moroccan chamomile	Mainly used by perfume industry, some antibacterial activity

Different Essential Oils from Different Parts of the Plant

Occasionally, different parts of the same plant can produce different essential oils. In the case of the bitter orange plant (*Citrus* × *aurantium* var. *amara*), three different types of essential oils can be obtained: petitgrain from the stems and leaves, neroli from the petals, and bitter orange from the fruit. Neroli-like and petitgrain-like essential oils can be obtained from the petals and leaves of other citrus species. Bergamot essential oil is obtained from the rind of a fruit that is a subspecies of the bittersweet orange. The shorthand for *Citrus aurantium* var. *bergamia* (bergamot) is *Citrus bergamia* (Guenther 1976).

Sometimes just the part of the plant is listed (e.g., cinnamon bark or cinnamon leaf). Cinnamon bark contains approximately 50% eugenol (a phenol). Cinnamon leaf contains 80 to 96% eugenol. Eugenol is strongly antimicrobial (Kamatou et al 2012). However, it can cause sensitization (Svedman et al 2012) and if used in high concentrations can burn the skin. It can also dissolve metal, false teeth, and pearls (Ryman 1991). Cinnamon bark and cinnamon leaf are used by the fragrance and pharmaceutical industries in very low dilutions.

Clones and Chemotypes

To complicate the situation a bit more, some plants have clones or cultivars. These will have different chemistries (Table 3-3). Clones or cultivars are manufactured and the essential oil has a specific chemical profile. This might make it more suitable for treating a particular ailment, or make it safer to use. Common thyme *(Thymus vulgaris)* has several chemotypes: linalol, geraniol, α-terpineol, thujanol-4, carvacrol, and thymol (Vernet & Gouyon 1976). The first four are all safe to use on the skin, because they are high in alcohols. However, thymol and carvacrol are phenols and can cause skin irritation. There are four different chemotypes of Lavandin (*Lavandula* × *intermedia* or *Lavandula hybrida*)—each with a different chemistry. Tea tree, eucalyptus, rosemary, and German chamomile are other essential oils that

TABLE 3-3 *Some Examples of Essential Oil Chemotypes*

Latin Name	Chemical Constituents	Research Paper
Achillea millefolium	Caryophyllene, farnesene, azulene-free	Hethelyi et al 1988 Oswiecimska 1974
Artemesia dracunculus	Methyl chavicol, sabinene	Tucker and Maciarello 1987
Ocimum basilicum	Linalool, methyl chavicol, eugenol	Sobti et al 1978
Matricaria recutita	Bisabolone oxide, bisabolol, chamazulene, chamazulene-free	Frantz 1993
Salvia officinalis	α- and β-thujone, cineole, thuhone-free	Tucker and Maciarello 1990

have commercial chemotypes. Chemotypes will become more common as aromatic plants are grown for the pharmaceutical or food industry.

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BASIC ESSENTIAL OIL CHEMISTRY

Chemistry makes an excellent handmaid but the worst possible mistress. Buhner 2012.

For this section, I am grateful to Professor K. Hüsnü Can Başer for his essential oil chemistry chapters plus numerous papers and to Ian Cambray-Smith for his chemistry course notes and creating most of the chemical drawings. I have tried to make what is an extremely complicated subject as simple and as relevant to aromatherapists, as possible. I have selected research papers to illustrate the wide range of potential properties of essential oil components. My intention is that the reader will look anew at essential oils they may have used previously for other outcomes. It is worth remembering that sometimes the minor components of essential oils can be important in aromatherapy. For example, the strong, sweet, floral smell of rose *(Rosa damascena)* is created by the high content of citronellol, geraniol modified by nerol (5 to 11%) and farnesol (0.2 to 1.4%) (Başer et al 2012). For possible toxicity and side effects please see Chapter 4.

ESSENTIAL OILS COMPONENTS

Essential oils are made up of terpenoids and nonterpenoid volatile hydrocarbons (Baser & Demirci 2011). These constituents contain a basic frame of carbon and hydrogen to which a "functional group" is added (Tisserand & Young 2013). A functional group is a term familiar to aromatherapists and means "a group of atoms the shape of which determines the characteristic chemical properties of the molecule" (Tisserand & Young 2013). There are six classes (functional groups) of organic compound that are important to aromatherapists (Cambray-Smith 2013). In alphabetical order, they are: alcohols, aldehydes, esters, ethers, ketones, and phenols.

Simple hydrocarbons such as alkanes, alkenes, and benzenoids are called nonterpenoid hydrocarbons due to the fact that their biosynthesis is not due to mevalonate or nonmevalonate (D-erythritol 4-phosphate [MEP]) pathways. Phenylpropanoids are synthesized through the Shikimic acid pathway (Tisserand & Young 2013). For more information, please see the biosynthesis section of this chapter. Please see Figure 3-1 for chemical drawings.

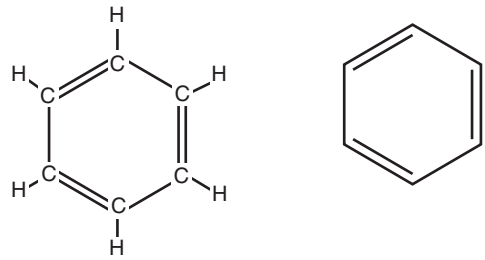


FIGURE 3-1 | Benzene rings (aromatic ring).

NONTERPENOID HYDROCARBONS

Terpenes

Terpenes—the largest single class of compounds found in essential oils, also called isoprenoids (Baser & Demirci 2011)—are made up of isoprene molecules. Each isoprene molecule (sometimes called isoprene unit) contains five carbon atoms with double bonds. The simplest terpenes are monoterpenes that contain two isoprene molecules. Sesquiterpenes have three isoprene molecules and diterpenes have four (Table 3-4). Because each isoprene molecule has five carbon atoms, it is easy to calculate the number of carbon atoms per molecule (Table 3-5). Terpenes can be subdivided into groups *acyclic* or *cyclic* which indicate their structure. Acyclic terpenes are linear, like the monoterpene β-myrcene. Cyclic terpenes form a ring, like the monoterpene *p*-cymene. Monocyclic, bicyclic, and tricyclic monoterpenes (meaning one, two, or three nonaromatic rings) occur in essential oils (Baser & Demirci 2007). All terpenes end in *-ene.*

Monoterpenes

Monoterpenes are light molecules that evaporate quickly and are called "top notes" by the perfume industry. Citrus oils, with the exception of bergamot, contain a high proportion of monoterpenes, in particular the optical isomer D-limonene, a cyclic form (Cambray-Smith 2013). D-Limonene is the most commonly found optical isomer or enantiomer of limonene and it is generally called limonene alone without mentioning its D-enantiomer. All monoterpenes have antiseptic properties and they are thought to be psychologically uplifting. Ocimene, α-pinene and limonene are monoterpenes. Some monoterpenes such as limonene and α-pinene have antitumoral properties (Rabi & Bishayee 2009), (Bhattachariee & Chatterjee 2013). Please see Table 3-6 for some chemical structures. Limonene also is effective for relief of heartburn and gastroesophageal reflux (GERD) due to its gastric acid neutralizing effect and its support

TABLE 3-4 *Structure of Terpenes*

Molecular Structure	Name	Example
Chain, no ring	Acyclic	α-Myrcene
One ring	Cyclic	D-Limonene
Two rings	Bicyclic	Thujane

TABLE 3-5 *Isoprene Units in Terpenes*

Chemical Constituent	Number of Isoprene Units	Number of Carbon Atoms
Monoterpene	2 isoprene units	10 carbon atoms
Sesquiterpene	3 isoprene units	15 carbon atoms
Diterpene	4 isoprene units	20 carbon atoms

of normal peristalsis (Sun 2007). Limonene occurs in most citrus oils and in dill *(Anethum graveolens)*. L-Limonene is present in spearmint oil and pine oil. Limonene oxidizes on air-exposure. Oxidized D-limonene can cause skin irritation (Christensson et al 2009). Because terpenes are insoluble in water, the perfume industry frequently removes them to produce "terpeneless" essential oils (Guenther 1972).

