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Essential oils as a source of bioactive molecules

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Summary

Nature gives us a large number of compounds with interesting biological properties, within them we have essential oils, which are an important source of new bioactive molecules, which can replace synthetic chemicals, since they are friendly to the environment and they are less toxic. Currently there are more than 20.000 publications in which essential oils are related to some biological activity, according to the search made in different databases until January 2018. This confirms the wide utility of essential oils as the main source of bioactive metabolites, which can be used in different areas of our life.

Keywords: Natural products, plants, terpenes, volatile compounds, biological activity, phenylpropanes.

Resumen

Aceites esenciales como fuentes de moléculas bioactivas

La naturaleza nos proporciona una gran cantidad de compuestos con interesantes propiedades biológicas, dentro de los cuales tenemos los aceites esenciales, los cuales son una fuente importante de nuevas moléculas bioactivas, que pueden reemplazar a los químicos sintéticos, ya que son amigables con el medio ambiente y son menos tóxicos. Actualmente existen más de 20.000 publicaciones en las que los aceites esenciales están relacionados con alguna actividad biológica, según la búsqueda realizada en diferentes bases de datos hasta enero de 2018. Esto confirma la amplia utilidad de los aceites esenciales como principal fuente de metabolitos bioactivos, que pueden ser utilizados en diferentes áreas de nuestra vida.

Palabras clave: Productos naturales, plantas, terpenos, compuestos volátiles, actividad biológica, fenipronanos.

Introduction

Essential oils (EOs) are complex mixtures of volatile organic compounds produced in the form of secondary metabolites in plants that can contain about 20-60 components in very different concentrations [1, 2]. They are characterized because they contain two or three main components in relatively high concentrations (20-70%) compared to other components present in minimal amounts [3]. They may consist of monoterpenes, sesquiterpenes, and phenylpropanes, which may contain different functional groups (alkanes, alcohols, aldehydes, ketones, esters and acids) [1, 2].

In nature, EOs plays an important role in the protection of plants such as antibacterial, antiviral, antifungal, insecticide and also against herbivores, reducing their appetite for these plants. They are also responsible for the characteristic smell of plants, which can attract some insects to favor the dispersal of pollen and seeds, or repel other undesirable ones [3]. Around 3000 of the essential oils are known and 10% of them having commercial importance in the cosmetic, food and pharmaceutical industries, and in agriculture [3, 4]. Therefore, they are generally recognized as safe by the FDA (Food and Drug Administration). Its composition can vary considerably between species of aromatic plants and varieties and within the same variety of different geographical areas [1].

Methodology

An exhaustive search was carried out in PubMed, Scopus, Google scholar and SciELO databases to find an article that related the different biological activities of essential oils and their components. The search was conducted until January 2018. A text-mining step was carried out in order to detect citation-associated relationships between essential oils and several biological activities. Taking into account the dates of publication and the country of origin.

These keywords were recognized through literature reviews using a wide variety of academic databases and search engines available online, such as GoPubmed (http://gopubmed.org/web/gopubmed/), pubGraph (http://datamining.cs.ucla.edu/cgi-bin/pubgraph.cgi), and Helioblast (http://helioblast.heliotext.com/) and the analysis of associations among these terms was done in the PubMed/Medline literature database was carried out using the Jaccard co-occurrence score, as a measure of the degree to which the two queries coincide among all publications. The information obtained was organized in order to identify the reported biological activity, the essential oil responsible for the activity and the biologically active concentration.

Results

Bioactivity of essential oils

The EOs has a wide application in pharmacology (see figure 1), especially for their antimicrobial properties [5, 6], the hydrocarbon and oxygenated monoterpenes are able to destroy the cellular integrity and therefore inhibit respiration and transport of ions [7]. The terpenes; Pine, myrcene, limonene, Ocimene, linalool, and verbenum are related to the antimicrobial activity of the essential oil of *Bidens pilosa* [7]. Essential oils with an abundance of phenylpropanoids and phenols inhibit platelet aggregation. The α-terpineol has cytotoxic properties, D-limonene, anticancer in male rats [1], perillic alcohol used in the treatment of different types of cancer, which is found in Phase I and II clinical studies [8], antiseptic, anti-inflammatory, antioxidant, antifungal, antidepressant, aphrodisiac and other properties present in a greater or lesser degree in all oils [1, 3, 9, 10]. They are also used for their relaxing or stimulating effects on the Central Nervous System, bronchial, urinary infections and those caused by cuts and burns [3, 11].

Many studies carried out with essential oils have reported that they have a broad microbiological activity such as: antifungal [12], antibacterial [13-15], acaricide [16], insecticide [17,18], antimalarial [19], quorum sensing [20], and antiviral [21]. They also have properties such as: analgesics [7], antipyretics [22], anti-inflammatories [7, 23], anticonvulsants [24], as an estrogenic agent [25], hepatoprotective [26], anticancer [27] and antimutagenic [28]. They are also used in the treatment of gastric ulcer and different types of cancer [3].

