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Essential Oil's Chemical Composition and Pharmacological Properties

Jean Baptiste Houndou Fokou, Pierre Michel Jazet Dongmo and Fabrice Fekam Boyom

Abstract

Essential oil, sent by nature, is a complex mixture of volatile secondary metabolites. Its composition varies along with many parameters that can lead to misunderstanding of its wonderful pharmacological property. In fact, from post-harvest treatment to the compound's identification through extraction approaches, the original chemotype of essential oils can be misdescribed. The pharmacological potentials of these oils are well known in the traditional system since time immemorial. Nowadays, some chemotypes of these oils had shown the effect against WHO's top 10 killer diseases. But the misuses of these essential oils are in part due to the lack of robust and easy analysis strategy that can allow the quality of the essential oils.

Keywords: essential oils, chemotype, Kovats indexes, FTIR, 10 leading death diseases

1. Introduction

Essential oils are a complex mixture of plant volatile compounds. Those compounds are essentially composed of terpenoids and phenolic compounds. The biosynthesis of these flavoring volatile compounds is done in dedicated cell types present in almost all parts of the plant, from the leaves or flower to the roots depending on the plant's genus. These cells are glandular trichome, adduct cavities and osmophores where the compounds are biosynthesized and accumulated [1]. According to the scent of these compounds, the plant that can produce those compounds that when extracted are called essential oils are then called aromatic plants. Aromatic plants are not specific to a given taxonomic group, but they are present widely across the plant kingdom. It must be mentioned that the composition of the essential oils is different from plant taxonomic group to another [2–5]. It should be noted as well that, in the plant, compounds that will later form the essential oils are considered as secondary metabolites with a volatile characteristic. The variation in chemical composition of the essential oil can change from plant to plant even in the same species. These changes in the chemical profile are associated with many factors such as abiotic and biotic factors, postharvest treatment, extraction methods, and conservation conditions.

Abiotic factors group all the nonliving factors that affect the plant's secondary metabolite production. This includes the soil hydrology, pH and salinity, and the climate in general but more interestingly the microclimate in which plant is growing [6–10].

Biotic factors group the living organisms that can affect the plant's metabolite productions. These factors include, in one part, soil organism and microorganism. In fact, secondary metabolites present in essential oils are produced to help the plant to fight against plant invaders, interact with the symbiotic organism, and attract insects for pollination, among others. In another part, biotic factors are inherent in the plant itself.

Postharvest treatment include all the procedure that occurs between the plant collection and essential oil extraction. There are numerous reports that highlight the fact that drying plant material before extraction increases drastically the yield of extraction [5, 11, 12]. The counterpart of this method is the fact that after plant collection, there is a biochemical reaction that occurs between secondary metabolites. The output of this biochemical interactions is the changes in the chemistry of the obtained essential oil in comparison with that originally present in plant. At that point, the balance is between biological activity and the yield [5, 11, 12].

The extraction method can also lead to significant modification of the chemical profile of the essential oil. There are a huge number of approaches that can help to obtain an extract from the aromatic plant, including distillation methods, expression, solvent extraction, enfleurage, and microwave-assisted extraction. Apart from hydrodistillation, microwave assisted, and expression (specifically the citrus pericarp expression), all the other methods lead to a product that is not recognized as essential oil *sensu stricto*. In fact, with all the other methods, the extract obtained usually contains nonvolatile compounds that are extractable by the process and must be further removed. Also, the hydrodistillation method can lead to the chemical transformation of the compounds such as ester and other compounds that are highly hydrolyzable due to the long stay of the essential oil in water in the extraction system [13–17].

Regarding the conservation method that group all the process between the extraction and chemical analysis, the nature of the oil can lead to some modifications. In fact, most of the compounds that are present in essential oils are unsaturated (contain double bound) and most of them are sensitive to light (photo-sensitive) and to oxygen (oxidable).

Essential oils are used for their wonderful biological properties. The biological properties include the effect on humans, animals, plants, insects, and microorganisms. In humans, every single part of the human life can be affected by essential oils. In fact, essential oil is employed in nutrition as a food preservative or flavoring, in cosmetics as an odorant part, and in pharmacology as an active ingredient. The essential oil's pharmacological properties comprise their effect on transmissible and non-transmissible diseases.

This chapter aims at going through the mechanism of essential secondary metabolite biosynthesis, essential oil extraction, essential oil chemical profile, and its pharmacological potential against the top list of human killer diseases as presented by WHO.

2. Chemical composition

2.1 Biosynthesis

Terpenoid and phenylpropanoid derivatives are the main components found in essential oils. In most plants, their essential oils contain terpenoids at around 80%. But the presence of phenylpropanoid derivatives affords the essential oils significant flavor, odor, and piquant. These two groups of compounds are derived from two different pathways from different primary metabolites [18].

2.1.1 Biosynthesis of terpenoids

The name terpene was first attributed to the compounds with molecular formula $C_{10}H_{16}$ by Kekule, a German chemist, due to its abundance in turpentine oil. The derivatives $C_{10}H_{16}O$ and $C_{10}H_{18}O$ were named generically camphor and related to terpenes. Wallach, Kekule's assistant, characterized pinenes, limonene, dipentene, phellandrene, fenchone, terpinolene, and sylvestrene, which at that period were recognized as artifacts for turpentine oil [19]. But nowadays, they are considered as compounds of some essential oils.

