

Nematollahi N, Kolev SD, Steinemann A 2018. Volatile chemical emissions from essential oils. Air Quality, Atmosphere & Health doi: <https://doi.org/10.1007/s11869-018-0606-0>

Volatile Chemical Emissions from Essential Oils

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This is a pre-print of an article published in Air Quality, Atmosphere & Health. The final authenticated version is available online at: <https://doi.org/10.1007/s11869-018-0606-0>

Volatile Chemical Emissions from Essential Oils

Essential oils, widely used in society, emit numerous volatile organic compounds (VOCs). Some of these VOCs are considered as potentially hazardous under federal regulations. However, essential oils are exempt from disclosure of their ingredients on their label. Thus, the public may lack information on emissions and potential hazards from essential oils. This study examined VOCs emitted from a range of commercial essential oils, including tea tree oils, lavender oils, eucalyptus oils, and other individual oils and mixtures of oils. Using headspace gas chromatography/mass spectrometry (GC/MS), the study analyzed 24 commercial essential oils, including 12 with claims of being "natural" or related terms, such as organic, 100% pure, or plant-based. Results identified 595 VOCs emitted from the 24 essential oils, representing 188 different VOCs. The most common VOCs emitted were alpha-pinene, limonene, acetone, linalool, alpha-phellandrene, beta-myrcene, and camphene. Among the 589 VOCs identified, 124 VOCs, representing 33 different VOCs, are classified as potentially hazardous. All natural and regular essential oils emitted one or more potentially hazardous VOCs, such as acetaldehyde, acetone, and ethanol. Toluene was also found in 50% of essential oils. Moreover, for the prevalent VOCs classified as potentially hazardous, no significant difference was found between regular and natural essential oils. This study provides insights and information about emissions of commercial essential oils that can be useful for public awareness and risk reduction.

Keywords: essential oils, fragrance, volatile organic compounds, emissions, ingredients

Introduction

Essential oils, such as lavender oil, orange oil, eucalyptus oil, and tea tree oil, are widely used in cosmetics, cleaning supplies, fragranced products, building systems, and aromatherapy. Essential oils are complex mixtures of various compounds such as terpenes (Huang et al. 2012). Exposure to compounds emitted from essential oils has been associated with adverse health effects such as skin irritation (Chiang et al. 2010; Sarkic and Stappen 2018), asthma exacerbation, decrease of pulmonary function, chest tightness, and wheezing (Su et al. 2007). Moreover, exposure to some of these compounds during pregnancy may potentially harm a developing fetus (Bagasra et al. 2013).

Numerous studies have examined essential oils, and most used their own extracted oils from plant leaves, roots or fruits (Isidorov and Jdanova 2002; Winters et al. 2009; Helmig et al. 2013; González-Rivera et al. 2016), instead of commercially available essential oils. In addition, studies on essential oils typically focus on providing information about anti-bacterial and anti-oxidant benefits (Lee et al. 2005, 2013) rather than emissions or possible risks.

Among the literature, a relatively small subset of studies examined VOC emissions from commercially available essential oils. For example, Chiang et al. (2010) analysed emitted compounds from five essential oils (i.e., lavender, lemon, rose, rosemary, and tea tree), and found the main carbonyl compounds were acetaldehyde, formaldehyde, acetone, and propionaldehyde. Chiu et al. (2009) analysed VOC emissions from five essential oils (i.e., rose, lemon, rosemary, tea tree, and lavender), and found the predominant VOCs were toluene, 1,2,3- trimethylbenzene, 1,2,4-trimethylbenzene, n-undecane, p-diethylbenzene, and m-diethylbenzene. Cheng and Lai (2014) analyzed by-products of tea tree essential oils, and

found alkane compounds such as propane and isobutane, as well as aromatic compounds such as ethylbenzene, m/p-xylene, 1,2,3-trimethylbenzene, 1,2,4 trimethylbenzene, 1,4-diethylbenzene, and acetone. Su et al. (2007) analyzed three essential oils (i.e., lavender, eucalyptus, and tea tree), and showed the main VOCs were linalool, linalyl arthanilate, eucalyptol, D-limonene, ρ -cymene, γ -terpinene, and terpinene-4-ol-, all from the family of terpenes. Francis and Stusdal (2014) analyzed three mint essential oils (i.e., peppermint oil, Japanese peppermint, and spearmint oil), and found the main compounds from peppermint and Japanese peppermint oil were menthone, menthol, limonene, 1,8-cineole, menthofuran, and neomenthol, and from spearmint oil were carvone, limonene, and 1,8-cineole. Collectively, these studies provide evidence that essential oils emit numerous VOCs, with some considered as potentially hazardous. However, most studies analyzed five or fewer essential oils rather than a range of types and brands, which is a contribution of this present study.

This study investigates the VOCs emitted from a variety of 24 commercial essential oils of different types and brands, including both regular and natural essential oils. In addition, this study compares the emitted VOCs from both regular and natural essential oils, and examines their classifications as potentially hazardous under federal regulations. "Essential oil" will be considered, for this paper, as an oil derived from or with the aroma of the essence of a plant substance. The term "Commercial essential oils" in this study refers to essential oils that are publicly available for purchase. The classifier "natural" for essential oils refers to oils or diffusers with the claim of "natural" or a related term such as "certified organic," "100% pure," "organic," "no petrochemicals," "non-toxic," or "plant-based," for the whole essential oil or individual ingredients. However, this study did not seek to authenticate the product claims of "natural." The classifier "regular" for essential oils refers to those not in the natural category.

Materials and methods

Headspace GC/MS was used to analyze VOCs emitted from 24 essential oils. Essential oils were in two categories: 12 regular and 12 natural. The regular category included 2 lavender oils, 2 jasmine oils, 1 orange oil, 1 English rose oil, 1 rose and grapefruit oil, 1 lemongrass oil, and 4 mixture of aromas oils. The natural category included 2 tea tree oils, 2 eucalyptus oils, 1 lavender oil, 1 orange oil, 1 peppermint oil, 1 lime and coconut oil, and 4 mixtures of aromas oils. Commercial essential oils in this study were purchased from supermarkets, aroma stores, organic stores, and pharmacies in Australia, and were from both domestic and international suppliers.

Headspace GC/MS analysis of the essential oils was performed using a Shimadzu GC/MS equipped with a BPX-VOL capillary column. The volatile components of samples were identified based on the mass spectral library of the National Institute of Standards and Technology NIST Version 2.0 (Stein 2008). More details about the GC/MS methods are described in Nematollahi et al. (2018). Although the chromatograms of most of the essential oils exhibited more than 100 peaks (see Supplementary Figure, available online), only the top 25 peaks for each of the samples were processed.

Emitted VOCs from essential oils were examined for classification as (i) potentially hazardous under Australian regulations or (ii) potentially carcinogenic under the World Health Organization. For (i), Safe Work Australia (SWA) provides a Hazardous Chemical Information System (HCIS) with a database of potentially hazardous compounds (SWA 2018). Although SWA uses the Globally Harmonised System of Classification and Labelling of Chemicals (GHS 2018) with concentration thresholds to determine a specific hazard class and category, overall risk depends on additional factors such as exposures. For (ii), the World Health Organization, International Agency for Research on Cancer (IARC) (World Health Organization (WHO) 2018), evaluates compounds for their potential

carcinogenic risk to humans. However, these two analyses do not suggest that the VOCs discussed in the current study are the only potentially hazardous compounds emitted from essential oils. Moreover, this study focused on individual compounds, and did not examine potential hazards of one or more compounds together in one essential oil.

Results and Discussion

VOCs emitted

Each essential oil emitted between 20 to 140 VOCs (see Supplementary Tables 1 and 2, available online). Table 1 shows the summary of VOCs emitted from "natural" and "regular" essential oils. In this paper, the term "VOC occurrences" represents the number of individual VOCs emitted from each essential oil corresponding to the top 25 chromatographic peaks. The term "VOC identities" represents the number of unique VOCs, which can be emitted from one or more of the essential oils. For all the 24 essential oils, the numbers of VOC occurrences and identities were 589 and 188, respectively. Supplementary Tables 3, 4, and 5 (available online) provide details about the VOCs emitted from all 24 essential oils, and subsets of "natural" essential oils and "regular" essential oils.