The EOs has shown antiviral activity against species of the Flavivirus genus. In fact, it has been shown that the EOs of *Lippia origanoides*, *Oreganum vulgare*, *Lippia alba* and Artemisia vulgaris have an antiviral effect against the yellow fever virus [29]. Nowadays, there are reports of the antiviral activity of essential oils against the dengue virus. Authors such as Pájaro-Castro *et al.* [30], Ocazionez *et al.* [31], Meneses *et al.* [32], Meneses *et al.* [33], Duschatzky *et al.* [34] and García *et al.* [35] has revealed the antiviral properties of these natural products. In the field of agriculture, EOs have been recognized for their repellent activity [36, 37], insecticide and fumigant [38-40]. Neiro *et al.*, [1] reported more than 80 different essential oils families with repellent activity for arthropod species.

Table 1. Biological activities reported for essential oils.

Bioactivity reported	Reference
Antibacterials	[13-15]
Antivirals	[30-35]
Antifungals	[12]
Antimalarial	[19]
Insecticides	[17-18]
Insect repellents	[36-37]
Antidepressant	[1,3]
Anticancer	[27]
Antimutagenic	[28]
Hepatoprotective	[26]
Antiinflammatory	[7, 23]
Antioxidant	[1, 3]
Analgesics and antipyretics	[7, 22]
Anticonvulsants	[24]

Taking into account that essential oils are complex mixtures of many molecules, it is important to establish if the biological activities identified in them are due to a single component or several of them, that is, if their biological effects are the result of a synergy of all the molecules or if they reflect only the main molecules present at the highest levels according to the gas chromatography analysis [1, 2]. The studies found in the literature generally do not answer this question. In general, it is found that the main components reflect fairly well the biological characteristics of the essential oils from which they were isolated, and their effects depend only on their concentration when each component is analyzed independently or in some cases of the mixture. Therefore, it is possible that the activity of the main components is modulated by other molecules that are in lower concentration in the essential oil. In that sense, for biological purposes, it is more informative to study a complete essential oil instead of some of its components because the concept of synergy seems to be more significant [3].

In the search carried out using the keyword essential oils, 73814 articles were observed until 2018. An increase in the number of public articles was observed, being 929 in the year 1994, this value has been increased every year until 5853 in the year 2017 and 1524 until January 2018. The journals that have most published articles related to essential oils are: *Food Chemistry* (1746), *Journal of Chromatography A.* (1350), *Industrial Crops and Products* (1307) and *Phytochemistry* (1159).

When the search was carried out using the keywords essential oils and biological activity, 27.021 articles published up to 2018 were found, as well as an increase in the number of publications each year, being 319 for the year 1994 and 2656 for the year 2017, being 713 publications so far in 2018. Table 1 shows some of the essential oils with their concentrations reported with some biological activity worldwide. Taking into account the Jaccard co-occurrence e (-1.0), there is a clear association between the essential oils and the different biological activities reported. The main journals that have published an article with these two key words were: *Food Chemistry* (643), *Industrial Crops and Products* (625), *Journal of Ethnopharmacology* (549), *Journal of Chromatography A* (434), *Food and Chemical Toxicology* (375) and *Phytochemistry* (326).

General considerations

According to the bibliographic search carried out, essential oils are an important and rich source of bioactive molecules, which can be used in different fields of pharmaceutical sciences. In fact, many of these studies are focused on evaluating the phytochemical profile of a particular essential oil. The main biological activity attributable to essential oils is the antioxidant activity with 17846 reports (24.2%) until January 2018. In these studies, this activity has been reported in more than 100 essential oils from different plant species.

Table 2. Essential oils with their concentrations reported with some biological activity.

Biological activity	Eos	Concentration	Country	Publication date	Reference
Antioxidant	*Bidens pilosa* Linn	**49.7 µg/mL**	Japan	2008	[7]
	Plectranthus amboinicus	**23.97 µg/mL**	Colombia	2015	[10]
	Citrus sinensis	**6-23%**	Mexico	2017	[28]
	Citrus latifolia	**22-71%**	Mexico	2017	[28]
Antiseptic action	*Eugenia caryophyllata*	**2%**	Colombia	2017	[9]
	Cinnamomum verum	**2%**	Colombia	2017	[9]
Antibacterial activity	*Citrus sinensis*	**600 mg/mL**	Colombia	2017	[13]
	C. aurantifolia	**600 mg/mL**	Colombia	2017	[13]
	C. reticulata	**600 mg/mL**	Colombia	2017	[13]
	C. paradisi	**600 mg/mL**	Colombia	2017	[13]
	Minthostachys mollis	**500 mg/mL**	Colombia	2016	[14]
	Thymus vulgaris	**300-800 ppm**	Colombia	2015	[15]
	Cinnamomum verum	**300-800 ppm**	Colombia	2015	[15]
	Eugenia caryophyllata	**300-800 ppm**	Colombia	2015	[15]
Antiquorum sensing activity	*Piper bredemeyeri*	**45.6 µg/mL**	Colombia	2011	[20]
	Piper brachypodom	**93.1 µg/mL**	Colombia	2011	[20]
	Piper bogotence	**513.8 µg/mL**	Colombia	2011	[20]
Acaricidal activity	*Syzygium aromaticum*	**2.5 mg/mL**	Brazil	2018	[16]
Fumigant toxicity	*Curcuma longa*	**11.36 mg/ liter air**	India	2002	[17]
Insecticidal activity	*Coriandrum sativum*	**5.25 µL/L air**	Colombia	2015	[30]
	Cymbopogon martinii	**37.2 µL/L air**	Colombia	2015	[40]
	Cymbopogon nardus	**0.03-0.04 µL/ cm^2**	Colombia	2015	[40]
Hepatoprotective	*Mentha piperita L*	**15 mg/kg**	Africa	2018	[26]
Antitrypanosomal activity	*C. citratus*	**1.83 µg/mL**	Benin	2014	[19]
	C. giganteus	**0.25 µg/mL**	Benin	2014	[19]
	C. nardus	**5.71 µg/mL**	Benin	2014	[19]
	C. schoenantus	**2.1 µg/mL**	Benin	2014	[19]