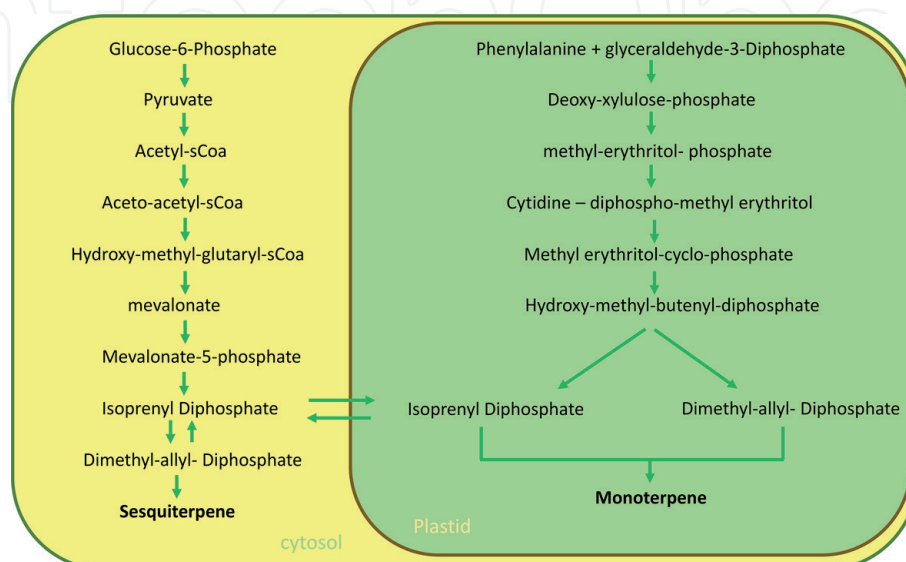
Terpenoids are a heterogeneous group of terpenes (compounds with double bonds) and their oxygenated derivative. Sensu stricto, an essential oil terpene, is a group of compounds derived from isoprene. Isoprene in its part is an organic scaffold with 5 carbon units with 1 double bond. Terpenoids are also called isoprenoids.

To start at the beginning, there are two pathways that lead to the synthesis of isoprene. These two pathways occur in the different parts of the upstate specialized cell. In the cytosol, the so-called mevalonic acid pathway is used, while in the plastid, the Rohmer or 1-deoxy-D-xylulose-5-phosphate is used. As this part is the most important part to understand the differences between essential oils' chemistry and thereby their pharmacological properties, let us walk you through some chemistry (**Figure 1**).

According to plant species and foremost to the plant enzymatic ability, there is interconversion between certain compounds. The most observed case is that of conversion of thymol into carvacrol or vice versa. This depends on what plants need and environmental conditions [22, 23]. This leads in some case to a huge difference between chemotype of the same plants collected in different areas or different period of time during the same day or during different maturity stages. This has been reported for *Allium sativum* [24–26] and for *Lavandula angustifolia* [14, 27–30] and *Melissa officinalis* [4, 12, 13, 16, 31–36].

2.1.2 Biosynthesis of phenylpropanoids

The synthesis of this class of compounds in aromatic plant leads to a wide variety of compounds, but in this chapter, we will focus on the pathway that leads to volatile compounds.



In comparison to isoprenoids, volatile phenylpropanoid compound synthesis occurs less often. But this is not the case for almost all plants; in fact for clove oil, eugenol is the major compounds [37].

The enzymatic arsenal involved in the synthesis of volatile compounds in the plant is not well known. Therefore, there are many approaches to explain the synthesis of those groups of compounds. But from a metabolite point of view, the starting point of these volatile phenols is the phenyl-alanine that is transformed into cinnamic acid by the phenylalanine amino lyase. The cinnamic acid in turn is transformed into para-COUMARIC acid. This latter compound depending on the enzymatic ability of the plants can undergo two different ways of synthesis (**Figure 2**).

2.2 Essential oil extraction

Essential oil extraction is one of the critical points that can affect the chemical profile of the essential oil. Sensu stricto, essential oils are a volatile odorant complex mixture obtained by distillation. Many techniques have been developed to obtain essential oil such as microwave-assisted extraction, expression, enfleurage, and solvent extraction. Most of these extraction methods lead most of the time to artefactual products as well as transformed products. To better understand, the next paragraphs will present the most used methods and their principal limit in the way of modification of the original chemical profile of the essential oil.

2.2.1 Distillation methods

Distillation methods are a group of methods using steam as compound vector or transporter. In fact, in distillation method, the plant material may be immersed or not in water, and after heating to water boiling point, the impression created in the reactor by steam as well as the high temperature will create the vaporization of these volatile compounds from their stockade cell to the environment of the reactor. The gas is pouched throughout a cooler. The condensation of the water and volatilized compounds from their vapor to water phase form a mixture that can be separated according to their density. There are two varieties of distillation methods: the hydrodistillation and the so-called steam distillation methods [38–40].