Sesquiterpenes

Sesquiterpenes are less volatile than terpenes, have a greater potential for stereochemical diversity (Waterman 1993) and have stronger odors. They are antiinflammatory (Jeena et al 2013) and have bactericidal properties (Ishnava et al 2013). Please see Table 3-7 for some chemical structures. Sesquiterpenes oxidize over time into sesquiterpenols. In patchouli oil, this oxidation is thought to improve the odor. One of the most antiinflammatory sesquiterpenes, chamazulene, only has 14 carbon atoms but is usually included with sesquiterpenes. Chamazulene and caryophyllene have strong antioxidant (Ornano et al 2013) and antitumor activity (Feraz et al 2013; Park et al 2011). Chamazulene is found in German chamomile. Sesquiterpenes can be monocyclic, bicyclic or tricyclic and are a very diverse group (Baser & Demirci 2007). Examples include α-bisabolene in black pepper (*Piper nigrum*) and β-caryophyllene in ylang ylang *(Cananga odorata)* (Cambray-Smith 2013). Some sesquiterpenes such as α-farnesene can be effective against the bacteria that cause tooth decay (Ishnava et al 2013).

Diterpenes

There are very few diterpenes in essential oils because they are big, heavy molecules with correspondingly high boiling points, so very few are present following the steam distillation process (Cambray-Smith 2013). Diterpenes are generally found in resins (Baser & Demirci 2007). An example is α-camphorene (Cambray-Smith 2013). Diterpenes can occur in solvent extracts.

TABLE 3-6 *Some Monoterpenes and Their Properties*

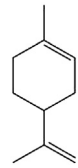
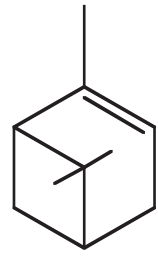
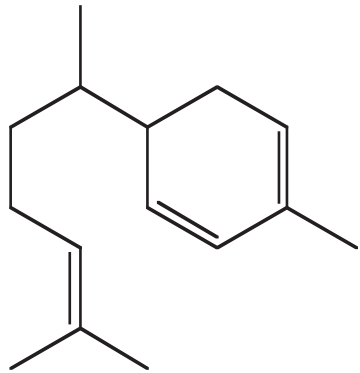
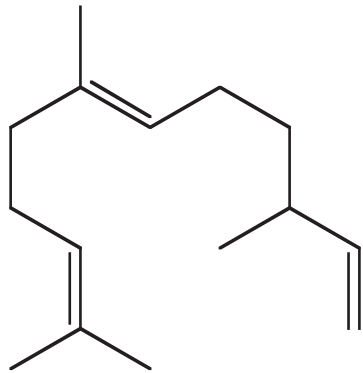
D-Limonene found in many citrus peel oils (60-90%)		Inhibit various cancer cell growths without toxicity (Rabi & Bishayee 2009) Dissolves gall stones (Sun 2007)
α-Pinene found in *Elettaria cardamom* (Cardamom)		Possible antitumoral activity (Bhattachariee & Chatterjee 2013)

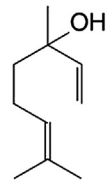
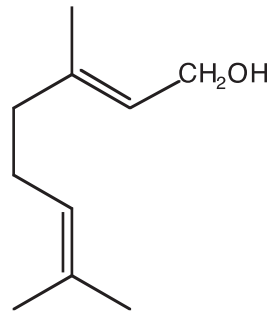
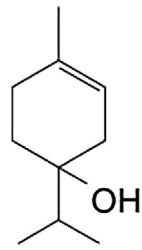
TABLE 3-7 *Some Sesquiterpenes and Their Properties*

α-Zingiberene found in *Zingiber officinalis* (ginger)		Antioxidant, increases glutathione production and reduces inflammation (Jeena et al 2013)
α-Farnesene in *Eucalyptus globulus* (blue gum eucalyptus)		Effective against cariogenic bacteria that cause tooth decay (Ishnava et al 2013)

Alcohols

Terpenic alcohols (terpenols) are found in many essential oils. Their names all end in *-ol*. Structurally, they have a hydroxyl group attached to one of their carbon atoms (Table 3-8). Monoterpenols are thought to be good antiseptics with some antibacterial, antifungal, and antiviral properties (Opaichenova & Obreshkova 2003), (Chiang et al 2005). Some alcohols, such as terpinen-4-ol, are uplifting; others like linalool are thought to be sedative (Yamamoto et al 2013). Usually essential oils with a high percentage of monoterpenols, for example, palma rosa *(Cymbopogon martini)*, are safe to use undiluted on the skin. Geraniol in *Cymbopogon martini* (palma rosa) is effective against *Escherichia coli* (Duarte et al 2007) and has antitumor and anticancer activity (Madankumur et al 2013). Terpinen-4-ol in *Melaleuca alternifolia* (tea tree) is effective against multidrug-resistant *Staphylococcus aureus* (MRSA) (Thomsen et al 2013), (Loughlin et al 2008) and also has antitumor properties (Calcabrini et al 2004). Terpinen-4-ol was also found to prevent the influenza virus from entering host cells by disturbing the normal viral membrane fusion procedure (Li et al 2013).

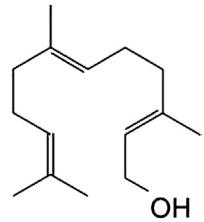
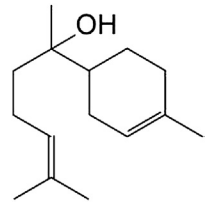
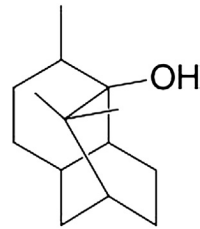
TABLE 3-8 *Some Monoterpenols and Their Properties*

Linalool in *Ocimum basilicum* (basil) Linalool in *Lavandula angustifolia* (lavender)		Effective against MRSA and resistant *Pseudomonas* (Opaichenova & Obreshkova 2003); antiviral (Chiang et al 2005) Inhaled linalool altered hypothalamic gene expression in rats under stress (Yamamoto et al 2013)
Geraniol in *Cymbopogon martini* (palma rosa)		Antitumor and anticancer activity (Madankumur et al 2013) Antimicrobial against *E. Coli* (Duarte et al 2007)
Terpinen-4-ol in *Melaleuca alternifolia* (tea tree)		Effective against MRSA (Loughlin et al 2008) Antitumor and anticancer activity (Madankumur et al 2013); inhibits growth of melanoma cells (Calcabrini et al 2004)

Sesquiterpenols

Sesquiterpenols have 15 carbon atoms and a variety of therapeutic effects (Table 3-9). Farnesol found in Australian sandalwood *(Santalum spicatum)* enhanced amphotericin B and caspofungin activity against *Candida* (Cordeiro et al 2013). It also appeared to protect lungs from the damage of cigarette smoke (Wajhul & Sarwat 2008). Patchoulol found in *Patchouli cablin* (patchouli) is effective against influenza (Kiyohara et al 2012) and also has antiinflammatory properties (Li 2011). α-Bisabolol found in *Matricaria recutita* (German chamomile) has its own antiinflammatory (Kamatou et al 2010) and antinociceptive-like action (de Miranda et al 2010). Nerolidol, found in *Melaleuca quinquenervia*, enhanced the insecticidal and ovicidal effect of 0.5% tea tree against hair nits (Di Campli et al 2012). The Amazonian Waiapi tribe treat malaria by inhaling the essential oil from the leaf of *Virola surinamensis.* Nerolidol is one of the active components of *Virola surinamensis* (Lopes et al 1999). Sclareol has shown significant cytotoxic activity against both human leukemic and breast cell lines

TABLE 3-9 *Some Sesquiterpenols and Their Properties*

Farnesol found in *Santalum spicatum* (Australian sandalwood)		Enhances amphotericin B and caspofungin activity against *Candida* (Cordeiro et al 2013); may protect lungs from cigarette smoke (Wajhul & Sarwat 2008)
α-Bisabolol found in *Matricaria recutita* (German chamomile)		Antiinflammatory (Kamatou et al 2010); possible peripheral topical analgesic (de Miranda 2010)
Patchoulol found in *patchouli cablin* (Patchouli)		Antiviral against influenza (Kiyohara et al 2012) Antiinflammatory (Li 2011)

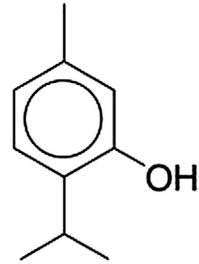
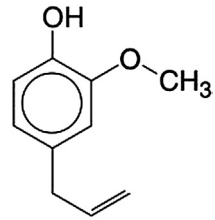
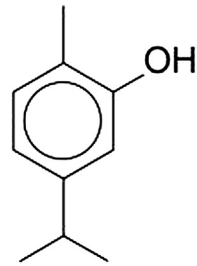
and also enhances the effect of anticancer drugs (doxorubicin, etoposide, and cisplatinum) against MDD2 breast cancer cell lines (Dimas et al 2006).

