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Volatile chemical emissions from essential oils with therapeutic claims

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Abstract

Essential oils emit many volatile organic compounds (VOCs), with some considered potentially hazardous. However, little is known about specific emissions from essential oils that make therapeutic claims for health and well-being. This study investigated VOCs emitted from 14 commercially available essential oils with therapeutic claims, such as beneficial for coughs, colds, flus, relaxation, sleep, tension, headaches, stress, or skin irritation. The essential oils were selected from different brands and types, such as tea tree oil, lavender oil, eucalyptus oil, geranium oil, peppermint oil, bergamot oil, orange oil, and oil blends. Analyses were performed using headspace gas chromatography/mass spectrometry (GC/MS). The analyses found 1034 VOCs emitted from the 14 essential oils, representing 378 VOC identities. The most prevalent VOCs (in more than 90% of the oils) were acetaldehyde, alpha-phellandrene, alpha-pinene, camphene, limonene, methanol, terpinolene, 3-carene, acetone, beta-phellandrene, ethanol, and gamma-terpinene. Among the 1034 VOCs emitted, 251 VOCs, representing 60 VOC identities, are classified as potentially hazardous. The most prevalent potentially hazardous VOCs were acetaldehyde, limonene, methanol, acetone, ethanol, and 3-carene. Toluene was found in more than 70% of the essential oils. Each of the essential oils emitted 9 or more potentially hazardous VOCs. Fewer than 1% of all VOCs identified and fewer than 1% of all potentially hazardous VOCs were listed on any essential oil label, safety data sheet, or website. Results from this study provide new findings on VOC emissions from essential oils with therapeutic claims, which can help to improve public awareness about potential exposures and risks.

Keywords Essential oils · Therapeutic · Emissions · Volatile organic compounds · Hazardous compounds · Fragrance · Ingredients

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Introduction

Essential oils with therapeutic claims are widely used in many public and private places for different purposes, such as aromatherapy, antibacterial effects, and alleviation of cold and flu symptoms. Essential oils, such as tea tree oil, lavender oil, eucalyptus oil, peppermint oil, and orange oil, are complex mixtures of many different compounds (e.g., Milhem et al. 2020; Nematollahi et al. 2018a; Huang et al. 2012).

Numerous studies have examined potential health benefits of essential oils. For example, Shaaban et al. (2012) reviewed bioactivities associated with essential oils, including antibacterial, antiviral, anti-inflammatory, and additional properties. More specifically, Cavanagh and Wilkinson (2002) reviewed the physiological and psychological effects associated with lavender oil.

However, relatively few studies have examined potential hazards of essential oils. Exposure to essential oils has been associated with adverse health effects such as skin irritation

Table 1 VOCs emitted from the 14 essential oils *

	Emitted		Listed (on product label, safety data sheet, or website)	
Number of essential oils	All emitted VOCs	Potentially hazardous VOCs	All listed VOCs	Potentially hazardous VOCs
14	1034 occurrences 378 identities	251 occurrences 60 identities	9 occurrences 8 identities	1 occurrence 1 identity

"VOC occurrences" refers to the number of individual VOCs emitted from the essential oils

"VOC identities" refers to the number of unique VOCs emitted from one or more of the essential oils

and allergic contact dermatitis (Sarkic and Stappen 2018). Milhem et al. (2020) detailed negative effects of essential oils on indoor air quality.

Furthermore, relatively few studies have analyzed VOCs emitted from commercially available essential oils. In prior analyses of essential oils, Nematollahi et al. (2018a) found the most prevalent VOCs (emitted from more than 70% of 24 oils) were alpha-pinene, limonene, and acetone. Chiang et al. (2010) found the most prevalent (> 40% of 5 oils) were limonene, eucalyptol, and camphor. Francis and Stusdal (2014) found the most prevalent (> 70% of 3 oils) were beta-pinene, *p*-cymene, limonene, menthone, menthofuran, neomenthol, menthol, 4-terpineol, menthyl acetate, and β-bourbonene. Chiu et al. (2009) found the most prevalent (> 60% of 5 oils) were limonene, eucalyptol, heneicosane, and alpha-terpineol. Thus, commonly emitted compounds were terpenes (e.g., limonene, beta-pinene, and alpha-pinene).

Table 2 Most prevalent VOCs emitted from the 14 essential oils

Compound	CAS no.	Prevalence (no. of products)
Acetaldehyde*	75-07-0	14
Alpha-phellandrene	99-83-2	14
Alpha-pinene	80-56-8	14
Camphene	79-92-5	14
Limonene*	138-86-3	14
Methanol*	67-56-1	14
Terpinolene	586-62-9	14
3-Carene*	13466-78-9	13
Acetone*	67-64-1	13
beta-Phellandrene	555-10-2	13
Ethanol*	64-17-5	13
Gamma-terpinene	99-85-4	13
Alpha-terpineol	98-55-5	12
Beta-pinene	127-91-3	12
Isovaleraldehyde	590-86-3	12
Linalool	78-70-6	12
Beta-myrcene*	123-35-3	11
Isobutyraldehyde	78-84-2	11
1,1-Dimethylallyl alcohol	115-18-4	10
2-Methylfuran	534-22-5	10
3-Methylfuran	930-27-8	10
Beta-trans-ocimene	3779-61-1	10
Toluene*	108-88-3	10
Caryophyllene	87-44-5	9
Eucalyptol	470-82-6	9
Pentane*	109-66-0	9

*Classified as potentially hazardous

Despite this prior work, little information exists on the specific VOCs, including potentially hazardous compounds, emitted from commercially available essential oils that make therapeutic claims for health and well-being.