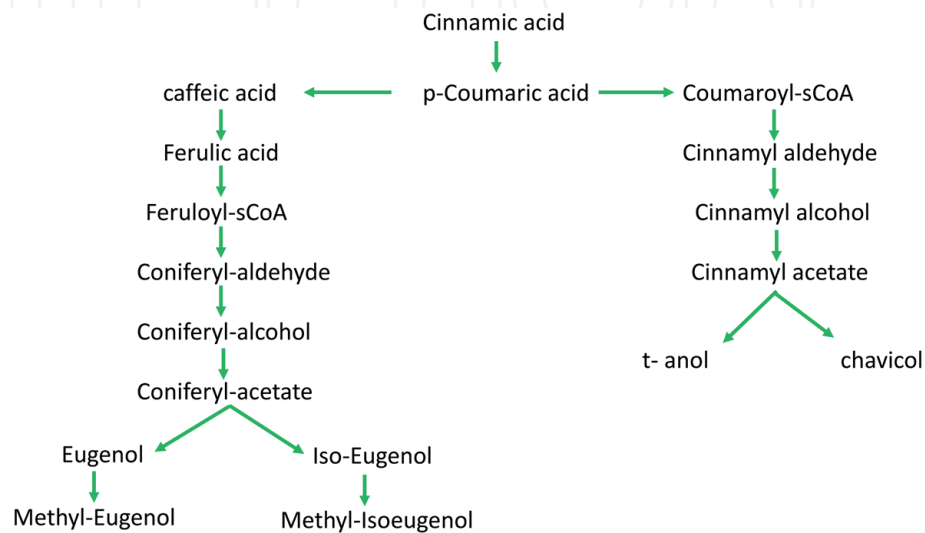


Figure 2.
Biosynthesis of phenylpropanoids summarized from [20].

Hydrodistillation is an essential oil extraction method in which the material is immersed in water, but in the steam distillation, the plant material is not in direct contact with water but will go through, for example, steam flow before entering the cooler.

The principal limits of this method regarding the impact on the chemical profile of the essential oil are as follow:

- The thermosensitive compounds will undergo a transformation or simply degradation. In fact, the high temperature can catalyze some chemical reactions that the normal cell will not, and this will lead to the chemical entities that were not present in the plants.
- Lasting contact with water increases hydrolysis. Esterified compounds are highly sensitive to water as they will be broken down into compounds that do not exist in the essential oil storage cells.
- When the glass Clevenger is used, the essential oil is exposed to light and can, therefore, undergo photo-oxidation and the chemical profile will reveal a high number of oxygenated derivatives that do not really exist in the plant.

Many reports have highlighted these observations and one of them is that of Kamii et al. [14]. In fact when analyzing the chemical profile of *Lavandula angustifolia* extract using two different technics including hydrodistillation, they obtained 25.3% of linalyl acetate, 16.4% of terpene-4-on, 13% of linalool, and 13.6% of ocimene for hydrodistillation and 30.6% of linalyl acetate, 14.1% of terpene-4-on, 8.4% of lavandulyl acetate, 7.3% of β -caryophyllene, and 7.2% of β -farnesene for supercritical fluid extraction as well as lavandulol and phytol that were solely present in that later method. Many other reports are available in the literature for many other plants [1, 15–17].

2.2.2 Microwave-assisted essential oil extraction

Microwave-assisted essential oil extraction is a variant of the distillation method where the heating source has been changed from the normal electric heating cap by the microwave. The plus here is the hypothetic increasing in extraction yield: hypothetic because the increase in yield is not as spectacular as tough [41–43]. It is true that it is better to crush the plant material, but in comparison to the classic distillation method, the essential oil yield is systematically the same. The principle of this method is based on the change of the polarity of water by the waves and of course the heating that will play the same role as in classic distillation method. This method has in addition the limit of the normal distillation method, the fact that the microwave can lead to chemical stereo switching from one isomer to another.

2.2.3 Expression

This method is specific for citrus pericarp. In fact, to avoid the thermal destruction, cold pressing of the citrus fruit rinds as the essential oil is store at that part of the plant has led to a good quality oil. The limit of this technique is the fact that it is not applicable to other parts of the plant [38–40].

2.2.4 Enfleurage

Enfleurage is an old technique of essential aroma extraction. It is based on the solubilization of the essential oil's component on a greasy wax. When using cold extraction, it can take more than a month, but this can be reduced to a few

hours by heating. The aromatized wax is then called concrete. This later undergoes solubilization in a polar solvent and then partitioned with absolute ethanol. The product obtained after this process is at most a part of the essential oil as present in plant, and it contains many other terpenes that can be solubilized in fats used; that is, while at the end, the product is not called essential oil but absolute.

2.2.5 Solvent extraction

This is the oldest method for obtaining crude extract from plants. The principle is based on the solubilization of the compounds in the cells by the solvent. This method also has two variants as it can be run in room temperature or in high temperature. But no matter whether the extraction was performed in room temperature or not, the solvent will be separated by Rotavapor regarding the volatility of the solvent. This method does not really lead to obtaining the essential oil as all the nonvolatile compounds are also extracted by this approach. Therefore, the chemical profile will not be that of the volatile fraction of the plants but for the compound that is soluble in the solvent used in the process [13–17].

2.2.6 Supercritical fluid extraction

This method is the most modern and sophisticated. It uses gases at their supercritical stage. The gas at supercritical stage is liquid due to the high pressure applied to it. Many solvents can be used as the method brings the solvent at its temperature and pressure above its thermodynamic critical point, but the most used is CO₂ for the reason that it needs less pressure to be liquified, it is less reactive than other, it is noninflammable, it is nontoxic and available at low cost with high purity, and most importantly it can be removed from the plant material using just the press release. This method is based on the fact that gas at the supercritical state can enter throughout the plant material like a gas and dissolve component like a liquid. After the extraction procedure, the essential oils compounds are mixed with the supercritical fluid (in liquid form). The separation is performed by reducing temperature and increasing the pressure up to room conditions [13–17]. The principal limit of this method is the complexity of the system.