Phenolic Terpenes

A phenol is a hydroxyl group that is bonded directly to one of the six carbon atoms in a benzene ring (Table 3-10). Like alcohols, phenol names end in *-ol,* but they should not be mistaken for the much gentler alcohols. Benzene (aromatic) rings can easily be formed from aliphatic (nonbenzene) rings, but the reverse reaction rarely occurs (Guenther 1972). Phenols are widespread in nature, for example, adrenaline and tetrahydrocannabinol (the hallucinogenic ingredient in marijuana) (Cambray-Smith 2013). There are two principal phenols found in essential oils: carvacrol and thymol. Carvacrol and thymol of oregano, satureja, thyme, etc., are isomeric monoterpenic phenols.

Phenols need to be treated with care because they are irritating to the skin and mucous membrane (Tisserand & Young 2013). Most have very strong antibacterial properties, with a stimulating effect on both the nervous system and the immune system. Thymol (from *Thymus vulgaris CT thymol*) has antimicrobial, antioxidant, and antitumoral properties (Nikolić et al 2014). It is effective against *Pseudomonas* and may be useful in cystic fibrosis (Helenicy et al 2012). Eugenol, found in *Syzygium aromaticum* (clove bud) and *Ocimum sanctum* (holy basil), is

TABLE 3-10 *Some Phenols and Their Properties*

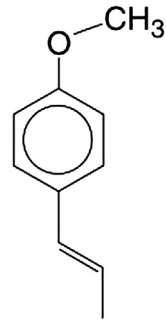
Thymol found in *Thymus vulgaris,* common thyme Thymol found in *Lippia sidoides* (pepper-rosmarin)		Antimicrobial, antioxidant, and antitumoral (Nikolić et al 2014) Effective against *Pseudomonas* and may be useful in cystic fibrosis (Helenicy et al 2012)
Eugenol found in *Syzygium aromaticum* (clove bud) Eugenol found in *Ocimum sanctum* (holy basil)		Vasorelaxant (Damiani et al 2003) Antimicrobial against *E. coli*, *S. aureus* (Walsh et al 2003) Antifungal against *Aspergillus* (Kumar et al 2010)
Carvacrol found in *Zataria multiflora* (Iranian thyme) Carvacrol found in *Origanum bilgeri* (Turkish oregano)		Effective against bacterial vaginosis (Simar et al 2008), vaginal candida (Islami et al 2004) Acaricidal against ticks (Koc et al 2013)

a vasorelaxant (Damiani et al 2003). It has antimicrobial properties, particularly against *E. coli* and *S. aureus* (Walsh et al 2003) and is also antifungal (Kumar et al 2010). Carvacrol found in *Zataria multiflora* (Iranian thyme), *Origanum vulgare* (oregano) and *Thymus vulgaris CT carvacrol* (thyme) is effective against bacterial vaginosis (Simar et al 2008) and vaginal candida (Islami et al 2004). Carvacrol is also acaricidal and effective against ticks (Koc et al 2013). Carvacrol also has anticarcinogenic effects (Baser 2008). The compound phenol (carbolic acid) is a disinfectant derived from coal tar and not found in essential oils (Tisserand & Young 2013).

Ethers (Phenolic) or Phenylpropanoids

Ethers found in essential oils are phenylmethyl ethers or phenolic ethers or, more scientifically, alkenylbenzenes (Cambray-Smith 2013). Ethers occur when a methyl or ethyl group is attached to a benzene ring via an oxygen molecule (Table 3-11). Examples (in alphabetical order) are anethole, apiol, eugenol, estragole, myristicin, and safrole (Tisserand & Young 2013). Estragole is sometimes called

TABLE 3-11 *An Ether and Its Properties*

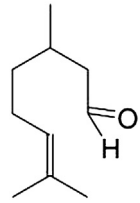
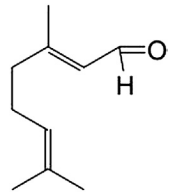
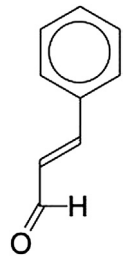
trans-Anethole in *Foeniculum vulgare* (fennel)		Estrogenic activity (Mazaheri et al 2013)

methyl-chavicol (Tisserand & Young 2013). Ethers are not widely distributed but are found in some common essential oils, for example: anise, basil, cinnamon leaf, and fennel. Ethers are less aggressive on the skin than phenols. However, some ethers like myristicin have hallucinogenic properties when taken orally (Ehrenpreis et al 2014). Myristicin (found in nutmeg) has a similar structure to MMDA a precursor to MDMA (ecstasy). *trans*-Anethole in *Foeniculum vulgare* (fennel) has estrogenic activity (Mazaheri et al 2013) as does anethole from several *Pimpinella* species (Baser et al 2007).

Aldehydes

An aldehyde is a partially oxidized primary alcohol (Tisserand & Young 2013). Structurally, it has an oxygen atom double bonded to a carbon atom at the end of a carbon chain (Table 3-12). The fourth bond is always a hydrogen atom (Bowles 2000). Aldehydes usually end in *-al* and often have sedative, calming effects, as well as being important to the aroma of the plant. Examples include citral in lemon balm *(Melissa officinalis)*, β-citronellal in lemongrass *(Cymbopogon citratus)*, geranial in lemon eucalyptus *(Eucalyptus citriodora)*, and neral in lemon verbena *(Aloysia triphylla)*. Geranial and neral are isomers. This means they have the same molecular make-up but the carboxyl molecule is in a different place. Geranial (α-citral) and neral (β-citral) occur naturally as a mixture of the two isomers in citral (Tisserand & Young 2013). Citral has strong antiseptic and antibacterial properties and is effective against MRSA (Saddiq & Khayyat 2010). It also has antiinflammatory properties and enhances the effect of naproxen (Ortiz et al 2010). Citronellal has antifungal properties (Mimica-Dukic et al 2004) especially against *Candida* (Zore et al 2011). In some interesting new research, citronellal may increase olfactory sensitivity in patients with Parkinson-impaired olfaction (Haehner et al 2013). Cinnamaldehyde found in *Cinnamomum zeylanicum* (cinnamon) has antimicrobial and antifungal properties (Unlu et al 2010). It is a potential antidiabetic agent (Subash et al 2007) and has been found to decrease muscle soreness after exercise (Mashhadi et al 2013). Isolated aldehydes can be

TABLE 3-12 *Some Aldehydes and Their Properties*

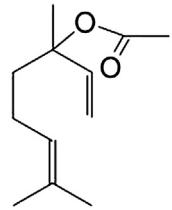
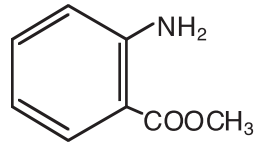
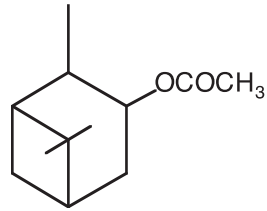
Citronellal found in *Eucalyptus citriodora* Citronellal found in *Melissa officinalis* (melissa)		Antifungal especially *Candida* (Zore et al 2011) Antifungal (Mimica-Dukic et al 2004) May increase olfactory sensitivity in patients with Parkinson-impaired olfaction (Haehner et al 2013)
Neral & geranial (citral) in *Cymbopogon citratus* (lemongrass)		Antibacterial against MRSA (Saddiq & Khayyat 2010) Enhances antiinflammatory effect of naproxen (Ortiz et al 2010)
Cinnamaldehyde in *Cinnamomum zeylanticum* (cinnamon)		Antimicrobial, antifungal (Unlu et al 2010) Potential antidiabetic agent (Subash et al 2007) Decreases muscle soreness after exercise (Mashhadi et al 2013)

dermal irritants, but when the whole essential oil is used the irritating effect of aldehydes appears to be ameliorated by the presence of terpenes, such as limonene or α-pinene (Opdyke & Letizia 1982).