Most prevalent VOCs

Among the 24 essential oils, the most prevalent VOCs (in at least 50% of all essential oils) were alpha-pinene, limonene, acetone, linalool, alpha-phellandrene, beta-myrcene, camphene, ethanol, beta-pinene, 3-carene, eucalyptol, acetaldehyde, beta-phellandrene, gamma-terpinene, m-cymene, beta-trans-ocimene, methanol, and terpinene. In "regular" essential oils, the most prevalent VOCs (in at least 50% of regular essential oils) were acetaldehyde, linalool, 1-(2-methoxy-1-methylethoxy)propan-2-ol, alpha-pinene, limonene, acetone, ethanol, and 1-(2-methoxypropoxy)propan-2-ol. In "natural" essential oils, the most prevalent VOCs (in at least 65% of natural essential oils) were alpha-pinene, alpha-phellandrene, beta-

pinene, limonene, 3-carene, beta-myrcene, eucalyptol, gamma-terpinene, camphene, acetone, beta-phellandrene, and m-cymene. Table 2 presents the most prevalent VOCs.

Regulatory classifications

All the essential oils emitted at least 1 VOC classified as potentially hazardous (Supplementary Table 1 and 2, available online). Among all the 589 VOC occurrences, 124 VOCs were classified as potentially hazardous under Australian regulations (Table 3). The most prevalent potentially hazardous compounds (in at least 40% of essential oils) were limonene, acetone, ethanol, acetaldehyde, and methanol.

Table 4 presents the most common potentially hazardous compounds, as classified under Safe Work Australia (SWA 2018), among all emitted compounds (not only those corresponding to the top 25 chromatographic peaks). These results indicate that acetaldehyde, acetone and ethanol were emitted from almost all (over 90%) of the essential oils studied. Toluene was also emitted from 50% of essential oils. Table 5 indicates the carcinogenic risks of compounds among all emitted compounds (not only those corresponding to the top 25 chromatographic peaks). Among these emitted compounds, 6 VOCs, representing 49 VOC occurrences, are classified as Group 1, 2, or 3 under the World Health Organisation (WHO 2018).

Potentially hazardous emissions

All "natural" essential oils emitted at least 3 VOCs classified as potentially hazardous, i.e., acetaldehyde, acetone, and methanol (Table 4). All "regular" essential oils emitted at least 1 VOC classified as potentially hazardous, i.e., acetaldehyde (Table 4.). The most prevalent potentially hazardous VOCs emitted by at least 50% of all "natural" and "regular" essential oils were the same. Interestingly, the prevalences of 3 out of 7 of the most prevalent

compounds were higher in "natural" essential oils than in "regular" essential oils. Moreover, for the prevalent VOCs classified as potentially hazardous (Table 4), no significant difference was found between regular and natural essential oils ($p < 0.05$, t-test).

Limitations

The current study was focused on identifying primary VOC emissions from essential oils, but other relevant phenomena such as the formation of secondary pollutants (e.g., formaldehyde) and the effect of VOC concentrations and exposures on the overall risk could also be investigated. In addition, while the study identified what VOCs were present, it did not seek to determine why those VOCs were present, which could be associated with factors such as sources and extraction methods. Finally, the study did not seek to authenticate whether the essential oils that claimed to be "natural" were in some way truly natural.

Conclusions

This study analysed VOCs emissions from 24 commercial essential oils of different types and brands. The results indicated that 589 VOCs, representing 188 different VOCs, were emitted, with 124 VOCs, representing 33 different VOCs, classified as potentially hazardous.

Furthermore, emissions of the most prevalent potentially hazardous VOCs from "regular" and "natural" essential oils were not significantly different. Essential oils are not required to disclose their ingredients on their labels. Thus, results from this study can improve public awareness about the emitted VOCs from essential oils.

Acknowledgments

The study received support from the Australian Government Research Training Program Scholarship (RTP), through the University of Melbourne; the Australian Department of Education and Training (Australian Postgraduate Award); and the Commonwealth Scientific and Industrial Research Organisation (CSIRO). This article is dedicated to the memory of Neda Yarmahmoudi.

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Table 1: VOCs emitted from 24 essential oils.

Type	Number of essential oils	All VOCs	Potentially hazardous VOCs
Regular	12	289 occurrences 132 identities	74 occurrences 27 identities
Natural	12	300 occurrences 95 identities	50 occurrences 16 identities
Total	24	589 occurrences 188 identities	124 occurrences 33 identities

Table 2: Most prevalent VOCs emitted by the 24 essential oils

Compound	CAS #	Prevalence (# of essential oils)		
		Total	Regular	Natural
<u>All essential oils (n=24)</u>				
alpha-Pinene	80-56-8	20	8	12
Limonene*	138-86-3	19	8	11
Acetone*	67-64-1	17	8	9
Linalool	78-70-6	16	9	7
alpha-Phellandrene	99-83-2	16	4	12
beta-Myrcene	123-35-3	15	5	10
Camphene	79-92-5	15	5	10
Ethanol*	64-17-5	15	8	7
beta-Pinene	127-91-3	15	3	12
3-Carene	13466-78-9	14	3	11
Eucalyptol	470-82-6	14	4	10
Acetaldehyde*	75-07-0	13	10	3
beta-Phellandrene	555-10-2	13	4	9
gamma-Terpinene	99-85-4	13	3	10
m-Cymene	535-77-3	11	3	8
beta-trans-Ocimene	3779-61-1	10	3	7
Methanol*	67-56-1	10	3	7
Terpinolene	586-62-9	10	3	7
<u>Regular essential oils (n=12)</u>				
Acetaldehyde*	75-07-0	10		
Linalool	78-70-6	9		
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7	8		
alpha-Pinene	80-56-8	8		
Limonene*	138-86-3	8		
Acetone*	67-64-1	8		
Ethanol*	64-17-5	8		
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7	6		
<u>Natural essential oils (n=12)</u>				
alpha-Pinene	80-56-8	12		
alpha-Phellandrene	99-83-2	12		
beta-Pinene	127-91-3	12		
Limonene*	138-86-3	11		

3-Carene	13466-78-9	11
beta-Myrcene	123-35-3	10
Eucalyptol	470-82-6	10
gamma-Terpinene	99-85-4	10
Camphene	79-92-5	10
Acetone*	67-64-1	9
beta-Phellandrene	555-10-2	9
m-Cymene	535-77-3	8
Linalool	78-70-6	7
beta-trans-Ocimene	3779-61-1	7
4-Carene	29050-33-7	7
Methanol*	67-56-1	7
Ethanol*	64-17-5	7
Terpinolene	586-62-9	7
alpha-Thujene	2867-05-2	6
alpha-Terpineol	98-55-5	6

*Classified as hazardous under Safe Work Australia, Hazardous Chemical Information System (SWA 2018)

Table 3: Compounds classified as potentially hazardous* among VOCs emitted from the essential oils

Compound	CAS #	Prevalence (# of essential oils)		
		Total	Regular	Natural
Limonene	138-86-3	19	8	11
Acetone	67-64-1	17	8	9
Ethanol	64-17-5	15	8	7
Acetaldehyde	75-07-0	13	10	3
Methanol	67-56-1	10	3	7
Ethyl acetate	141-78-6	4	4	0
Ethyl formate	109-94-4	4	3	1
Methyl acetate	79-20-9	4	4	0
2-Methylpropene	115-11-7	3	3	0
Acetaldehyde diethyl acetal	105-57-7	3	3	0
cis-3,7-Dimethyl-2,6-octadien-1-ol	106-25-2	3	3	0
Methyl formate	107-31-3	3	2	1
(S)-(-)-propylene oxide	16088-62-3	2	2	0
(Z)-citral	106-26-3	1	1	0
Butane	106-97-8	3	0	3
Citral	5392-40-5	2	1	1
Isoamyl acetate	123-92-2	1	0	1
(R)-(-)-2-butanol	14898-79-4	1	1	0
1-Hexanol	111-27-3	2	0	2
1-Octanol	111-87-5	1	0	1
2,4-Dimethylhexane	589-43-5	1	0	1
2-Butene	107-01-7	1	1	0
Benzaldehyde	100-52-7	1	1	0
Benzyl alcohol	100-51-6	1	1	0
Benzyl benzoate	120-51-4	1	1	0
Butyl butyrate	109-21-7	1	0	1
Carbon disulphide	75-15-0	1	1	0
Cyclohexane	110-82-7	1	1	0
Ethyl methyl ether	540-67-0	1	1	0
Ethylbenzene	100-41-4	1	0	1
Isopropyl alcohol	67-63-0	1	0	1
Propylene glycol butyl ether	5131-66-8	1	1	0
p-Xylene	106-42-3	1	1	0

*Classified as hazardous under Safe Work Australia, Hazardous Chemical Information System (SWA 2018)

Table 4: Most common compounds classified as potentially hazardous* among all VOCs emitted from the essential oils.