2.3 Method for chemical analysis

There is a myriad of technics and methods for essential oil chemical profiling. All the methods used in organic chemistry can be used here. Due to their volatility nature, the compounds that constitute essential oil are preferably analyzed by gas chromatography (GC). Gas chromatography alone does not provide enough data for good chemical proofing. Therefore, many other analytical tools have been used such as mass spectrometry (MS), infrared spectroscopy (IR), and nuclear magnetic resonance (NMR). As well, many technics have been used to make the GC a better tool for chemical profiling, and these include chiral selective GC and multidimensional GC. Advances in liquid chromatography have highlighted the usefulness of high-pressure liquid chromatography (HPLC) as a tool for essential oil analysis. Many variants are available to date as multidimensional HPLC, HPLC-MS, and HPLC-GC. The following section will walk you through gas chromatography and gas chromatography coupled with mass spectrometry for their popularity and the Fourier transform infrared spectroscopy for its simplicity and for being environment-friendly and long-term cost-effectiveness.

2.3.1 Gas chromatography and variant in essential oil analysis

Gas chromatography is an old essential oil chemical profiling method. As all the chromatographic methods, it is based on the single compound separation from a complex matrix between two phases regarding their affinity between the phases, their shape, and mass. The mobile phase is the one which moves by capillarity or pressure transporting compounds faster or slower toward the fixed phase. In GC, the mobile phase is a gas and the fixed phase is a solid at room temperature, but at a high temperature, this phase will be slightly melted but will remain fixed on the column.

For analysis, the essential oil is mixed with a solvent (mostly hexane or pentane) and introduced into the injector room set at 200°C with the help of a syringe. The mixture is carried by the mobile phase into the column. Here the temperature drops down to about 50°C. All the compounds settle down at different distance in the column. This column itself is placed in an oven set with gradient increasing temperature (1–5°C/min). Each compound has its vaporization point and therefore when the oven temperature will reach this point, it will be volatilized thereby take off from the stationary (fixed) phase and carry and spit off out of the column.

Usually, the column is connected to a detector, which in the case of essential oil analysis is the flame ionization detector (FID). In this case, when the compound comes out of the column, it is burned and the increasing temperature in the flame, proportional to the compound scaffold, is detected and transformed into a peak. The compound identification is done by using the retention time and/or the Kovats index. The following formula as presented in Adams is used to calculate the Kovats index.

$$KI_{(x)} = 100 P_z + 100 \left(\frac{\log RT_x - \log RTP_z}{\log RTP_z - \log RTP_{z+1}} \right) \quad (1)$$

$KI_{(x)}$ is the Kovats indices of compounds x , P_z is the paraffin with z carbon atoms, $P_{(z+1)}$ is the paraffin with $z + 1$ carbon atom, and RT is the retention time.

The linearization of this formula presented in Adams is as follows:

$$AI_{(x)} = 100 P_z + 100 \left(\frac{RT_x - RTP_z}{RTP_z - RTP_{z+1}} \right) \quad (2)$$

$AI_{(x)}$ is the arithmetic index of compounds x , P_z is the paraffin with z carbon atom, $P_{(z+1)}$ is the paraffin with the $z + 1$ carbon atom, and RT is the retention time.

After calculation of index, the value is compared with that of the online libraries or the Adams library [45].

When the GC is connected to MS, the compound is accelerated and ionized into the different compartment of its scaffold and detected as bands.

Table 1 summarizes few retention or Kovats indexes reported in the literature for randomly selected plant and randomly selected papers. The diversity of chemotype obtained per essential oil is interesting. But the question about the accuracy of this profiling method has come up. Moreover, the Internet-based data bank proposes a huge range of retention indexes for the same compounds. For illustration matter, let us take the eucalyptol also called cineol-1,8. In the NIST database in the slightly polar column, here dimethyl-silicone with 5% phenyl group (DIMS 5P), this compound have a retention indexes ranging from 1021 to 1044 [44]. This range represents 23 units in the retention indexes. Taking into consideration the Kovats or Van Den Dool and Kartz formula, this range (8 min 57 s to 9 min 44 s) represents a gap of 47 s. For the same column, in terms of polarity, in Adams Database, during this period, 24 single compounds can be identified [45]. More complexly, there are overlappings in