Esters

Esters are a combination of an acid and an alcohol and take their name from the acid and alcohol (Table 3-13). Hence, acetic acid and linalool produce linalyl acetate. Acids do not occur in essential oils but can be found in floral waters. Esters end in *–ate* and have antispasmodic (Ou et al 2012) and calming properties (Igarashi 2013). Some are also antifungal. They often smell very fruity. Examples include linalyl acetate in lavender *(Lavandula angustifolia)*, clary sage *(Salvia sclarea)* and bergamot (*Citrus aurantium* subsp. *bergamia*), and geranyl acetate in sweet marjoram *(Origanum majorana)*. An essential oil with a very high ester content (85%) is Roman chamomile *(Chamaemelum/Anthemis nobilis)*. Esters are usually safe in high amounts except for methyl salicylate. Methyl salicylate occurs at approximately 98% in sweet birch (*Betula lenta*) and wintergreen (*Gaultheria procumbens*) essential oils. Methyl anthranilate found in mandarin (*Citrus reticulata*) has antiandrogenic potential that could be useful in prostate cancer (Roell et al 2011). Bornyl

TABLE 3-13 *Some Esters and Their Properties*

Linalyl acetate found in *Lavandula angustifolia* (lavender)		Reduces stress in pregnant women (Igarashi 2013) Pain relief in primary dysmenorrhea (Ou et al 2012) Reduce serum cortisol in healthy men (Shiina et al 2008)
Methyl anthranilate found in *Citrus reticulata* (mandarin)		Antiandrogenic potential for prostate cancer (Roell et al 2011)
Bornyl acetate found in *Picea mariana* (black spruce)		Possible preventive agent for lung inflammatory diseases (Chen et al 2014)

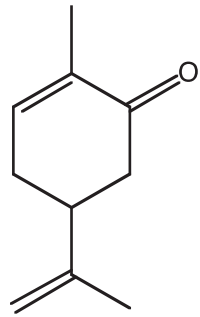
acetate found in *Picea mariana* (black spruce) is a possible preventive agent for lung inflammatory diseases (Chen et al 2014). Linalyl acetate found in lavender (*Lavandula angustifolia*) reduced serum cortisol in healthy men (Shiina et al 2008).

Ketones

Ketones contain the carbonyl group (–C=O) and so are related to the aldehydes. Ketones and aldehydes are both found in biological molecules, e.g., progesterone and testosterone (Cambray-Smith 2013). A ketone is derived from an alcohol by oxygenation and has an oxygen atom double bonded to a carbon atom that is also bonded to two other carbon atoms (Table 3-14) (Bowles 2000). Ketones end in *-one* with a single exception: camphor. This substance has no relation to the plant camphor. Some ketones can produce adverse effects when taken orally and, because ketones are resistant to metabolism, this adverse effect can build up in the liver. The most cited toxic ketone is D-pulegone (found in pennyroyal), which caused the death of a 23-year-old woman in 1897 after she drank 15 mL of undiluted essential oil (Allen 1897). That is a large amount to swallow. A child who developed hepatic malfunction and severe epileptic encephalopathy after swallowing a large amount of unknown essential oil tested positive for pulegone (Bakerink et al 1996).

Examples of essential oils that contain large amounts of ketones (in alphabetical order) are: caraway, frankincense, hyssop, peppermint, rosemary, sage, and spearmint (Cambray-Smith 20130. Clearly caution should be used when these

TABLE 3-14 *A Ketone and Its Properties*

L-Carvone found in *Mentha* × *spicata* (spearmint)		Possible chemopreventive agent against colon cancer (Vinothkumar et al 2013)

are ingested. Ketones that are beneficial to the skin include jasmone in jasmine *(Jasminum officinale)* and isomenthone in geranium *(Pelargonium graveolens)*. Other useful ketones are D-carvone in spearmint *(Mentha × spicata)*, fenchone in fennel (*Foeniculum vulgare* var. *dulce*) and verbenone in rosemary *(Rosmarinus officinalis)*. D-Carvone is a possible chemopreventive agent against colon cancer (Vinothkumar et al 2013). Carvone occurs in two mirror images or enantiomers: *R*(–)-carvone (or L(-)carvone) smells like spearmint. Its mirror image, *S*-(+)-carvone (or D-carvone), smells like caraway.

Two unusual ketones (italidione and beta-diketone) are found only in "everlasting" (sometimes called "immortelle")—*Helichrysum italicum* (Stewart 2005). A diketone contains two ketone groups. Both italidione and beta-diketone contribute to the unusual fragrance of *Helichrysum* and its remarkable antihematoma properties. I have used *Helichrysum* occasionally undiluted on the skin for bruises and contusions with excellent results, but I could find no published research, which is rather surprising.

Oxides

In chemical terminology, an oxide is called an ether or a peroxide. However, using the term *ether* might be confusing because there is group of phenolic ethers in aromatherapy that have different properties. The use of the term *oxide* in aromatherapy is a little more general because the carbons are not neighbors. (Oxides in organic chemistry typically involve an oxygen bridge between two neighboring carbon atoms.) In aromatherapy, an 'oxide' has an oxygen atom in a chain of carbons, that forms a non aromatic ring (Table 3-15). The most common oxide is cineole—a strong expectorant. Both 1,4-cineole and 1,8-cineole occur in essential oils (Tisserand & Young 2014). 1,8 cineole is sometimes called eucalyptol and is found in blue gum *(Eucalyptus globulus)*, rosemary *(Rosmarinus officinalis CT cineole)*, and bay laurel *(Laurus nobilis)*. Research indicates that 1,8-cineole, found in *Eucalyptus globulus* (blue gum) is a possible antiinflammatory agent for neurodegenerative disease (Khan et al 2014). Other oxides are ascaridole found

TABLE 3-15 *An Oxide and Its Properties*

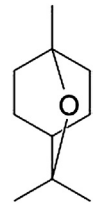
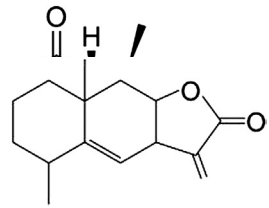
1,8-Cineole found in *Eucalyptus globulus* (blue gum)		Possible antiinflammatory agent in neurodegenerative disease (Khan et al 2014)

TABLE 3-16 *Lactones and Their Properties*

Nepetalactone found in *Nepeta parnassica* (giant catnip) Alantolactone found in *Inula helenium* root (elecampane)		Mosquito repellant (Gkinis et al 2014) Antimicrobial against *Staphylococcus aureus* (Stojanović-Radić et al 2012) Anticancer activity in some cancer lines (Khan et al 2013)

in wormseed (*Chenopodium ambrosioides* var. *anthelminticum*) and rose oxide found in both geranium *(Pelargonium graveolens)* and rose *(Rosa damascena)*. Ascaridole shows interesting antitumor activity in sarcoma cells (Bezerra 2009).

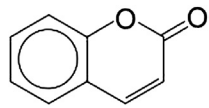
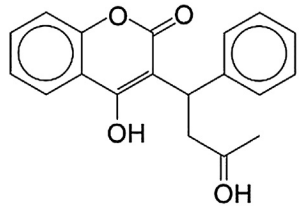
Lactones

Lactones are mainly found in expressed oils and some absolutes like jasmine (Clarke 2002). They are cyclic esters derived from lactic acid (Baser & Demirci 2007) and have an oxygen atom double bonded to a carbon atom. The carbon atom is attached to another oxygen atom that is part of a closed ring (Table 3-16). Lactones tend to end in *-lactone* or *-ine*. The percentage of lactones present may be low, but they are traditionally thought to play an important role as mucolytics (Clarke 2002; Schnaubelt 2011; Rhind 2012). Alantolactone is present in elecampane *(Inula helenium)* and is effective against *Staphylococcus aureus* (Stojanović-Radić et al 2012). It also has anticancer activity in some cancer lines (Khan et al 2013). However, elecampane is linked to skin sensitization, as are many lactones (Tisserand & Young 2013). Nepetalactone, found in catnip *(Nepeta cataria)*, is a mosquito repellant (Gkinis et al 2014). It is also feline attractant.