Compound	CAS #	Prevalence (# of essential oils)		
		Total	Regular	Natural
Acetaldehyde	75-07-0	24	12	12
Acetone	67-64-1	22	10	12
Ethanol	64-17-5	22	11	11
Methanol	67-56-1	18	6	12
Methyl acetate	79-20-9	14	8	6
Toluene	108-88-3	12	4	8
Ethyl acetate	141-78-6	12	7	5
Ethyl formate	109-94-4	8	4	4
Isopropyl alcohol	67-63-0	7	2	5
1-Hexanol	111-27-3	6	1	5
2-Butene	107-01-7	4	1	3
Hexane	110-54-3	4	2	2
Methyl isobutyl ketone	108-10-1	4	0	4
Ethylbenzene	100-41-4	1	0	1
Benzene	71-43-2	1	0	1
p-Xylene	106-42-3	1	1	0
Benzyl alcohol	100-51-6	1	1	0

*Classified as hazardous under Safe Work Australia, Hazardous Chemical Information System (SWA 2018)

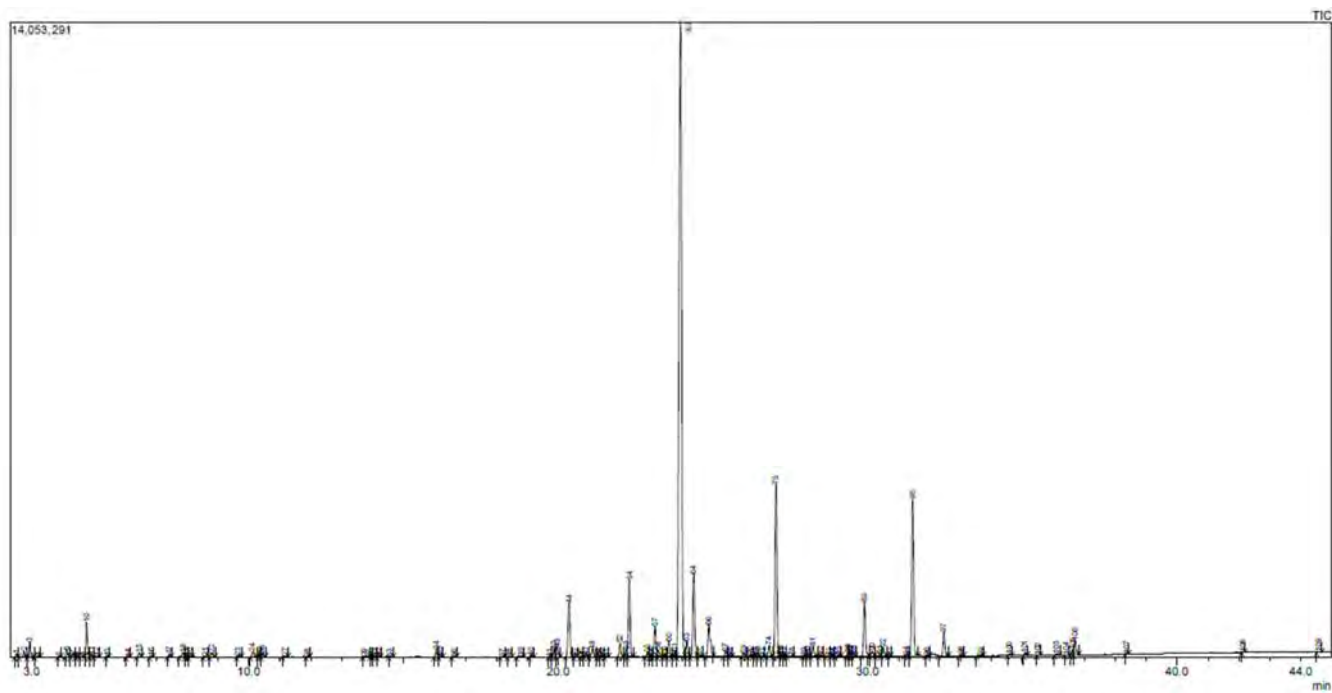
Table 5: Compounds classified for carcinogenic risk among all VOCs emitted from the essential oils.

Compound	CAS #	Classification group*	Prevalence (# of essential oils)		
			Total	Regular	Natural
Acetaldehyde	75-07-0	2B	24	12	12
Toluene	108-88-3	3	12	4	8
Isopropyl alcohol	67-63-0	3	7	2	5
Methyl isobutyl ketone	108-10-1	2B	4	0	4
Benzene	71-43-2	1	1	0	1
Ethylbenzene	100-41-4	2B	1	0	1

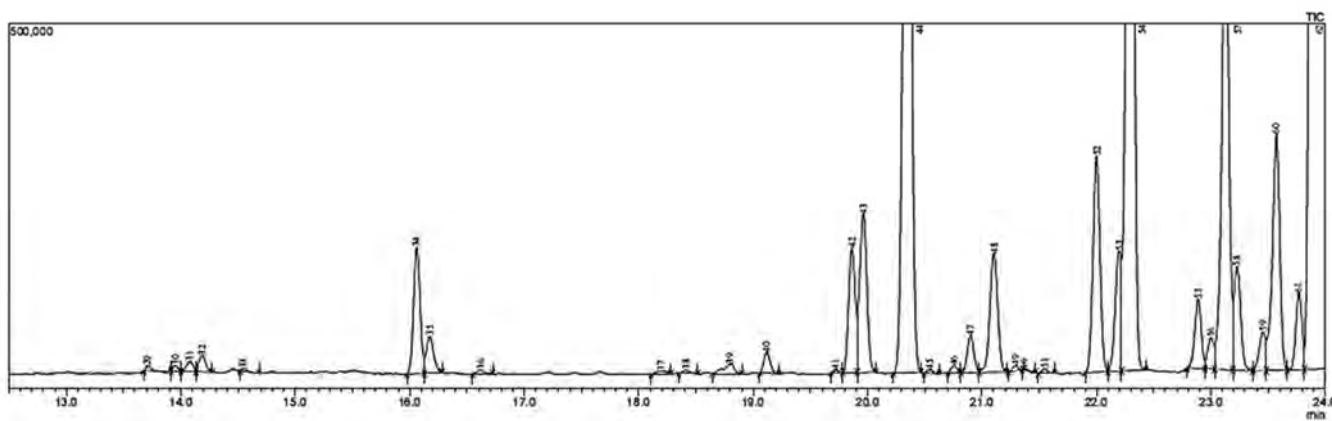
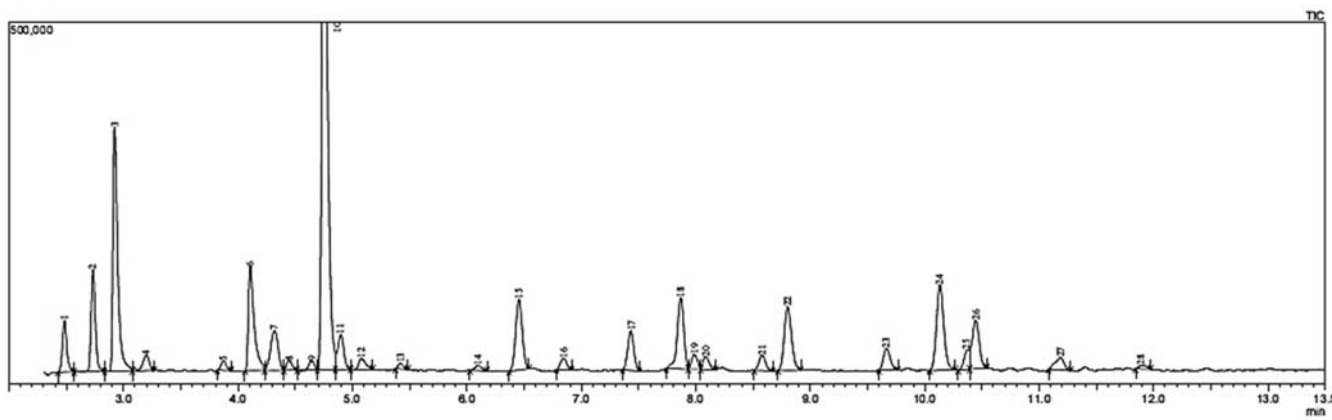
*Group 1: Carcinogenic to humans, Group 2A: Probably carcinogenic to humans, Group 2B: Possibly carcinogenic to humans, Group 3: Not classifiable as to its carcinogenicity to humans (WHO 2018).