This study investigates VOCs emitted from 14 therapeutic essential oils, with four main objectives: (1) to analyze VOC emissions from individual essential oils with therapeutic claims, (2) to identify VOCs classified as potentially hazardous, (3) to determine the most prevalent VOCs and potentially hazardous VOCs, and (4) to compare differences between the VOCs emitted and the ingredients listed on essential oil labels, safety data sheets, and manufacturers' websites.

Materials and methods

For this study, a set of 14 essential oils were analyzed, representing different brands and aromas, including lavender oil, eucalyptus oil, tea tree oil, geranium oil, peppermint oil, bergamot oil, orange oil, and oil blends. Essential oils were selected based on claims of therapeutic benefits, such as the following: alleviates symptoms of colds, coughs, and flus; provides calming and relaxing effects; eases tension, headaches, stress, anxiety, depression, and anger; offers a natural antiseptic; soothes irritated skin; and promotes peaceful sleep for both adults and babies. Essential oils in this study were purchased from aromatherapy stores, supermarkets, pharmacies, and organic stores, in both Australia and the United States.

Headspace GC/MS was used to analyze VOCs emitted from the essential oils using a capillary column and an automated injection system. Details about the analytic methods are provided in Nematollahi et al. (2018b).

Table 3 Potentially hazardous VOCs emitted from the 14 essential oils

Compound	CAS no.	Prevalence (no. of products)	SWA	Prop65	HAPs	Asthmagens
Acetaldehyde**	75-07-0	14	✓	✓	✓	
Limonene	138-86-3	14	✓			
Methanol	67-56-1	14	✓	✓	✓	
Acetone	67-64-1	13	✓			
Ethanol	64-17-5	13	✓			
3-Carene	13466-78-9	13				✓
Beta-myrcene	123-35-3	11		✓		
Toluene	108-88-3	10	✓	✓	✓	
Pentane	109-66-0	9	✓			
2-Methylpropan-1-ol	78-83-1	8	✓			
Butanone	78-93-3	8	✓			
Ethyl acetate	141-78-6	8	✓			
2-Methyl-1-propene	115-11-7	7	✓			
Isopropyl alcohol	67-63-0	7	✓			
Methyl acetate	79-20-9	7	✓			
1-Hexanol	111-27-3	6	✓			
Methyl isobutyl ketone	108-10-1	6	✓	✓	✓	
Propanal	123-38-6	6	✓		✓	
Butyl butyrate	109-21-7	5	✓			
Methyl formate	107-31-3	5	✓			
Ethyl formate	109-94-4	4	✓			
Fenchyl alcohol	1632-73-1	4	✓			
2,4-Dimethylhexane	589-43-5	3	✓			
2-Methylpropyl ester	110-19-0	3	✓			
3-Methylhexane	589-34-4	3	✓			
Butane	106-97-8	3	✓			
Butyl acetate	123-86-4	3	✓			
Hexane	110-54-3	3	✓	✓	✓	
Isopentane	78-78-4	3	✓			
(Z)-but-2-ene	590-18-1	2	✓			
2-Butanol	78-92-2	2	✓			
2-Butene	107-01-7	2	✓			
2-Methylpentane	107-83-5	2	✓			
Isoamyl acetate	123-92-2	2	✓			
Isoprene (stabilized)	78-79-5	2	✓	✓		
Tetracarbonylnickel	13463-39-3	2	✓	✓		✓
(E)-citral	141-27-5	1	✓			
(R)-(−)-2-butanol	14898-79-4	1	✓			
1-Heptanol	111-70-6	1	✓			
1-Methoxy-2-propanol	107-98-2	1	✓			
1-Octanol	111-87-5	1	✓			
2,2-Dimethylbutane	75-83-2	1	✓			
2,3,4-Trimethylpentane	565-75-3	1	✓			
2-Methoxy-1-methylethyl acetate	108-65-6	1	✓			
2-Methylbutyl acetate	624-41-9	1	✓			
3-Ethyl-3-methylpentane	1067-08-9	1	✓			
3-Methylpentane	96-14-0	1	✓			
3-Pentanone	96-22-0	1	✓			
Acetaldehyde diethyl acetal	105-57-7	1	✓			

Table 3 (continued)