Coumarins

Coumarins are a subgroup of lactones. They have an oxygen atom double bonded to a carbon atom. That carbon atom is attached to another oxygen (that is part of a closed ring) and they also have a benzene ring attached (Table 3-17). Coumarins usually end in *-one* (pronounced *own*), as in umbelliferone, or

TABLE 3-17 *Structural Similarities between Coumarin and Warfarin*

Coumarin		May have potential use in Alzheimer's (Huang et al 2013)
Warfarin		Anticoagulant (Cavallari et al 2011)

with *-in*, as in coumarin. Coumarins are present in very small amounts in essential oils. There is sometimes confusion between the functional group, coumarin, and the chemical dicoumarol (Mills 1991). Dicoumarol is created naturally by the breakdown of the sweet clover plant. Synthetic dicoumarol is the basis of the anticoagulant drug warfarin (Cavallari et al 2011). The chemical drawing (see Figure 3-18) shows a coumarin structure within warfarin. Some coumarins may reduce clotting time if taken internally. Ramesh & Pugalendi (2007) found that umbelliferone normalized prothrombin, clotting and bleeding time in diabetic rats. Previously, they had found umbelliferone to be antihyperglycemic (Ramesh et al 2006) and antidiabetic (Ramesh et al 2005). Coumarins may have a future role to play in Alzheimer's disease as coumarins are important acetylcholinesterase (AChE) inhibitors. Chinese research found a coumarin derivative was a 100 times better than the conventional drug donepezil (Huang et al 2013).

Furanocoumarins

Furanocoumarins (FCs) are present (<2%) in citrus-peel oils and a few other essential oils, for example: angelica *(Angelica archangelica)* root and rue *(Ruta graveolens)*. FCs react in the presence of ultraviolet light to produce a phototoxic effect, resulting in burns or erythema. Even small dilutions (0.03%) applied to the skin can result in phototoxicity (Tisserand & Young 2013). A phototoxic effect was also produced with a 2.4% concentration on pale skin and 15% concentration on dark brown or black skin. Sometimes, the pigmentation can remain for life. Extensive burns can also result from oral ingestion of FCs in combination of UV exposure (Tisserand & Young 2013). Common FCs include bergapten (found in expressed bergamot, bitter orange, grapefruit, lemon, lime (and in steam distilled angelica root), and bergamottin (found in expressed bergamot, grapefruit, lemon and lime). Bergamottin is antitumoral in human fibrosarcoma HT-1080 cells (Hwang et al 2012).

APART FROM CHEMISTRY

Some people believe there is more to an essential oil than the sum of its parts: that there is a synergy of all those parts working together. Some people believe there is an energy or vibration to an essential oil and this plays a major role in healing. Some people think essential oils have yin- and yang-like qualities. Others think the effect of essential oils is purely chemical so by isolating the part, the effect will be grasped. Whatever your view, I hope this short overview of chemistry for aromatherapists, has been useful. There are some excellent chemistry chapters, books, and courses relevant to aromatherapy available for those wanting to delve further.

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EXTRACTION, BIOSYNTHESIS, AND ANALYSIS

"All we have yet discovered is but a trifle in comparison with what still lies hid in the great treasury of nature." Anton von Leeuwenhoek. 1679.

EXTRACTION

There are several ways of extracting volatile components from plants. Some methods produce classic essential oils, others produce extracts. See Figure 3-2 and Table 3-18 for comparisons of the extraction procedures used for aromatic extracts and essential oils. Traditionally aromatherapy has specified only the use of essential oils (from distillation or expression), but some extracts are now becoming acceptable.

Essential oils are either distilled or expressed (Arctander 1960). Distillation can mean water distillation, water-and-steam distillation, steam distillation, or steam-and-vacuum distillation (Arctander 1960). To give some idea of yield, 200 kg of *Lavandula angustifolia* flowers will produce 1 kg of essential oil. However, between 2 and 5 metric tons of rose petals are needed to produce the same amount of rose oil.

Distillation (Steam)

The design of the distillation plants varies from region to region. Traditional and sometimes rather simple methods are still being used in some developing countries. Industrialized nations tend to use more technologically advanced equipment that

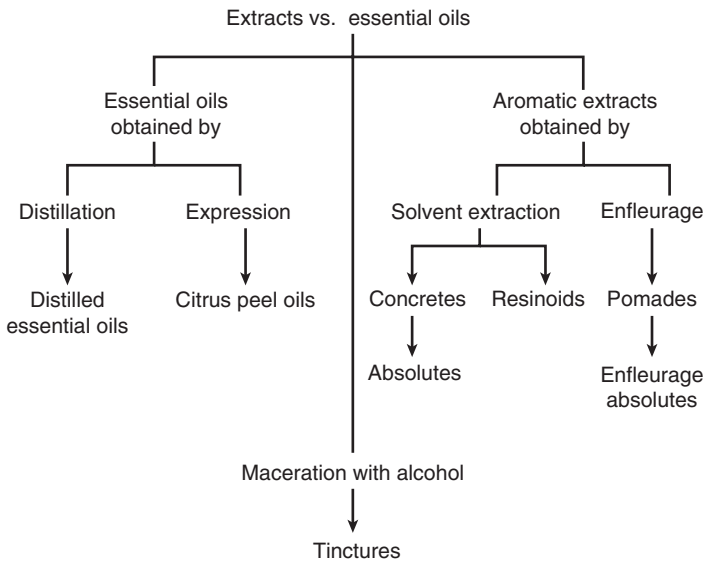

FIGURE 3-2 | Essential oils versus extracts. (Adapted from Williams D. Lecture Notes on Essential Oils. With kind permission of Eve Taylor, London. 1989.)

is computer-controlled with software that can monitor the product throughout the distillation process. Nevertheless, excellent quality oils can be obtained even with a basic distillation apparatus. The aromatic plant material is placed on a grid through which steam passes, usually at a temperature not above 100° C (Bowles 2000). See Figure 3-3 for more details. The water boils at temperatures between 88° C and 100° C depending on the altitude at the distillation site.

High-pressure steam is the fastest way of distilling essential oils with high-boiling constituents like vetiver, sandalwood, and clove. The steam loosens the volatile non-polar constituents of the plant and they pass, with the steam, into a condenser that cools the mixture. Steam also alters some of the components within an essential oil, for example, turning matricin to chamazulene. Some of the polar components from the plant dissolve in the water, producing floral water. The mixture of floral water and essential oil is cooled and becomes liquid. As essential oils and floral water do not mix, they quickly separate—the majority of essential oils float above the floral water, but some sink, depending on their specific gravity.