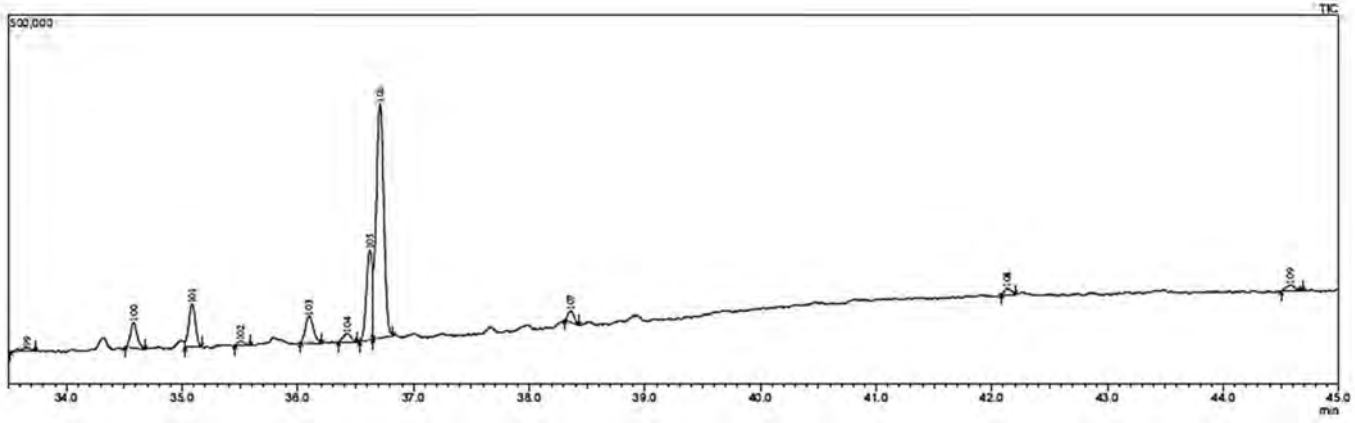
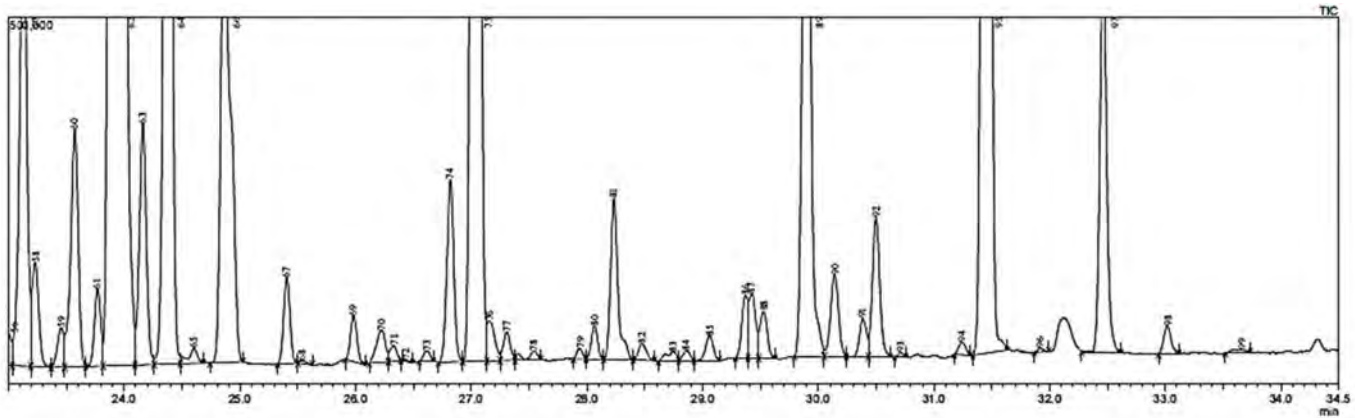
Supplementary Figure:

Full-scan chromatograms for one of the essential oils showing 109 peaks:



Detailed Chromatograms:





Green Essential Oils:

1. Tea tree oil

Compounds	CAS#
Acetone*	67-64-1
alpha-Pinene	80-56-8
beta-Pinene	127-91-3
beta-Myrcene	123-35-3
Limonene*	138-86-3
beta-Phellandrene	555-10-2
4-Terpineol	562-74-3
gamma-Terpinene	99-85-4
4-Carene	29050-33-7
Ethanol*	64-17-5
m-Cymene	535-77-3
Terpinolene	586-62-9
Eucalyptol	470-82-6
alpha-Phellandrene	99-83-2
Ocimenol	5986-38-9
Isobutyraldehyde	78-84-2
3-Carene	13466-78-9
Alloaromadendrene	25246-27-9
(+)-Ledene	21747-46-6
delta-Cadinene	483-76-1
Butane*	106-97-8
2-Methylbutyraldehyde	96-17-3
alpha-Gurjunene	489-40-7
Ethyl acetate*	141-78-6
Acetaldehyde*	75-07-0

*Classified as hazardous under Safe Work Australia, Hazardous Chemical Information System (HCIS)

2. *Eucalyptus oil*

Compounds	CAS#
Eucalyptol	470-82-6
alpha-Pinene	80-56-8
Limonene*	138-86-3
m-Cymene	535-77-3
beta-Pinene	127-91-3
gamma-Terpinene	99-85-4
3-Carene	13466-78-9
alpha-Thujene	2867-05-2
alpha-Terpineol	98-55-5
Ethanol*	64-17-5
beta-Myrcene	123-35-3
4-Carene	29050-33-7
alpha-Phellandrene	99-83-2
Camphene	79-92-5
4-Terpineol	562-74-3
Acetone*	67-64-1
beta-Phellandrene	555-10-2
Isovaleraldehyde	590-86-3
Linalyl isobutyrate	78-35-3
(+)-Camphene	5794-03-6
Isoamyl alcohol	123-51-3
2,4-Thujadiene	36262-09-6
Terpinolene	586-62-9
Methanol*	67-56-1
Isoamyl acetate*	123-92-2

*Classified as hazardous under Safe Work Australia, Hazardous Chemical Information System (HCIS)

3. *Eucalyptus oil*

Compounds	CAS#
Eucalyptol	470-82-6
Limonene*	138-86-3
alpha-Pinene	80-56-8
gamma-Terpinene	99-85-4
m-Cymene	535-77-3
3-Carene	13466-78-9
beta-Pinene	127-91-3
alpha-Thujene	2867-05-2
beta-Myrcene	123-35-3
4-Carene	29050-33-7
alpha-Terpineol	98-55-5
Terpinolene	586-62-9
Isovaleraldehyde	590-86-3
Ethanol*	64-17-5
4-Terpineol	562-74-3
beta-trans-Ocimene	3779-61-1
Acetone*	67-64-1
Pentylidenecyclopentane	53366-55-5
alpha-Pinene oxide	1686-14-2
Linalool	78-70-6
Isoamyl alcohol	123-51-3
alpha-Phellandrene	99-83-2
Methanol*	67-56-1
Camphene	79-92-5
2-Isopropenyltoluene	7399-49-7

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4. Peppermint oil

Compounds	CAS#
Menthone	89-80-5
Menthol	1490-04-6
Eucalyptol	470-82-6
Limonene*	138-86-3
beta-Pinene	127-91-3
alpha-Pinene	80-56-8
4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran	494-90-6
beta-Phellandrene	555-10-2
DI-Menthyl acetate	16409-45-3
D,l-Menthol	15356-70-4
m-Cymene	535-77-3
Acetone*	67-64-1
4-Carene	29050-33-7
gamma-Terpinene	99-85-4
Methanol*	67-56-1
2-Isopropylidene-5-methylcyclohexanone	15932-80-6
Caryophyllene	87-44-5
Isovaleraldehyde	590-86-3
2-Methylbutyraldehyde	96-17-3
alpha-Phellandrene	99-83-2
Camphene	79-92-5
2,5-Diethyl tetrahydrofuran	41239-48-9
alpha-Thujene	2867-05-2
Butane*	106-97-8
(R)-(+)-pulegone	89-82-7