Retention indexes								
<i>Allium sativum</i>								
Compounds	AP	SAPC	PC	[26]	[25]	[24]	[85]	[86]
Diallyl sulfide	835–872	831–872	1118–1177	855	784	—	846	854
Allyl methyl disulfide	891–915	887–928	1241–1322	916	918	—	908	915
Diallyl disulfide	1054–1078	1048–1095	1436–1526	1080	1111	1085	1079	1084
Allyl methyl trisulfide	1100–1132	1123–1165	1587–1605	1138	1116	1145	1126	1131
Diallyl trisulfide	1266–1292	1277–1320	1775–1822	1301	1207	1311	1301	1305
<i>Lavandula angustifolia</i>								
Compounds	AP	SAPC	PC	[5]	[28]	[29]	[30]	[14]
Ocimene	1027–1050	1028–1047	1211–1251	1030	—	1043	—	1043
Linalool	1074–1098	1088–1109	1507–1564	1092	—	1107	1100	1101
Terpineol	1148–1180	1178–1203	1655–1687	1167	1179	—	—	1181
Linalyl acetate	1234–1254	1238–1268	1532–1570	1246	—	1256	—	1258
Borneol	1134–1172	1152–1177	1653–1717	1155	1167	1170	1144	1169
<i>Melissa officinalis</i>								
Compounds	AP	SAPC	PC	[4]	[13]	[16]	[12]	[33]
Neral	1211–1240	1231–1269	1641–1706	—	—	1246	1245	1240
Nerol	1206–1239	1216–1250	1752–1832	—	—	1228	—	—
Geranial	1236–1260	1252–1291	1680–1750	—	—	1278	1271	1270
Geraniol	1231–1256	1238–1269	1795–1865	1185	1252	1258	—	—
Caryophyllene	1400–1442	1405–1440	1569–1632	—	1417	1405	1421	1418
Germacrene D	1458–1491	1446–1493	1676–1726	—	1484	1480	1489	1480
Cadinene	1506–1542	1503–1541	1734–1803	—	1523	1538	1514	—
<i>Ocimum basilicum</i>								
Compounds	AP	SAPC	PC	[87]	[88]	[89]	[90]	[17]
Eucalyptol	1013–1039	1021–1044	1186–1231	1031	1031	1027	1029	1026
Ocimene	1027–1050	1028–1047	1211–1251	1038	1045	—	1048	1034
Linalool	1074–1098	1088–1109	1507–1564	1111	1120	1085	1116	1095
Eugenol	1323–1372	1345–1375	2100–2198	—	—	1377	1376	1330
Humulene	1439–1459	1436–1456	1637–1689	1447	1455	1430	1459	1445
Cadinene	1506–1542	1503–1541	1734–1803	1519	—	1497	—	1505
<i>Peper nigrum</i>								
Compounds	AP	SAPC	PC	[3]	[89]	[91]	[92]	[15]
a-Pinene	924–951	921–944	1008–1039	938	930	931	931	939
b-Phellandrene	1005–1036	995–1013	1148–1186	1040	978	1024	1021	1003
g-Terpinene	1035–1062	1049–1069	1222–1266	—	1049	1051	1050	1060
a-Cubebene	1345–1359	1438–1480	1438–1480	1357	—	1377	1352	1351
Farnesene	1484–1509	1488–1493	1627–1668	1455	1518	1453	1445	1443
b-Caryophyllene	14,000–1442	1405–1440	1569–1632	1437	1395	1419	1419	1419

Retention indexes								
<i>Rosmarinus officinalis</i>								
Compounds	AP	SAPC	PC	[6]	[7]	[8]	[10]	[93]
a-Pinene	924–951	921–944	1008–1039	931	936	1075	961	939
Myrcene	975–991	980–995	1140–1175	980	991	1174	991	991
Camphene	936–965	936–959	1043–1086	944	952	1102	943	954
Eucalyptol	1013–1039	1021–1044	1186–1231	1021	1031	1221	1032	1031
Camphor	1106–1153	1127–1155	1481–1537	1122	1148	1547	1088	1144
Verbenone	1167–1198	1190–1224	1696–1735	1183	1209	—	1119	1207
Bornyl acetate	1259–1209	1264–1297	1549–1597	1272	1292	1612	1277	—
<i>Salvia officinale</i>								
Compounds	AP	SAPC	PC	[89]	[36]	[9]	[94]	[95]
Myrcene	975–991	980–995	1140–1175	981	988	—	980	992
a-Thujone	1076–1104	1099–1117	1385–1441	1104	1101	1105	—	1102
Camphor	1106–1153	1127–1155	1481–1537	1122	1141	1143	1108	1142
Eucalyptol	1013–1039	1021–1044	1186–1231	1027	1026	1034	1191	1032
b-Caryophyllene	1400–1442	1405–1440	1569–1632	1395	1417	1418	—	1418
Humulene	1439–1459	1436–1456	1637–1689	1430	1452	—	1430	1454
Viridiflorol	1561–1598	1569–1604	2041–2110	—	—	—	1587	—
<i>Syzygium aromaticum</i>								
Compounds	AP	SAPC	PC	[96]	[97]	[98]	[99]	[89]
Eugenol	1323–1372	1345–1375	2100–2198	1392	1353	1370	1354	2098
b-Caryophyllene	14,000–1442	1405–1440	1569–1632	1458	1428	1426	1421	—
Eugenyl acetate	1472–1493	1514–1531	2252–2277	1552	1538	—	1522	2107
Humulene	1439–1459	1436–1456	1637–1689	1579	—	1460	1455	—
<i>Thymus vulgaris</i>								
Compounds	AP	SAPC	PC	[22]	[100]	[23]	[98]	[101]
a-Terpinene	1001–1024	1007–1026	1154–1195	—	1010	1016	1019	1019
p-Cymene	1004–1029	1011–1033	1246–1291	1029	1014	1024	1026	1033
Limonene	1012–1038	1019–1039	1178–1219	—	1022	1028	1031	—
Terpineol	1148–1180	1178–1230	1655–1687	—	1162	1194	1190	1177
g-Terpinene	1035–1062	1049–1069	1222–1266	1064	1049	1057	1062	1060
Linalool	1074–1098	1088–1109	1507–1564	—	1084	1099	1100	1107
Thymol	1260–1289	1272–1304	2100–2205	—	—	1288	1296	1315
Carvacrol	1272–1300	1291–1344	2140–2246	1308	1286	1296	1305	—
b-Caryophyllene	14,000–1442	1405–1440	1569–1632	—	—	1419	1419	1423
<i>Zingiber officinale</i>								
Compounds	APC	SPC	PC	[102]	[103]	[104]	[105]	[106]
a-Pinene	1001–1024	1007–1026	1154–1195	939	—	926	943	935
Camphene	936–965	936–959	1043–1086	953	—	944	954	950
Linalool	1074–1098	1088–1109	1507–1564	—	1112	—	—	1103

Retention indexes								
Eucalyptol	1323–1372	1345–1375	2100–2198	1033	1060	1015	1027	1032
Neral	1211–1240	1231–1269	1641–1706	—	1265	1249	1227	1247
Geranial	1236–1260	1252–1291	1680–1750	—	1292	—	1252	1379
Germacrene D	1458–1491	1446–1493	1676–1726	1481	1532	—	1469	—
b-Farnesene	14,000–1442	1405–1440	1569–1632	—	1518	—	—	1458
Zingiberene	1463–1494	1485–1509	1696–1743	1495	1521	1492	1487	1508
APC, apolar column; SPC, slightly polar column; PC, polar column.								