The degree of heat and the amount of time are vital parts of the distillation process as some components of plants are very sensitive to heat and others take much longer to distill (Guenther 1974). The distillation process for *Lavandula angustifolia* is approximately one hour, but it is considerably longer for sandalwood or vetiver. The length of the distillation process will affect the chemical composition of the essential oil (Guenther 1976). Steam distillation is suitable for the highly volatile components such as the monoterpenes, but heavier molecules like di or sesquiterpenes take longer. Some floral waters (hydrolats) can also be used therapeutically. Portable distillation equipment is simple to make and can

TABLE 3-18 *Advantages and Disadvantages of Various Extraction Processes*

Extraction Process	Advantages	Disadvantages
Distillation	Economical	Changing constituents
	Large quantities can be processed	Depending on time/temp
	Little labor needed	
Expression	No heat required	Some flavoring left
	Simple apparatus	Only citrus peel oils
		Oxidize quickly
Enfleurage	Low temperature needed	Time consuming
		Labor intensive
		Expensive
CO_2 extraction	Constant product	Expensive
	No heat used	Different chemistry to essential oil
Solvent extraction	Constant product	Solvent residues
		Different chemistry to essential oil

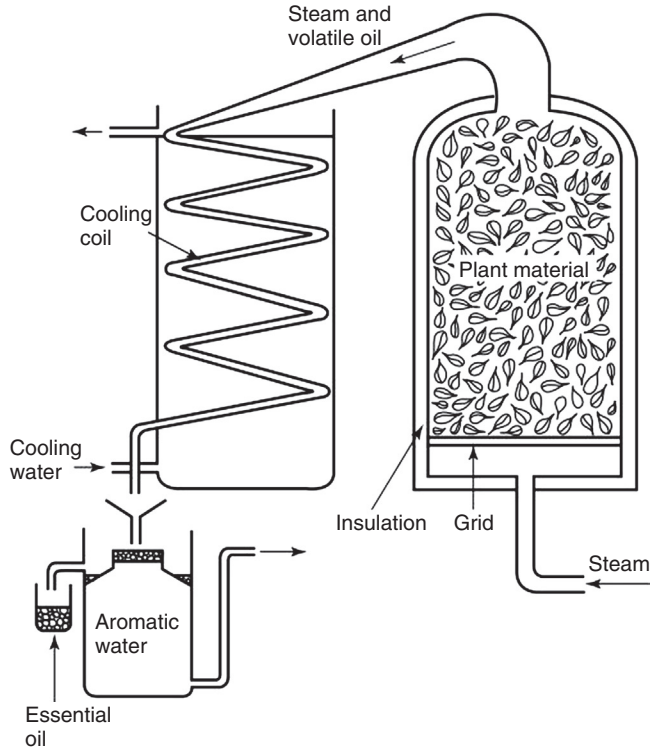

FIGURE 3-3 | Steam distillation. (Reproduced from Price S. Practical Aromatherapy, with the kind permission of Harper Collins, London. 1983.)

be used for small quantities of plants when essential oils must be distilled on site (Alkaire & Simon 1992).

Variations of Steam Distillation

1) **Cohobation:** The water used in the distillation process is reused (Guenther 1974).
2) **Fractional distillation:** The essential oil is distilled at specific temperatures for specific lengths of time to collect different factions (or functional groups) within the essential oil. For example, peppermint contains menthol (a monoterpene) that is less volatile than other peppermint monoterpenes (e.g., α-pinene, β-pinene, sabinene and limonene) and other low boiling hydrocarbons. Monoterpenes evaporate at different temperatures, but many of the peppermint monoterpenes evaporate below 150° to 185° C, so this temperature can be used to "get rid" of lower boiling monoterpenes in order to obtain a high-quality peppermint flavor (Gafner 2014). Nowadays, fractional distillation is often done at reduced pressure in order to lower the boiling temperature.
3) **Rectification:** This aims to separate the volatile and nonvolatile components of an essential oil. If an essential oil contains impurities, it can be purified by

redistillation. This process is called rectification. Sometimes peppermint and caraway seed oils can take on an unpleasant odor if they have been in contact with the wall of a hot still. This aroma can be removed through rectification (Guenther 1974).

4) **Steam-plus-vacuum distillation:** This method uses steam with partial vacuum (Arctander 1960). The pressure used is typically 100 to 200 mm Hg. The advantage of this method is speed. The disadvantage is a fast method of cooling is required.

Expression

In expression, the production of essential oils (by mechanically pressing the product) involves mainly the peel of citrus plants, like oranges, lemons, or grapefruit. The peel of the fruit is racked or abraded by mechanical scrapers, and the essence collected by centrifugal separation. Sometimes the whole fruit is crushed before the essential oil is separated from the juice and peel. Expressed oils will naturally contain a proportion of waxes, and citrus oils may include other components such as bergapten, a coumarin that can cause phototoxicity (Tisserand & Young 2013).

Methods for Producing Aromatic Extracts (not essential oils)

There are other methods of extraction that produce compounds called *absolutes*. These are mainly used by the fragrance and cosmetics industry. Rose absolute is yellow, viscous, and sticky. Rose essential oil is clear and solid at room temperature. The essential oil is ten times the price of the absolute. Residual solvents in extracts can produce adverse reactions.

Enfleurage

This method was used on fragile blossoms like jasmine and tuberose. It is rarely used today as it is very labor intensive. I watched this process in Grasse, France. Animal fat is pounded until soft, then glass plates are coated with the fat. Each fat-covered glass plate is called a *chassis*. Fresh blossoms are placed close together on the *chassis* and left until the fat becomes saturated with essential oil. The chassis are constantly being replenished with fresh blossoms, and the old blossoms discarded. This process can take days or even weeks. The resulting oil/fat mixture is called a *pomade*. The *pomade* is washed with alcohol to remove the fat. The remaining extract is called an absolute. However, 99% of jasmine and tuberose extract is now produced by solvent extraction.

Supercritical Fluid Extraction

Supercritical fluid extraction (SFE) with carbon dioxide has been available since the 1980s. When the temperature of CO_2 is maintained at approximately 31° C, under pressure, it acts like a fluid and dissolves the CO_2-soluble constituents of an herb. The interest in SFE has increased in recent years because of legal limitations of solvent residues and solvents (Vagi et al 2005). However, the chemistry of the resulting extract is different to a steam-distilled essential oil because (a) less heat is used and (b)

some different components are absorbed by CO_2 extraction (Guan Hou et al 2007). For example, steam-distilled German chamomile *(Matricaria recutita)* essential oil is dark blue because heat converts matricine (found in the plant) to chamazulene—a sesquiterpene. However, matricine is present in the SFE extract. SFE extracts are not available for every plant used in aromatherapy but there is no reason not to use them, provided the chemistry is known and the components are relevant to the clinical goal being targeted. Volatile oils can also be extracted with other solvents. The use of benzene has declined but it is still used (Tisserand & Young 2013). Hexane is commonly used [cyclohexane and *n*-hexane (Tisserand & Young 2013)]. Such extracts are called "volatile oils" to differentiate them from essential oils (Coelho et al 2012).

Resinoids

Resinoids are obtained from resins (amber and mastic), balsams (benzoin) or gum-like exudates (frankincense and myrrh). Frequently resinoids are extracted by solvents. However, frankincense and myrrh can also be obtained by steam distillation or SFE. Resins are soluble in alcohol but not in water. Gums are soluble in water but not in alcohol.

Notes (Aroma Intensities)

The aromas of essential oils have variable intensities, and these may last for different periods of time. The perfume industry calls these properties "notes" (Teixeiry et al 2013). Poucher developed a classification method based on a perfume's evaporation rate (1 to 100) that is still used today (Poucher 1993). Scents that evaporate quickly (1 to 15) are called top notes, for example, mandarin (2) and nutmeg (11). Middle notes (16 to 69) include marjoram (18), ylang ylang (24), and rose (43). Base notes last the longest (70 to 100), for example, angelica (94). Perfumes with the highest ratings last the longest and evaporate the slowest, for example, frankincense, patchouli, sandalwood, and vetiver). A top note might last for a few hours, a middle note for a couple of days, and a base note may last for several weeks.

Oxidation

The odor of an essential oil deteriorates as a result of oxidation. When an essential oil has contact with air, certain components within it react with the oxygen. For example, alcohols can react with oxygen to become aldehydes (Bowles 2000).The rate of oxidation is dependent on the exposure to oxygen and the reactivity of each individual component of the essential oil. Heat and sunlight can speed up oxidation. The oxidization of an essential oil will affect its chemistry and thus its therapeutic potential.

TERPENE BIOSYNTHESIS: HOW AND WHY PLANTS MAKE ESSENTIAL OILS

Biosynthesis is the production of all plant secondary metabolites: alkaloids, bitters, glycosides, gums, saponins, steroids, and essential oil components. Only 1% of flowering plants produce an essential oil in any significant amount, and for a

long time essential oils were thought to be unimportant to the plant. The number of identified volatile chemicals synthesized by various plants exceeds 1000 and is likely to grow as more plants are examined (Pichersky et al 2006). The largest class of essential oil components is derived from isoprenoid pathways. The two basic pathways are called the malonic acid pathway and the shikimic acid pathway (Taiz & Zeiger 2014). Terpenoids are formed by malonic pathways and most phenylpropanoids and benzenoids derive from the shikimic acid pathway (Yang et al 2009).