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5. Lavender oil

Compounds	CAS#
Linalool	78-70-6
Linalyl butyrate	78-36-4
Eucalyptol	470-82-6
Ocimene	13877-91-3
3-Octanone	106-68-3
(-)-Terpinen-4-ol	20126-76-5
Hexyl methyl ether	4747-07-3
alpha-Pinene	80-56-8
Acetone*	67-64-1
beta-Myrcene	123-35-3
Hexyl acetate	142-92-7
Camphor	76-22-2
3-Carene	13466-78-9
alpha-Phellandrene	99-83-2
Camphene	79-92-5
cis-1,2-Dimethylcyclopropane	930-18-7
Neryl acetate	141-12-8
Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	242794-76-9
Methanol*	67-56-1
beta-Pinene	127-91-3
gamma-Terpinene	99-85-4
m-Cymene	535-77-3
1-Octen-3-yl-acetate	2442-10-6
Ocimenol	5986-38-9
Isovaleraldehyde	590-86-3

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6. Mixture of oils

Compounds	CAS#
Eucalyptol	470-82-6
Propylene glycol	57-55-6
alpha-Pinene	80-56-8
Limonene*	138-86-3
beta-Pinene	127-91-3
gamma-Terpinene	99-85-4
m-Cymene	535-77-3
Camphene	79-92-5
Menthol	1490-04-6
3-Carene	13466-78-9
alpha-Thujene	2867-05-2
beta-Myrcene	123-35-3
alpha-Terpineol	98-55-5
Camphor	76-22-2
4-Carene	29050-33-7
alpha-Phellandrene	99-83-2
Methyl salicylate	119-36-8
gamma-Terpineol	586-81-2
Terpinolene	586-62-9
beta-trans-Ocimene	3779-61-1
beta-Terpineol	138-87-4
Pentylidenecyclopentane	53366-55-5
Caryophyllene	87-44-5
Borneol	10385-78-1
Dihydrocarveol	619-01-2

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7. Mixture of oils

Compounds	CAS#
Ethanol*	64-17-5
Eucalyptol	470-82-6
Linalyl butyrate	78-36-4
Limonene*	138-86-3
Linalool	78-70-6
beta-Myrcene	123-35-3
alpha-Pinene	80-56-8
3-Octanone	106-68-3
Camphene	79-92-5
Caryophyllene	87-44-5
Hexyl methyl ether	4747-07-3
beta-Pinene	127-91-3
Hexyl acetate	142-92-7
m-Cymene	535-77-3
alpha-Phellandrene	99-83-2
beta-trans-Ocimene	3779-61-1
gamma-Terpinene	99-85-4
3-Carene	13466-78-9
Camphor	76-22-2
Terpinolene	586-62-9
Hexyl butyrate	2639-63-6
Butyl butyrate*	109-21-7
beta-Phellandrene	555-10-2
Neryl acetate	141-12-8
4-Terpineol	562-74-3

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8. Mixture of oils

Compounds	CAS#
Limonene*	138-86-3
Linalool	78-70-6
Linalyl butyrate	78-36-4
(Z)-beta-ocimene	3338-55-4
beta-Myrcene	123-35-3
alpha-Pinene	80-56-8
(-)-Terpinen-4-ol	20126-76-5
Ethyl 2-methylcyclopropanecarboxylate	20913-25-1
3-Octanone	106-68-3
Acetone*	67-64-1
Neryl acetate	141-12-8
Hexyl acetate	142-92-7
Caryophyllene	87-44-5
3-Carene	13466-78-9
beta-Phellandrene	555-10-2
1-Octen-3-yl-acetate	2442-10-6
Methanol*	67-56-1
Iso-amyl-senecioate	56922-73-7
alpha-Phellandrene	99-83-2
alpha-Terpineol	98-55-5
Camphene	79-92-5
Hexyl methyl ether	4747-07-3
Isobutyl butyrate	539-90-2
beta-Pinene	127-91-3
beta-trans-Ocimene	3779-61-1

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9. Mixture of oils

Compounds	CAS#
Limonene*	138-86-3
alpha-Pinene	80-56-8
Linalool	78-70-6
Linalyl butyrate	78-36-4
Eucalyptol	470-82-6
beta-Pinene	127-91-3
Camphene	79-92-5
beta-Myrcene	123-35-3
Benzyl acetate	140-11-4
Acetone*	67-64-1
beta-Phellandrene	555-10-2
Caryophyllene	87-44-5
Methyl benzoate	93-58-3
Borneol	10385-78-1
3-Carene	13466-78-9
alpha-Phellandrene	99-83-2
Isomenthone	491-07-6
Citronellyl formate	105-85-1
3-Octanone	106-68-3
Hexyl acetate	142-92-7
beta-Citronellol	106-22-9
beta-trans-Ocimene	3779-61-1
Isopropyl alcohol*	67-63-0
Acetaldehyde*	75-07-0
Octanal	124-13-0

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10. Sweet orange oil^C

Compounds	CAS#
Limonene*	138-86-3
beta-Pinene	127-91-3
alpha-Pinene	80-56-8
beta-Phellandrene	555-10-2
3-Carene	13466-78-9
beta-trans-Ocimene	3779-61-1
Methanol*	67-56-1
Acetone*	67-64-1
Octanal	124-13-0
Linalool	78-70-6
Ocimene	13877-91-3
Ethanol*	64-17-5
alpha-Thujene	2867-05-2
1,1-Dimethylallyl alcohol	115-18-4
1-Octanol*	111-87-5
(+)-Limonene oxide	1195-92-2
Methyl formate*	107-31-3
Decanal	112-31-2
alpha-Terpineol	98-55-5
gamma-Terpinene	99-85-4
(+)-(E)-limonene oxide	6909-30-4
Nonanal	124-19-6
1-Hexanol*	111-27-3
alpha-Phellandrene	99-83-2
Camphene	79-92-5

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11. Tea tree oil

Compounds	CAS#
(-)-Terpinen-4-ol	20126-76-5
gamma-Terpinene	99-85-4
4-Carene	29050-33-7
m-Cymene	535-77-3
alpha-Pinene	80-56-8
Eucalyptol	470-82-6
Terpinolene	586-62-9
alpha-Phellandrene	99-83-2
Ethanol*	64-17-5
Limonene*	138-86-3
alpha-Terpineol	98-55-5
beta-Pinene	127-91-3
beta-Myrcene	123-35-3
3-Carene	13466-78-9
Alloaromadendrene	25246-27-9
Isobutyraldehyde	78-84-2
alpha-Thujene	2867-05-2
(+)-Ledene	21747-46-6
delta-Cadinene	483-76-1
beta-Phellandrene	555-10-2
gamma-Muurolene	30021-74-0
Butane*	106-97-8
Acetone*	67-64-1
2-Methylbutyraldehyde	96-17-3
alpha-Gurjunene	489-40-7

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12. Lime and coconut oil

Compounds	CAS#
Acetaldehyde*	75-07-0
Methanol*	67-56-1
Ethanol*	64-17-5
Ethyl formate*	109-94-4
Ethyl 2-methylbutyrate	7452-79-1
Ethylbenzene*	100-41-4
alpha-Phellandrene	99-83-2
alpha-Pinene	80-56-8
Camphene	79-92-5
beta-Phellandrene	555-10-2
beta-Pinene	127-91-3
beta-Myrcene	123-35-3
beta-trans-Ocimene	3779-61-1
4-Carene	29050-33-7
Limonene*	138-86-3
3-Carene	13466-78-9
Eucalyptol	470-82-6
gamma-Terpinene	99-85-4
Terpinolene	586-62-9
Linalool	78-70-6
Decanal	112-31-2
Citral*	5392-40-5
gamma-Octalactone	104-50-7
Heneicosane	629-94-7
gamma-Nonanolactone	104-61-0

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Regular Essential Oils:

1. Lavender oil

Compounds	CAS#
Ethanol*	64-17-5
Eucalyptol	470-82-6
Limonene*	138-86-3
Linalyl formate	115-99-1
alpha-Pinene	80-56-8
Carbon disulphide*	75-15-0
Linalool	78-70-6
beta-Myrcene	123-35-3
Camphene	79-92-5
gamma-Terpinene	99-85-4
beta-Pinene	127-91-3
m-Cymene	535-77-3
Camphor	76-22-2
Benzyl benzoate*	120-51-4
N-butylbenzenesulfonamide	3622-84-2
alpha-Phellandrene	99-83-2
2-Methyl-1-butene	563-46-2
Terpinolene	586-62-9
beta-Phellandrene	555-10-2
Acetaldehyde*	75-07-0
3-Carene	13466-78-9
Ethyl acetate*	141-78-6
beta-trans-Ocimene	3779-61-1
3-Octanone	106-68-3
3,5,5-Trimethylhexyl acetate	58430-94-7

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2. Lavender oil

Compounds	CAS#
Ethanol*	64-17-5
Methanol*	67-56-1
Limonene*	138-86-3
alpha-Pinene	80-56-8
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Terpinolene	586-62-9
beta-Myrcene	123-35-3
Linalyl acetate	115-95-7
Camphor	76-22-2
D,l-isobornyl acetate	92618-89-8
Camphene	79-92-5
4-Carene	29050-33-7
Linalool	78-70-6
Iso-camphane	473-19-8
gamma-Terpinene	99-85-4
2-Methylpropene*	115-11-7
1-Ethoxy-1-methoxyethane	10471-14-4
Dihydromyrcenol	18479-58-8
3-Carene	13466-78-9
2-Carene	554-61-0
Acetaldehyde*	75-07-0
alpha-Phellandrene	99-83-2
Methyl formate*	107-31-3
Acetone*	67-64-1

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3. Orange oil

Compounds	CAS#
Limonene*	138-86-3
beta-Myrcene	123-35-3
alpha-Pinene	80-56-8
3-Carene	13466-78-9
beta-Phellandrene	555-10-2
1,1'-dimethyldiethyleneglycol	110-98-5
2-(2-Hydroxypropoxy)-1-propanol	106-62-7
2,2'-Oxydipropanol	108-61-2
beta-trans-Ocimene	3779-61-1
Acetaldehyde*	75-07-0
2-Butanol,3,3'-oxybis	54305-61-2
alpha-Phellandrene	99-83-2
Octanal	124-13-0
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
(Z)-beta-ocimene	3338-55-4
Camphene	79-92-5
2-Butene*	107-01-7
Acetone*	67-64-1
alpha-Thujene	2867-05-2

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4. English rose oil

Compounds	CAS#
1,1'-dimethyldiethyleneglycol	110-98-5
2-(2-Hydroxypropoxy)-1-propanol	106-62-7
2,2'-Oxydipropanol	108-61-2
2-Butanol,3,3'-oxybis	54305-61-2
(Z)-rose oxide	16409-43-1
Benzyl alcohol*	100-51-6
beta-Citronellol	106-22-9
Acetaldehyde*	75-07-0
cis-3,7-Dimethyl-2,6-octadien-1-ol*	106-25-2
Limonene*	138-86-3
Triacetin	102-76-1
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Phenylethyl alcohol	60-12-8
Diethyl phthalate	84-66-2
Acetone*	67-64-1
(+)-trans-Rose oxide	876-18-6
Eucalyptol	470-82-6
Diphenyl ether	101-84-8
(-)-Camphene	5794-04-7
Benzaldehyde*	100-52-7
D,l-isobornyl acetate	92618-89-8
alpha-Pinene	80-56-8
(R)-(-)-2-butanol*	14898-79-4
Geranyl bromide	35719-26-7
3,5,5-Trimethylhexyl acetate	58430-94-7

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5. Jasmine oil

Compounds	CAS#
Ethyl isovalerate	108-64-5
Benzyl acetate	140-11-4
1,1'-dimethyldiethyleneglycol	110-98-5
Di(propylene glycol) methyl ether	34590-94-8
Dl-2-methylbutyrate	7452-79-1
2,2'-Oxydipropanol	108-61-2
Diethyl malonate	105-53-3
2-Butanol,3,3'-oxybis	54305-61-2
Eucalyptol	470-82-6
Limonene*	138-86-3
Triacetin	102-76-1
Linalool	78-70-6
2-tert-Butylcyclohexanol	13491-79-7
alpha-Pinene	80-56-8
Citronellyl acetate	150-84-5
4-Phenyl-2-butanone	2550-26-7
Diethyl phthalate	84-66-2
Acetaldehyde*	75-07-0
Methyl acetate*	79-20-9
4-Carene	29050-33-7
2-(2-Hydroxypropoxy)-1-propanol	106-62-7
Benzyl isobutyrate	103-28-6
2,2,3,3-Tetramethylpentane	7154-79-2
Ethanol*	64-17-5
Heptylhexyl ether	7289-40-9

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6. Rose and grapefruit oil

Compounds	CAS#
Ethanol*	64-17-5
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7
Di(propylene glycol) methyl ether	34590-94-8
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Dihydromyrcenol	18479-58-8
Benzyl acetate	140-11-4
2-Cyclohexene-1-acetaldehyde, 3-methyl-	129993-40-4
Linalool	78-70-6
1-(4-Methyl-1-cyclohex-3-enyl)ethanone	70286-20-3
Octanal dimethyl acetal	10022-28-3
Ethyl acetate*	141-78-6
4-Hexen-1-ol, acetate	72237-36-6
Acetaldehyde*	75-07-0
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3
beta-Ionone	79-77-6
cis-3,7-Dimethyl-2,6-octadien-1-ol*	106-25-2
Decanal	112-31-2
alpha-Ionone	6901-97-9
2-(1-ethoxyethoxy)-3-methyl-1,4-butanediol	88481-54-3
2-methyl-2-(4-methylpent-3-enyl)cyclopropane-1-carbaldehyde	97231-35-1
Acetone*	67-64-1
Ethyl formate*	109-94-4
Methyl acetate*	79-20-9
Acetaldehyde diethyl acetal*	105-57-7
Ethyl methyl carbonate	623-53-0

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7. Freesia and jasmine oil

Compounds	CAS#
Propylene glycol butyl ether*	5131-66-8
3,5,5-Trimethylhexyl acetate	58430-94-7
Dihydromyrcenol	18479-58-8
Hexanal	66-25-1
trans-3-Hexenyl acetate	3681-82-1
4-tert-Butylcyclohexyl acetate	32210-23-4
Dl-4-hydroxy-3-methoxymandelic acid	928-96-1
Benzyl acetate	140-11-4
Acetaldehyde dibutyl acetal	871-22-7
Phenylethyl alcohol	60-12-8
Methyl phenylcarbinyl acetate	93-92-5
2-tert-Butylcyclohexanol	13491-79-7
2-Cyclohexene-1-acetaldehyde, 3-methyl-	129993-40-4
Ethyl butyrate	105-54-4
2-Methyl-5-propylnonane	31081-17-1
Ethyl 2-methylpentanoate	39255-32-8
2,6-Dimethyl-5-heptenal	106-72-9
5-(2-Methylpropyl)nonane	62185-53-9
4-Methylanisole	104-93-8
(Z)-rose oxide	16409-43-1
3,7-Dimethyldecane	17312-54-8
5,6-Dimethylundecane	17615-91-7
2,6,11-Trimethyldodecane	31295-56-4
cis-3,7-Dimethyl-2,6-octadien-1-ol*	106-25-2
4-Methyldodecane	6117-97-1

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8. Mixture of oils

Compounds	CAS#
beta-Pinene	127-91-3
alpha-Pinene	80-56-8
Eucalyptol	470-82-6
Linalool	78-70-6
Linalyl butyrate	78-36-4
Camphor	76-22-2
Camphene	79-92-5
Acetone*	67-64-1
Limonene*	138-86-3
4-Terpineol	562-74-3
Borneol	10385-78-1
m-Cymene	535-77-3
Methanol*	67-56-1
cis-1,2-Dimethylcyclopropane	930-18-7
alpha-Phellandrene	99-83-2
beta-Phellandrene	555-10-2
(+)-Camphene	5794-03-6
Ethanol*	64-17-5
Neryl acetate	141-12-8
1-Octen-3-yl acetate	2442-10-6
Carane	554-59-6
3-Octanone	106-68-3
beta-trans-Ocimene	3779-61-1
1-Hexanol*	111-27-3
beta-Myrcene	123-35-3