Table 1.
Retention indexes of important compounds from 10 randomly selected essential oils.

the range proposed by the NIST as reported by Babushok [44] as it can be observed in **Table 1**; for the same DIMS5P column, α pinene (921–944) is overlapping with camphene (936–959) and eucalyptol (1021–1044) is overlapping with ocimene (1028–1047) and camphor (1127–1155). These observations are the real pitfalls of these identification approaches and can lead to misuses of the valuable data from those data banks. In fact, these overlappings lead to compound identification oriented to the chemotype available in the literature rather than the real chemotype that is analyzed. And the previous paragraph had highlighted that the chemical profile thereby the pharmacological profile can change because of a myriad of factors. All these lead to questioning the robustness of this actual gold essential oil chemical profiling strategy not in the view of the provided database or analytic tools but in the view of data interpretation by the users.

2.3.2 Infrared spectroscopy and chemometric analysis

The idea besides the spectroscopy analysis is the fact that, in the electromagnetic radiation, there is a range of a tiny part of visible light that exists as a wave. This light moves in a straight line if the part of this light is not reflected, refracted, or absorbed by the matter. In biology and chemistry, this technique is used to produce an infrared spectrum in the case of infrared spectroscopy by passing an infrared radiation through a given sample knowing that the atom constituting the sample will lead to absorption of a part of the light energy. When a part of the molecule present in the sample absorbs this energy, it will become unstable and will react by twisting, stretching, bending, rocking, wagging, or scissoring depending on the bond linking these atoms with the rest of the molecule. The energy absorbed, the different reactions of the atom lead to the appearance of a specific peak on the spectrum [46–49].

The spectrum can be at least qualitatively interpreted without prior or additional chemometric algorithm as it provides a high level of specific information on the molecular aspect of the essential oil [50]. In fact, the spectrum regions are known and correspond to established characteristic group absorbances [47] and therefore the assignment can lead to specific chemical identification (**Figure 3**). But this is when the sample is a single compound. When the mixture is analyzed, the peak cannot be simply attributed to the compounds as it is most of the time the result of the overlapping small vibration of different closely related groups from a different molecule in the mixture.

For the quality purpose, the fingerprint region is most important. In fact, the fingerprint region is a unique vibrational signature that a given essential oil can have. It is as specific as the fingerprint is specific to a human. But to be more

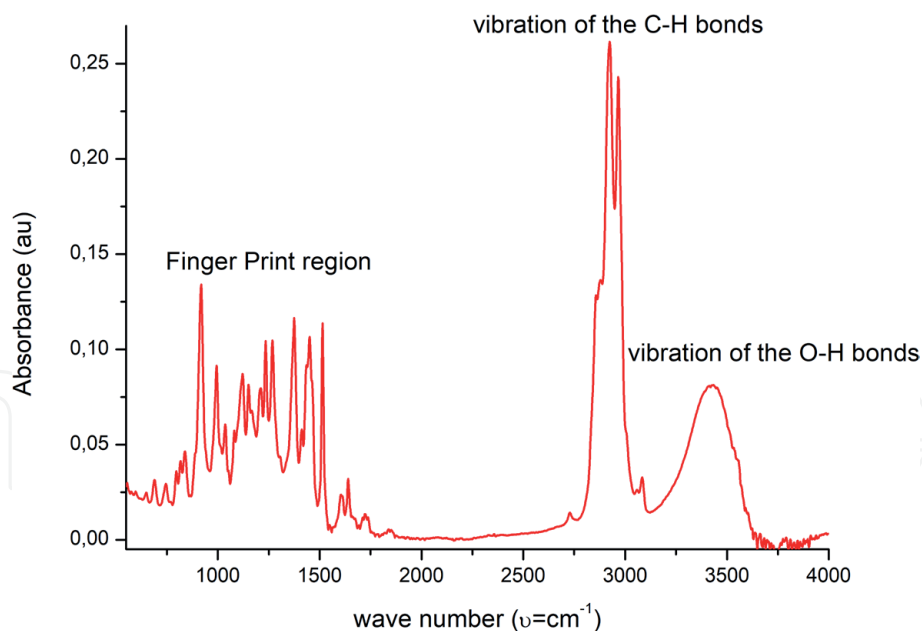


Figure 3.
 Infrared spectrum of *Ocimum basilicum* essential oil obtained from Fourier transform infrared spectroscopy.