Compound	CAS no.	Prevalence (no. of products)	SWA	Prop65	HAPs	Asthmagens
Benzene***	71-43-2	1	✓	✓	✓	
Butyl formate	592-84-7	1	✓			
Butyraldehyde	123-72-8	1	✓			
Furan	110-00-9	1	✓	✓		
Isobutyl methacrylate	97-86-9	1	✓			
Isopentyl formate	110-45-2	1	✓			
Isopropyl propionate	637-78-5	1	✓			
Methyl isopropyl ketone	563-80-4	1	✓			
Sec-butyl acetate	105-46-4	1	✓			
(R)-(+)-pulegone	89-82-7	1		✓		
Dimethyl phthalate	131-11-3	1			✓	

SWA, Safe Work Australia (SWA) contains a Hazardous Chemical Information System ("HCIS") with a database of chemicals and hazard classifications (SWA 2020); *Prop65*, California Proposition 65 (OEHHA 2020); *HAPs*, Hazardous Air Pollutants (HAPs), United States Environmental Protection Agency (EPA 2017), including carcinogenic HAPs (EPA 2018)

**Classified as possibly carcinogenic (2B) (EPA 2018)

***Classified as carcinogenic (1) (EPA 2018)

Asthmagens: Association of Occupational and Environmental Clinics (AOEC 2020)

"Potentially hazardous VOCs were identified according to classifications of (i) hazardous air pollutants (HAPs), United States Environmental Protection Agency (EPA 2017), including carcinogenic HAPs (EPA 2018), (ii) Hazardous Chemical Information System (HCIS), Safe Work Australia (SWA 2020), and (iii) asthmagens, Association of Occupational and Environmental Clinics (AOEC 2020)" following Steinemann et al. (2020). This classification approach, however, is not intended as an assessment of safety or hazard from use of the essential oils.

Results and discussion

VOCs emitted

The VOCs emitted from this group of essential oils are summarized in Table 1. In this paper: "The term 'VOC occurrences' refers to the number of individual VOCs emitted from the products, such that each VOC occurrence represents a single volatile ingredient in a single product. The term 'VOC identities' refers to the number of distinctly named VOCs emitted from the products, such that each VOC identity represents a compound, according to name and CAS number, that occurs in one or more of the products" following Steinemann et al. (2020).

Among the 14 essential oils, 1034 VOC occurrences, representing 378 VOC identities, were emitted. Each essential oil emitted between 40 to 116 VOCs. Detailed information about the VOCs emitted from each of the essential oils is provided in Supplementary Tables 1 and 2.

Most prevalent VOCs

Among the 14 essential oils, the most prevalent VOCs (in more than 90% of all essential oils) were acetaldehyde, alpha-phellandrene, alpha-pinene, camphene, limonene, methanol, terpinolene, 3-carene, acetone, beta-phellandrene, ethanol, and gamma-terpinene (Table 2).

Potentially hazardous emissions

All essential oils emitted at least 9 VOCs classified as potentially hazardous, and 50% of the oils emitted at least 20 potentially hazardous VOCs (Supplementary Table 1). Among the 14 essential oils, the most prevalent potentially hazardous VOCs (in more than 90% of all essential oils) were acetaldehyde, limonene, methanol, acetone, ethanol, and 3-carene (Table 3). To note, acetaldehyde, limonene, and methanol were emitted from all of the essential oils.

Regulatory classifications

Among the 1034 VOCs emitted, 251 VOC occurrences (60 VOC identities) are classified as potentially hazardous under one or more criteria (Table 3). Specifically, among the 251 VOCs, 225 VOCs (56 identities) are classified as potentially hazardous under Safe Work Australia (SWA 2020); 65 VOCs (11 identities) under California Proposition 65 (OEHHA 2020); 55 VOCs (8 identities) as Hazardous Air Pollutants (EPA 2017), including 15 VOCs (2 identities) as carcinogenic HAPs (EPA 2018); and 15 VOCs (2 identities) as asthmagens under the Association of Occupational and Environmental Clinics (AOEC 2020).

Listing of ingredients

Among all the 1034 VOC occurrences, only 9 VOCs were listed on any essential oil label, safety data sheet, or website. Thus, fewer than 1% of all identified VOCs were disclosed. Moreover, among all the 251 VOCs classified as potentially hazardous, only 1 VOC was listed, on a website. Thus, fewer than 1% of all identified potentially hazardous VOCs were disclosed.

Conclusions

This study analyzed VOC emissions from a variety of 14 essential oils that make therapeutic claims. The analyses found the oils collectively emitted 1034 VOCs, representing 378 VOC identities. Among these emissions, 251 VOCs, representing 60 VOC identities, are classified as potentially hazardous. The most prevalent VOCs emitted (in all 14 oils) were acetaldehyde, alpha-phellandrene, alpha-pinene, camphene, limonene, methanol, and terpinolene. Most prevalent potentially hazardous VOCs emitted (in all 14 oils) were acetaldehyde, limonene, and methanol. Results from this study provide new information on volatile compounds emitted from therapeutic essential oils, which can help to improve public awareness about potential exposures and risks.

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