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9. Lemongrass oil

Compounds	CAS#
Ethanol*	64-17-5
Limonene*	138-86-3
gamma-Terpinene	99-85-4
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7
Di(propylene glycol) methyl ether	34590-94-8
m-Cymene	535-77-3
Dihydromyrcenol	18479-58-8
(Z)-citral*	106-26-3
alpha-Pinene	80-56-8
Undecane	1120-21-4
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Linalool	78-70-6
alpha-Terpineol	98-55-5
Terpinolene	586-62-9
Acetaldehyde*	75-07-0
Acetone*	67-64-1
2-Methyl-2-hepten-6-one	110-93-0
4-tert-Butylcyclohexyl acetate	32210-23-4
Ethyl formate*	109-94-4
beta-Pinene	127-91-3
2-methyl-2-(4-methylpent-3-enyl)cyclopropane-1-carbaldehyde	97231-35-1
Citral*	5392-40-5
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3
Camphene	79-92-5
Decanal	112-31-2

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10. Mixture of oils

Compounds	CAS#
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7
Di(propylene glycol) methyl ether	34590-94-8
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Propyl 2-methyl butyrate	37064-20-3
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3
Tripropylene glycol monomethyl ether	20324-33-8
2-(1-ethoxyethoxy)-3-methyl-1,4-butanediol	88481-54-3
2-(2-Methoxypropoxy)propan-1-ol	13588-28-8
Phenylethyl alcohol	60-12-8
Cyclohexane*	110-82-7
Acetaldehyde*	75-07-0
Glutaric acid dimethyl ester	1119-40-0
4-tert-Butylcyclohexanol	98-52-2
Hexyl acetate	142-92-7
4-Hexen-1-ol, acetate	72237-36-6
Linalool	78-70-6
4-tert-Butylcyclohexyl acetate	32210-23-4
Ethyl methyl ether*	540-67-0
Methylcyclopentane	96-37-7
Methyl formate*	107-31-3
Methyl acetate*	79-20-9
4-Methoxybenzaldehyde	123-11-5
p-Xylene*	106-42-3
Dimethyl adipate	627-93-0
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-	24555-40-6

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11. Mixture of oils

Compounds	CAS#
Ethanol*	64-17-5
Limonene*	138-86-3
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Ethyl formate*	109-94-4
4-tert-Butylcyclohexanol	98-52-2
Linalool	78-70-6
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3
4-tert-Butylcyclohexyl acetate	32210-23-4
Ethyl acetate*	141-78-6
Benzyl acetate	140-11-4
Acetaldehyde*	75-07-0
Acetone*	67-64-1
2-(1-ethoxyethoxy)-3-methyl-1,4-butanediol	88481-54-3
alpha-Pinene	80-56-8
alpha-Guaiene	3691-12-1
(S)-(-)-propylene oxide*	16088-62-3
Methyl acetate*	79-20-9
Acetaldehyde diethyl acetal*	105-57-7
beta-Phellandrene	555-10-2
beta-Myrcene	123-35-3
2-(2-Methoxypropoxy)propan-1-ol	13588-28-8
Linalyl acetate	115-95-7
(+)-Cycloisositivene	22469-52-9
2-Methylpropene*	115-11-7

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12. Mixture of oils

Compounds	CAS#
Ethanol*	64-17-5
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7
Di(propylene glycol) methyl ether	34590-94-8
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7
Benzyl acetate	140-11-4
Ethyl acetate*	141-78-6
Linalool	78-70-6
DL-lactic acid	50-21-5
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3
4-Hexen-1-ol, acetate	72237-36-6
(S)-(-)-propylene oxide*	16088-62-3
2-(1-ethoxyethoxy)-3-methyl-1,4-butanediol	88481-54-3
Acetone*	67-64-1
Methyl phenylcarbinyl acetate	93-92-5
Acetaldehyde*	75-07-0
Methanol*	67-56-1
Acetaldehyde diethyl acetal*	105-57-7
2-(2-Methoxypropoxy)propan-1-ol	13588-28-8
Tripropylene glycol monomethyl ether	20324-33-8
2-Methylpropene*	115-11-7

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Supplementary Table 3: VOCs emitted from all "regular" and "natural" essential oils (n=24):

Compound	CAS #	Prevalence (# of essential oils)
alpha-Pinene	80-56-8	20
Limonene*	138-86-3	19
Acetone*	67-64-1	17
Linalool	78-70-6	16
alpha-Phellandrene	99-83-2	16
beta-Myrcene	123-35-3	15
Camphene	79-92-5	15
Ethanol*	64-17-5	15
beta-Pinene	127-91-3	15
3-Carene	13466-78-9	14
Eucalyptol	470-82-6	14
Acetaldehyde*	75-07-0	13
beta-Phellandrene	555-10-2	13
gamma-Terpinene	99-85-4	13
m-Cymene	535-77-3	11
beta-trans-Ocimene	3779-61-1	10
Methanol*	67-56-1	10
Terpinolene	586-62-9	10
4-Carene	29050-33-7	9
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7	8
alpha-Terpineol	98-55-5	7
alpha-Thujene	2867-05-2	7
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7	6
3-Octanone	106-68-3	6
Benzyl acetate	140-11-4	6
Camphor	76-22-2	6
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3	5
4-Terpineol	562-74-3	5
Caryophyllene	87-44-5	5
Hexyl acetate	142-92-7	5
Di(propylene glycol) methyl ether	34590-94-8	5
Linalyl butyrate	78-36-4	5
4-tert-Butylcyclohexyl acetate	32210-23-4	4
Decanal	112-31-2	4

Dihydromyrcenol	18479-58-8	4
Ethyl acetate*	141-78-6	4
Ethyl formate*	109-94-4	4
Isovaleraldehyde	590-86-3	4
Methyl acetate*	79-20-9	4
Neryl acetate	141-12-8	4
2-(1-ethoxyethoxy)-3-methyl-1,4-butanediol	88481-54-3	4
(-)-Terpinen-4-ol	20126-76-5	3
Borneol	10385-78-1	3
2-(2-Hydroxypropoxy)-1-propanol	106-62-7	3
1,1'-dimethyldiethyleneglycol	110-98-5	3
1-Octen-3-yl-acetate	2442-10-6	3
2-(2-Methoxypropoxy)propan-1-ol	13588-28-8	3
2,2'-Oxydipropanol	108-61-2	3
2-Butanol,3,3'-oxybis	54305-61-2	3
2-Methylpropene*	115-11-7	3
3,5,5-Trimethylhexyl acetate	58430-94-7	3
4-Hexen-1-ol, acetate	72237-36-6	3
Acetaldehyde diethyl acetal*	105-57-7	3
cis-3,7-Dimethyl-2,6-octadien-1-ol*	106-25-2	3
Hexyl methyl ether	4747-07-3	3
Methyl formate*	107-31-3	3
Octanal	124-13-0	3
Phenylethyl alcohol	60-12-8	3
2-Methylbutyraldehyde	96-17-3	3
Butane*	106-97-8	3
(S)-(-)-propylene oxide*	16088-62-3	2
(+)-Camphene	5794-03-6	2
(Z)-rose oxide	16409-43-1	2
Isobutyraldehyde	78-84-2	2
2-Cyclohexene-1-acetaldehyde, 3-methyl-	129993-40-4	2
2-methyl-2-(4-methylpent-3-enyl)cyclopropane-1-carbaldehyde	97231-35-1	2
2-tert-Butylcyclohexanol	13491-79-7	2
4-tert-Butylcyclohexanol	98-52-2	2
cis-1,2-Dimethylcyclopropane	930-18-7	2
Citral*	5392-40-5	2
D,l-isobornyl acetate	92618-89-8	2
Diethyl phthalate	84-66-2	2
Ocimenol	5986-38-9	2
beta-Citronellol	106-22-9	2