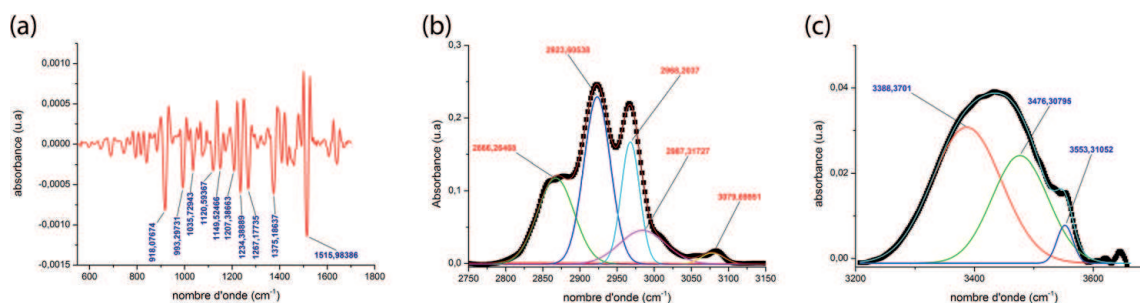


Figure 4.
 Spectral processing of fingerprint (a), C-H (b) and O-H (c) regions of *Ocimum basilicum* essential oil's FTIR spectrum [51].

efficient in the analysis of the area, chemometric tool should be used such as derivation. This approach is a simple application of the derivate formula to the equation of the fingerprint region or a given region. This technique provides with key benefits. In fact, it enhances the resolution for the first derivative and the second derivative gives negative peaks of each band in the examined region [47] an example from **Figure 3** is given in **Figure 4A**. It is also possible to apply other data processing such as baseline correction, smoothing, or curve fitting [47].

Using this approach, an increasing number of authors have succeeded in discriminating the essential oil of various plants based on their chemotype [46, 51–56]. Those authors have suggested that for a known essential oil, the fingerprint of the oil should be used as a tool for rapid essential oil quality control.

3. Pharmacological property of essential oils

This part of the chapter is huge and covers various aspects of human and animal care. It will be easier to find a disease that no essential oil as a whole or its component can exert any effect. Essential oils are used to manage even diseases that are not scientifically measurable these days. These include protecting against misfortune and bad spirit and protecting the soul after death. This aspect of the therapeutic use of the essential oil will not be described here. The following paragraphs will be

devoted to the review of essential oil use against top 10 human killers. Regarding the classification of 10 global causes of death around the world as published by WHO [57], ischemic heart disease, stroke, chronic obstructive pulmonary disease, lung cancer, diabetes, lower respiratory infection, diarrheal disease, tuberculosis, HIV/AIDS, and road injuries were respectively the most important human killers in 2016. Unfortunately, this chapter could not review the potential of essential oils against road accident.

3.1 Essential oil against ischemic heart disease and stroke

During the last 18 years, ischemic heart disease had won the gold medal in killing a human. In the second position with silver medal comes the stroke. In 2016, these affections were incriminated in 15.2 million human death [57]. This is clear, known, and localizable but a silent terrorist against which all efforts should be focused on. These two affections share the same origin but different target. In fact, they are both cardiovascular diseases. Cardiovascular disease is known as a disease that affects the heart and blood vessels of the circulatory system [58]. In this case, ischemic heart disease and stroke are specific to blood vessels. Ischemic heart disease is a class of cardiovascular disease that appears on the vessels that supply the heart cells with blood in terms of nourishing rather than pumping for other organs [58]. Stroke on its part can be defined as neurological shortfall caused by crucial injury of the central nervous system. The reason behind is the cerebral infarction or intracerebral hemorrhage. Ischemic stroke accounts for 80% [59] of all types of stroke this chapter will focus on these later on.

Death happens when cells of these two vital organs are not supplied with nutrients and oxygen and are not free from their metabolic wastes. The main cause is the obstruction of the vessels by a clot (thrombus) from venal or upper artery atherosclerosis in coronary (in the heart) or arterioles (in the brain) and/or atherosclerosis on these two vessels [58, 59]. It is therefore clear that targeting specific clot dissolution or arteriosclerosis can help to manage ischemic heart and stroke disease.

In that regards, a massive number of essential oils have been studied for their effect on cardiovascular diseases. These reports were previously reviewed by Grenier et al. [60] for the vasodilatation effect. The major compounds from these essential oils were eucalyptol (*Croton nepetaefolius*); piperitenone oxide (*Mentha × Villosa*); terpineol (*Alpinia zerumbet*); eugenol and methyl eugenol (*Ocimum gratissimum* and *Aniba canelilla*); anethole and estragole (*Croton zehntneri*); α pinene, caryophyllene, and eucalyptol (*Hyptis fruticose*); geraniol, citronellol, and citronellal (*Cymbopogon winterianus*); and many other essential oils containing linalool, bisabolol, and β pinene [60]. For the anti-arteriosclerotic effect, these same authors reviewed 17 essential oils that have been reported for their anti-arteriosclerotic effect both *in vitro* and *in vivo*. These plants include *Allium sativum*, *Ocimum sanctum*, *Melissa officinalis*, and *Lavandula angustifolia*.

3.2 Chronic obstructive pulmonary disease and lower respiratory infection other than tuberculosis

Chronic obstructive pulmonary disease and lower respiratory infection other than tuberculosis are respectively the third and the fourth leading causes of death worldwide. These diseases caused cumulatively 6 million deaths in 2016. The lower respiratory infection disease owns the gold medal in communicable disease. It is important to notice that, in the developing world, the lower respiratory infectious disease is the first leading cause of death [57].

The chronic obstructive pulmonary disease (COPD) can be defined as a progressive respiratory condition clinically characterized by dyspnea, cough, and sputum production. This is the manifestation of alveolar enlargement and destruction as well as inflammation of lung parenchyma airways [61]. *In fine*, this disease can be categorized as the inflammation of the lung. Essential oils or their components have been reported to have a positive effect on lung inflammation. In fact, eucalyptol, a main component of eucalyptus essential oil, has shown evidence on the resolution of pulmonary inflammation in humans [62, 63] and in rats [64]; myrtle, eucalyptus, and citrus essential oils have significantly reduced the inflammatory response *ex vivo* [65].