Mevalonic Acid Pathway

Aromatic plants contain enzymes called terpene synthases (TPSs). These enzymes: dimethylallyl pyrophosphate (DMAPP), geranyl pyrophosphate (GPP), farnesyl pyrophosphate (FPP) and geranyl pyrophosphate (GPP), act as catalysts in the formation of mono-, sesqui-, and diterpene essential oil components (Pichersky et al 2006). The plant first converts mevalonic acid to a 5-carbon structure called isoprene. Isoprene, known as methylbuta-1,3-diene to chemists, is a branched chain hydrocarbon containing five carbon atoms and two double bonds. Isoprene is then converted with GPP—an enzyme catalyst—to a 10-carbon molecule like a terpene (Cambray-Smith 2013). This process can continue with another enzyme catalyst, FPP, to produce a 15-carbon molecule like a sesquiterpene. Once the plant has formed GPP, the substance can be converted into alcohols or aldehydes as well as terpenes.

Shikimic Acid Pathway

Shikimic acid (3,4,5-trihydroxy-1-cyclohexene-1-carboxylic acid), another enzyme, is an important catalyst in this second pathway of biosynthesis. This enzyme is proceeded by another enzyme, phenylalanine ammonia lyase (PAL). The pathway is complex, but ultimately leads to the second largest class of essential oil components that contain an aromatic ring, such as phenols (Mann 2001a). Please see Figure 3-4.

Storage of Essential Oils in Plants

Essential oils are stored in specific parts of a plant (Table 3-19). For example, rose essential oil is found in the petals of the flowers, not the roots, leaves, or stem. However, sometimes an essential oil is found in different parts of the same plant, as in the case of angelica *(Angelica archangelica)* root and angelica seed, when the chemistry of each essential oil is different. The essential oil from the root of angelica can cause a skin reaction when ultraviolet light is used on the skin within 24 hours of applying topically, but the essential oil from the seed does not.

Secretory and Storage Structures of Essential Oils in Plants

Essential oils are stored in special secretory structures (Table 3-20). These can be on the surface of the plant or within the plant tissue, and are found in many kinds of plant: perennial, annual, biennial, evergreen and deciduous (Svoboda & Svoboda 2001). Secretory structures vary and include oils cells, secretory ducts or cavities and glandular hairs (Baser & Demirci 2007). Often the whole

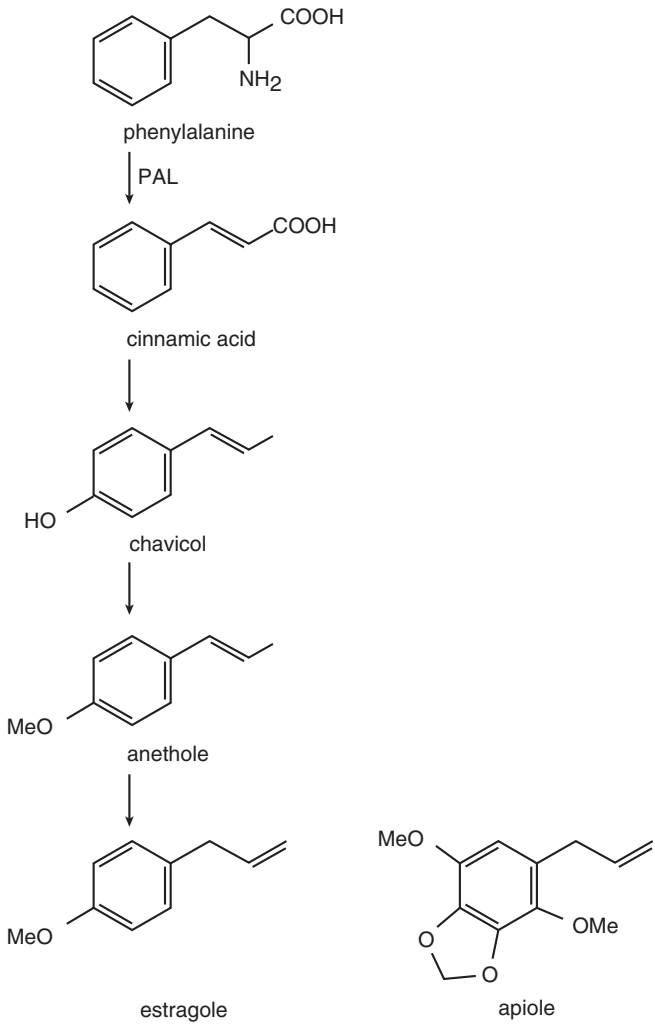

FIGURE 3-4 | Biosynthesis. (Adapted from Waterman P. 1993. The Chemistry of volatile oils. In Hay R, Waterman P (eds.), Volatile Oil Crops: Their Biology, Biochemistry and Production. Essex, UK: Longman Scientific and Technical, 47-61.)

family, or genus, of a plant will have a similar secretory system. This can be useful in plant identification.

Single, secretion-containing cells are common in many aromatic plants like the leaves of lemongrass, rhizome of ginger, seed coat of cardamom, fruit wall of black pepper, bark of cinnamon, and root of valerian. Secretory ducts are elongated cavities found in plants like coriander, cumin, angelica, dill, anise, and fennel (all members of the Umbelliferae family). Secretory cavities are prevalent in the fruit and leaves of lemon, orange and bergamot in the Citrus

TABLE 3-19 *Parts of Plant Where Essential Oils Are Stored*

Plant	Location Where Oil Is Stored
Angelica	Root, seed
Black pepper	Seed
Cinnamon	Bark, leaf
Clove	Leaf, bud
Eucalyptus	Leaf
Juniper	Berry
Mandarin	Fruit peel
Myrrh	Resin
Pine	Needles
Rose	Flower
Rosemary	Whole herb
Sandalwood	Wood

TABLE 3-20 *Secretory Parts of Plants*

Part	Plant
Single secretion cells	Ginger, black pepper, cardamom, valerian, lemongrass
Secretory cavities	Citrus fruits, clove, myrrh, frankincense
Secretory ducts	Tarragon, angelica, aniseed, pine
Secretory hairs	Many plants in the Lamiaceae and Geraniaceae families

family. They are also found in the bark of myrrh, frankincense and in clove buds. Glandular hairs are found on leaves and stems of plants such as basil, lavender, and marjoram in the Lamiaceae family. Epidermal cells diffuse essential oil directly through the cytoplasm and cell wall to the outside, and the amount of essential oil diffused is very low. Examples of aromatics with epidermal cells are rose and jasmine.

The function of essential oils in plants is not fully understood. Some may protect a plant from being eaten by plant-eating animals or insects by repelling them (Pichersky & Gershenzon 2002). For example, wild tobacco *(Nicotiania sylvestris)* can increase its production of nicotine by three or four times when under attack, and the bitter taste deters predators (Mann 2001b). Sometimes an essential oil component can reduce the growth, or maturation, of an insect that is eating the plant. Grasshoppers eating *Cyperus iria* become sterile. Tenulin (a sesquiterpene lactone) in *Helenium amarum* disrupts the growth and development of insect larvae (Mann 2001b). Many animals find the aroma (and taste) of essential oil components repellent and will not eat aromatic plants. Voles (a small rodent common in Europe) will not eat pine needles. However, there are exceptions. Australian possums and

kangaroos are two mammals that have adapted to live off a diet of Eucalyptus leaves. I saw this personally when I visited Australia in 2013.

Certain plants exude aromas that deter insects. The Lamiaceae family has two well-known plants, pennyroyal and peppermint, that deter insects. The mosquito that carries yellow fever is repelled by mugwort *(Artemisia vulgaris)*. Clinical studies found that mosquitoes carrying malaria or Dengue fever are repelled by *Artemisia annua* (Sharma et al 2014).