(*Continúa*)

Table 2. Essential oils with their concentrations reported with some biological activity (*continuación*).

Biological activity	Eos	Concentration	Country	Publication date	Reference
Anti-nociceptive activity	*Globba sessiliflora*	**100 mg/kg**	India	2017	[22]
Anti-inflammatory activity	*Globba sessiliflora*	**100 mg/kg**	India	2017	[22]
Antipyretic activity	*Globba sessiliflora*	**100 mg/kg**	India	2017	[22]
Anticonvulsant activity	*Laurus nobilis*	**1 mL/kg**	Iran	2002	[24]
Estrogenic activity	*Pimpinella. isaurica*	**45 - 650 mcg/mL**	Turkey	2004	[25]
	P. peucedanifolia	**45 - 650 mcg/mL**	Turkey	2004	[25]
Anticancer activity	*Elsholtzia ciliata*	**0.017–0.021%**	Lithuanian	2017	[27]
Antimutagenic activity	*Citrus sinensis*	**5 µg/pl**	Mexico	2017	[28]
	Citrus latifolia	**5 µg/pl**	Mexico	2017	[28]
Antiviral effect	*Lippia origanoides*	**1.1 mcg/mL**	Colombia	2009	[29]
	Lippia alba	**100 mcg/mL**	Colombia	2009	[29]
	Oreganum vulgare	**100 mcg/mL**	Colombia	2009	[29]
	Artemisia vulgaris	**100 mcg/mL**	Colombia	2009	[29]
	L. citriodora	**1.9-33.7 mcg/mL**	Colombia	2009	[31]
	Heterothalamus alienus	**44.2 ppm**	Argentina	2010	[34]
	Buddleja cordobensis	**39.0 ppm**	Argentina	2010	[34]
	Lippia junelliana	**14-20 ppm**	Argentina	2003	[35]
	Lippia turbinate	**14-20 ppm**	Argentina	2003	[35]
Repellent activity	*Ocimum campechianum*	**0.00006 µL/cm^2**	Colombia	2014	[37]
	P. pseudolanceifolium	**0.0001 µL/cm^2**	Colombia	2014	[37]
	Cananga odorata	**0.2 µL/cm^2**	Colombia	2011	[41]
	Lippia alba	**0.0002 µL/cm**	Colombia	2011	[41]

Table 2. Essential oils with their concentrations reported with some biological activity (*continuación*).

Biological activity	Eos	Concentration	Country	Publication date	Reference
	Tagetes minuta	**0.0021 mg**	Kenya	2014	[42]
	Tithonia diversifolia	**0.263 mg**	Kenya	2014	[42]
	Lippia pedunculosa	**60 ppm**	Brazil	2017	[43]

The second biological activity that has been most reported for essential oils is the antimicrobial activity with 8815 (11.9%), followed by insecticidal and repellent activity with 7827 (10.6%), and the least reported activities are anticancer, estrogen, hepatoprotective, anticonvulsant, antimutagenic, antiviral, antipyretic, acaricide, antinoceptive, antitripanosomal, anti-inflammatory activity, from major to minor.

The above indicates the great potential of essential oils as sources of bioactive molecules, however it is important to consider the complex chemical composition of these natural products, and the interaction of these to have a certain activity. So, the mechanism of action of essential oils is difficult to understand and in some cases is not completely elucidated. In fact, it has been reported that some essential oils have a synergistic effect [44-49]. An example of this is the use of essential oils in the development of biopesticides with different mechanisms of action and that often exhibit mutual synergistic relationships, which can be effective in preventing the development of populations of pathogens and resistant pests. However, it is important to establish relationships between individual substances in EOs and the effects of sublethal concentrations in white and non-white organisms [50]. In addition, essential oils are very useful, although it is a challenge to identify if a certain action is by individual components or by mixtures of them, as well as to elucidate their mechanism of action.

Conclusions

In summary, EOs are an excellent source of metabolites with a wide range of bioactive molecules that can be used in different areas of our lives, because they have been shown to be safe for humans and the environment.

Disclosure statement

No potential conflict of interest was reported by the authors.

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