Lower respiratory infection disease is mainly caused by microorganisms including bacteria (other than *Mycobacterium*), fungi and viruses. A myriad of reports has proved the potential of essential oils as a possible source or as a drug against pathogens causing respiratory infection. Essential oils from *Pimpinella anisum*, *Foeniculum vulgare*, *Eucalyptus globulus*, *Mentha piperita*, *Melaleuca alternifolia*, and *Thymus vulgaris* were reviewed by Horvath and Acs from European Pharmacopeia [66] and had an effect *in vitro*, *in vivo*, and on a human. *Syzygium aromaticum*, *Cinnamomum zeylanicum* Nees., Batch, *Eucalyptus globulus*, *Thymus vulgaris* L., *Pinus sylvestris*, and *Mentha piperita* have been reported for their inhibitory effect on bacteria that cause lower and upper respiratory infections [67].

3.3 Lung cancer

Lung cancer is the fifth leading cause of death worldwide, and in 2016, WHO estimated that 1.7 million persons were dying from lung cancer. It is established that there is an urgent need for anticancer drugs due to the high selectivity that anticancer drug should possess. There are an important number of publications in the literature on the anticancer effect of the essential oils. More specifically, a certain number of essential oils have been claimed to possess anticancer effect against lung cell line; all these experiments are as per now *in vitro* or in an animal model [68–70].

3.4 Diabetes

Diabetes is the sixth leading cause of death worldwide. In 2016, this affection caused 1.6 million deaths with an increase of 0.6 million compared to 2000. As the number of affected persons is increasing, this means that the management method is not that efficient, and alternatives are needed. Essential oils have been analyzed for their antidiabetic effect. *Lavandula angustifolia*, *Melissa officinalis*, *Ocimum basilicum*, *Peper nigrum*, *Rosmarinus officinalis*, *Saliva officinale*, and *Thymus vulgaris* were analyzed of their stimulation of glucose consumption. And *Melissa officinalis* essential oils present better effect compared to insulin [71]; moreover, *in vivo* studies have also been reported [72–76].

3.5 Diarrheal disease

Diarrhea is a disease caused by infection of the gastrointestinal tract by bacteria, fungi, virus, and ameba. The manifestation includes the urination of more than 3 liquid stools per day. The epidemiology of diarrheal disease has decreased from 200 with 2.4 million death cases to 1.4 million cases in 2016 [57]. This reduction is mostly made by hygiene management. Essential oils have been analyzed for their beneficial effect in the therapeutic management of diarrheal infection [77–80]. Some components as linalool, eucalyptol, terpineol, geraniol, thymol, carvacrol, spathulenol, caryophyllene, elemene, viridiflorol, bisabolol, eugenol, t-anetol,

cinnamaldehyde, and allyl isothiocyanate were used to optimize the effect of the available drugs against some of the pathogens with successful results [78].

3.6 Tuberculosis

Tuberculosis is the infection of the lung by *Mycobacterium tuberculosis*, and it caused 1.3 million deaths in 2016. Many drugs are available, and control by quarantining the affected person had caused a reduction in this affection during the last 19 years [57]. Essential oils can also play an important role in the management of this affection. In fact, *Salvia aratocensis*, *Lippia Americana*, *Turnera diffusa* [81], *Cuminum cyminum*, *Eugenia caryophyllata*, *Cinnamomum verum*, *Laurus nobilis*, *Pimpinella anisum* [82], and *Hyptis suaveolens* [83], among others have been analysed successfully for their effect against *Mycobacterium tuberculosis*.

3.7 HIV/AIDS

HIV/AIDS is the acquired immunodeficiency syndrome, caused by human immunodeficiency virus. The disease is the ninth more important terrorist worldwide, killing in 2016 1 million persons [57]. The mortality due to this virus has decreased along the years due to the generations of antiretrovirals as well as the protective measures adopted by the populations. There are only a few publications available on the effect of the essential oils on this virus. The reason can be the fact that this virus is very dangerous, and the testing equipment must be sophisticated to allow this test. However, *Ridolfia segetum* and *Oenanthe crocata* have been analyzed successfully for their effect on RNA-dependent DNA polymerase and ribonuclease H [84].

4. Conclusion

Essential oils are the oil of nature, sent by nature, the spirit of nature, and the soul of the forest. Their scent depends on their composition that in turn depends on the enzymatic package of the plant species. This enzymatic package can be influenced by external factors that can be biotic, depending on a living organism, or abiotic depending on molecules or climate and geography. The pharmacological potential of this spirit of the forest is a fact. But the scientific proof of that fact is subject to misunderstanding or misinterpretation. That may be why it is difficult to have essential oil recommended as an official drug for a disease. In fact, there are many variations that could affect the chemical composition not in the plant but during essential oil processes from plant collection time to the analytic method and the data interpretation. As well, Aromatic plants containing these scent of the nature are mostly present in tropical part of the world, and most of those tropical countries are developing countries and as such they do not have robust technology equipment to test and prove the whole efficiency of that essential oils, spirit of nature. To solve these small but crucial issues, scientists should come along with a robust analytical tool (FTIR, for example) and standard postharvest and extraction protocols for standardization of all essential oils not only in few local pharmacopeias but on a world level.

Conflict of interest

The authors declare no conflict of interest.

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