Other essential oils are thought to increase pollination by attracting insects. Many chemical compounds found in the odor glands of insects are also found in flower fragrances. Usually it is a mixture of compounds that generates the aroma the insect is seeking. Each part of the fragrant area of the plant may present a different volatile profile. The rose, for example, produces different aromas in its petals than in the sepals and stamens. Odor is thought to be more important to a pollinating insect than color. This is obvious with night-flying creatures as some flowers are pollinated by bats or moths. Insects can discern a scent at 1/100 the level compared with a human. Floral fragrances such as monoterpenes are important insect attractants. Some plants, such as *Datura innoxia*, produce a narcotic, so the hawkmoth becomes addicted and returns regularly for "fixes" (Mann 2001a). Insects live in a world where actions are triggered by smell, rather than noise or light.

Plants may produce secondary metabolites to protect them from bacteria, viruses and fungi. Plants respond to attack by producing stress metabolites called phytoalexins. Some synthetically produced phytoalexins are now used to protect crops from parasites (Holscher et al 2014).

Allelopathy

Allelopathy is the ability of a plant to prevent other plants from growing too close to it. Bracken and ferns leach germinating inhibitors (usually phenols) into the ground to deter other species from germinating or growing too close. Aromatic plants can use essential oils such as camphor to protect the land around them from other plants. Terpenes are the largest group of chemical components found in aromatic plants, and many terpenes can inhibit the respiration of other plants (Mann 2001b). The sage bush *(Salvia leucophylla),* which is prolific in the near-desert terrain of southern California, contains chemical compounds 1,8-cineole and camphor that deter other plants from germinating.

One of the other ideas suggested or why plants make essential oils is their antitranspirant activity. Essential oils aid survival in difficult climatic conditions when a haze of volatile oils may influence stomatal closure, and thus prevents excess water loss from the leaves.

Quality of Essential Oils

There are many factors that can affect the quality of an essential oil (Box 3-1). The chemical make-up of all living plants depends on climate and environmental conditions (such as rainfall, sunlight, soil acidity, altitude and pollution) (Guenther 1972). The chemistry of the same species of rose grown in Bulgaria will be subtly

BOX 3-1 *Factors Affecting Quality of Essential Oil*

Age of plant
Altitude
Climate
Genetics
Geography
Length of time essential oil is distilled
Number of times essential oil is distilled
Soil type
Temperature at which essential oil is distilled
Time of harvest (including both time of year and time of day)
Use of fertilizers and pesticides

different from the same one grown in England. Similarly, *Lavandula angustifolia* grown high in the mountains will contain more esters, which are thought to have a greater antispasmodic effect, than *Lavandula angustifolia* grown closer to sea level. If *Lavandula angustifolia* is distilled at a high altitude this will also increase the amount of esters. *Lavandula angustifolia* essential oil with a higher percentage of esters will have an aroma that is softer and fruitier. There are so many variables that the simplest way to be sure of the composition of the essential oil is to use modern analytical methods as well as the nose.

Analysis Tests for Purity in Essential Oils

There are several methods that are used to analyze the composition of an essential oil: the most frequently used is gas chromatography (GC). Other important analytical methods include high-performance liquid chromatography (HPLC) and nuclear magnetic resonance (NMR) (Tisserand & Young 2013).

Gas Chromatography

GC is a technique to separate the individual components in the essential oil (e.g., α-pinene, β-myrcene and linalyl acetate). The instrument is linked to a detector, most often a flame ionization detector (FID) or a mass spectrometer (MS). The individual constituents are shown in a computerized printout as a succession of peaks, and the peak size can be correlated to the amount of the constituent in the oil. The lighter molecules will show up first. The MS detector can be used to identify the peaks based on a comparison of the mass spectrum with data from a library. This is particularly useful for the detection and identification of pesticides. Although using a GC/MS will allow identifying and quantifying most of the chemical components, it may not always identify synthetic chemicals that have been added to extend, or alter the essential oil. Two-dimensional gas chromatographs (GC × GC) can show which way molecules rotate (Tisserand & Young 2013). This can help detect synthetic additives.

HPLC

HPLC is another separation technique, which can be used to analyze a much wider range of components, including nonvolatile molecules which cannot be analyzed by GC. HPLC is most often connected to an ultraviolet/visible (UV/Vis) detector, but MS detectors have become more and more popular due to the additional information that can be obtained.

NMR

The NMR is a high-end technique that is mainly used to determine the structure of pure compounds, but can also be used to get a view of the totality of the essential oil (fingerprint). Comparing such NMR fingerprints to fingerprints of authentic essential oils by statistical means can be a good way to detect adulteration of essential oils.

Optical Rotation

Molecules within essential oils have the ability to rotate a plane of polarized light. Molecules that rotate counterclockwise are called levorotatory, or L for short. Those that rotate clockwise are called dextrorotatory, or D. This ability is indicated in the name of the molecule, for example, D-limonene. Almost all essential oils show optical activity. Optical rotation can reveal synthetic compounds that alter the optical rotation. Synthetic menthol rotates in a different way to menthol from the mint plant (Stewart 2005).

Refractive Index

When light passes through a liquid it is refracted. This refraction can be measured and is consistent for a given essential oil. In scientific terms, it is the ratio of the speed of light of a given frequency in a vacuum to the speed of light in a medium of some kind, at a specified temperature. It is important that the test be carried out at the same temperature as the reference (the standard).

Infrared Spectroscopy

When infrared light is passed through an essential oil it produces a spectrum that is like the fingerprint of the essential oil. Similar to NMR, a comparison of the fingerprint to authentic materials will help to detect adulteration of the oil.

The Nose (Organoleptic Evaluation)

This is an underestimated but important part of analysis. When you first start you may find it hard to notice differences between synthetic and real essential oils, or pure and adulterated ones. However, with patience the nose does learn. Never smell directly from the bottle. Put one or two drops on to a special smell strip (made from paper a little like blotting paper). Recap the bottle. Hold the smell strip approximately 6 inches in front of your face. The sense of smell may be different from one nostril to the other as the aroma reaches different parts in the brain, so move the

strip back and forth several times. One nostril may detect a sweeter smell than the other. Close your eyes and concentrate. Rate the aroma on a scale of 0 to 10: when 0 means you dislike the odor intensely, and 10 means the odor is very pleasant. Write down a word that describes the aroma. When testing essential oils from an unknown source, first try one known to be authentic to "fix" the smell imprint in your brain. Then try the new one. Also, since the sense of smell adapts quickly to an odor, care should be taken to allow for sufficient time in between smelling consecutive samples in order to avoid olfactory fatigue. The trained human nose plays an important role in analysis. If your nose says the oil doesn't smell quite right, pay attention!

BUYING ESSENTIAL OILS

Essential oils can be purchased in a great many places, as well as online. Just remember that essential oils are easy to dilute or adulterate, and if the price sounds too good to be true, it probably is. The most common method of dilution is by adding vegetable oil or alcohol. The most common adulteration is adding a small amount of a cheaper oil, for example, adding geranium to rose, or petitgrain to neroli. Real melissa oil is very difficult to find, because it is frequently adulterated with lemongrass or citral. Sometimes particular components are added, such as citronella, geraniol, or linalool. Sometimes individual components are mixed in a test tube and the result is labeled "natural essential oil." Several countries can produce the same essential oil but they may be of varying quality. For example, rose is grown (and distilled) in France, Bulgaria, Turkey, China, and Morocco. Some essential oils may not be suitable for clinical use because they have been grown with pesticides.

If essential oils are being used clinically, they should be from a reputable supplier who can state the following: country of origin, botanical name, part of the plant, wild-crafted or organic, method of extraction, batch number, expiry date and the chemotype (when relevant). Reputable suppliers are happy to provide gas-chromatography/mass spectrometry (GCMS) information and material safety data sheets (MSDS).

Bottles should contain integral droppers and be made of colored glass. "Pure 100 percent essential oil" should be clearly marked. Basic safety precautions such as "do not take by mouth," "keep away from children," and "avoid contact with eyes" should be on the label. Apart from the product description, label and price, use your common sense and your nose. Long established, reputable companies would lose too much by compromising themselves on quality and are usually proud they can prove the authenticity of their oils. I have used the same small group of companies for 20 years. They are listed at the back of the book and also on www.rjbuckle.com. I have never sold essential oils. I do not have my own brand (although I have been asked to create one many times) so I can be completely independent. I dislike the cult-like behavior that some multilevel marketing seems to produce.

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