Isoamyl alcohol	123-51-3	2
Linalyl acetate	115-95-7	2
Menthol	1490-04-6	2
Methyl phenylcarbinyl acetate	93-92-5	2
alpha-Gurjunene	489-40-7	2
Alloaromadendrene	25246-27-9	2
delta-Cadinene	483-76-1	2
Ocimene	13877-91-3	2
Pentylidenecyclopentane	53366-55-5	2
Triacetin	102-76-1	2
Tripropylene glycol monomethyl ether	20324-33-8	2
1-Hexanol*	111-27-3	2
(+)-Ledene	21747-46-6	2
(+)-trans-Rose oxide	876-18-6	1
(R)-(-)-2-butanol*	14898-79-4	1
(R)-(+)-pulegone	89-82-7	1
(Z)-beta-ocimene	3338-55-4	1
(Z)-beta-ocimene	3338-55-4	1
1-(4-Methyl-1-cyclohex-3-enyl)ethanone	70286-20-3	1
1-Ethoxy-1-methoxyethane	10471-14-4	1
1-Octanol*	111-87-5	1
2-Methyl-2-hepten-6-one	110-93-0	1
2,2,3,3-Tetramethylpentane	7154-79-2	1
2,4-Dimethylhexane*	589-43-5	1
2,4-Thujadiene	36262-09-6	1
2,5-Diethyl tetrahydrofuran	41239-48-9	1
2,6,11-Trimethyldodecane	31295-56-4	1
2,6-Dimethyl-5-heptenal	106-72-9	1
2-Butene*	107-01-7	1
2-Carene	554-61-0	1
2-Isopropenyltoluene	7399-49-7	1
2-Isopropylidene-5-methylcyclohexanone	15932-80-6	1
2-Methyl-1-butene	563-46-2	1
2-Methyl-5-propylnonane	31081-17-1	1
3,7-Dimethyldecane	17312-54-8	1
4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran	494-90-6	1
4-Methoxybenzaldehyde	123-11-5	1
4-Methylanisole	104-93-8	1
4-Methyldodecane	6117-97-1	1
4-Phenyl-2-butanone	2550-26-7	1
5-(2-Methylpropyl)nonane	62185-53-9	1

5,6-Dimethylundecane	17615-91-7	1
Acetaldehyde dibutyl acetal	871-22-7	1
alpha-Guaiene	3691-12-1	1
alpha-Ionone	6901-97-9	1
alpha-Pinene oxide	1686-14-2	1
Benzaldehyde*	100-52-7	1
Benzyl alcohol*	100-51-6	1
Benzyl benzoate*	120-51-4	1
Benzyl isobutyrate	103-28-6	1
beta-Ionone	79-77-6	1
beta-Terpineol	138-87-4	1
Bicyclo[5.2.0]nonane, 2-methylene- 4,8,8-trimethyl-4-vinyl-	242794-76-9	1
Butyl butyrate*	109-21-7	1
Carane	554-59-6	1
Carbon disulphide*	75-15-0	1
Citronellyl acetate	150-84-5	1
Citronellyl formate	105-85-1	1
Cyclohexane*	110-82-7	1
Diethyl malonate	105-53-3	1
Dihydrocarveol	619-01-2	1
Dimethyl adipate	627-93-0	1
Diphenyl ether	101-84-8	1
DI-2-methylbutyrate	7452-79-1	1
DI-4-hydroxy-3-methoxymandelic acid	928-96-1	1
DI-lactic acid	50-21-5	1
DI-Menthyl acetate	16409-45-3	1
Ethanone, 1-(6,6- dimethylbicyclo[3.1.0]hex-2-en-2-yl)-	24555-40-6	1
Ethyl 2-methylbutyrate	7452-79-1	1
Ethyl 2-methylpentanoate	39255-32-8	1
Ethyl butyrate	105-54-4	1
Ethyl isovalerate	108-64-5	1
Ethyl methyl carbonate	623-53-0	1
Ethyl methyl ether*	540-67-0	1
Ethylbenzene*	100-41-4	1
gamma-Murolene	30021-74-0	1
gamma-Nonanolactone	104-61-0	1
gamma-Octalactone	104-50-7	1
gamma-Terpineol	586-81-2	1
Geranyl bromide	35719-26-7	1
Glutaric acid dimethyl ester	1119-40-0	1

Heneicosane	629-94-7	1
Heptylhexyl ether	7289-40-9	1
Hexanal	66-25-1	1
Hexyl butyrate	2639-63-6	1
Isobutyl butyrate	539-90-2	1
Iso-camphane	473-19-8	1
Isomenthone	491-07-6	1
Isopropyl alcohol*	67-63-0	1
Linalyl formate	115-99-1	1
Linalyl isobutyrate	78-35-3	1
Menthone	89-80-5	1
Methyl benzoate	93-58-3	1
Methyl salicylate	119-36-8	1
Octanal dimethyl acetal	10022-28-3	1
Propyl 2-methyl butyrate	37064-20-3	1
Propylene glycol	57-55-6	1
Propylene glycol butyl ether*	5131-66-8	1
p-Xylene*	106-42-3	1
trans-3-Hexenyl acetate	3681-82-1	1
Undecane	1120-21-4	1
(+)-Cycloisositivene	22469-52-9	1
(+)-(E)-limonene oxide	6909-30-4	1
D,l-Menthol	15356-70-4	1
(+)-Limonene oxide	1195-92-2	1
(Z)-citral*	106-26-3	1
1,1-Dimethylallyl alcohol	115-18-4	1
Ethyl 2-methylcyclopropanecarboxylate	20913-25-1	1
Isoamyl acetate*	123-92-2	1
Methylcyclopentane	96-37-7	1
N-butylbenzenesulfonamide	3622-84-2	1
Nonanal	124-19-6	1
(-)-Camphene	5794-04-7	1
Iso-amyl-senecioate	56922-73-7	1

*Classified as hazardous under Safe Work Australia, Hazardous Chemical Information System (SWA 2018)

Supplementary Table 4: VOCs emitted from all "natural" essential oils (n=12).

Compound	CAS #	Prevalence (# of essential oils)
alpha-Pinene	80-56-8	12
alpha-Phellandrene	99-83-2	12
beta-Pinene	127-91-3	12
Limonene*	138-86-3	11
3-Carene	13466-78-9	11
beta-Myrcene	123-35-3	10
Eucalyptol	470-82-6	10
gamma-Terpinene	99-85-4	10
Camphene	79-92-5	10
Acetone*	67-64-1	9
beta-Phellandrene	555-10-2	9
m-Cymene	535-77-3	8
Linalool	78-70-6	7
beta-trans-Ocimene	3779-61-1	7
4-Carene	29050-33-7	7
Methanol*	67-56-1	7
Ethanol*	64-17-5	7
Terpinolene	586-62-9	7
alpha-Thujene	2867-05-2	6
alpha-Terpineol	98-55-5	6
Caryophyllene	87-44-5	5
Hexyl acetate	142-92-7	4
3-Octanone	106-68-3	4
4-Terpineol	562-74-3	4
Isovaleraldehyde	590-86-3	4
Linalyl butyrate	78-36-4	4
Acetaldehyde*	75-07-0	3
Camphor	76-22-2	3
Neryl acetate	141-12-8	3
(-)-Terpinen-4-ol	20126-76-5	3
Hexyl methyl ether	4747-07-3	3
2-Methylbutyraldehyde	96-17-3	3
Butane*	106-97-8	3
Octanal	124-13-0	2
Borneol	10385-78-1	2
Isobutyraldehyde	78-84-2	2

(+)-Ledene	21747-46-6	2
delta-Cadinene	483-76-1	2
Alloaromadendrene	25246-27-9	2
Ocimenol	5986-38-9	2
Isoamyl alcohol	123-51-3	2
Pentylidenecyclopentane	53366-55-5	2
alpha-Gurjunene	489-40-7	2
Ocimene	13877-91-3	2
Menthol	1490-04-6	2
Decanal	112-31-2	2
1-Octen-3-yl-acetate	2442-10-6	2
1,1-Dimethylallyl alcohol	115-18-4	1
Ethyl 2-methylcyclopropanecarboxylate	20913-25-1	1
beta-Citronellol	106-22-9	1
Isoamyl acetate*	123-92-2	1
1-Octanol*	111-87-5	1
Isopropyl alcohol*	67-63-0	1
Benzyl acetate	140-11-4	1
Ethyl 2-methylbutyrate	7452-79-1	1
Hexyl butyrate	2639-63-6	1
(+)-Limonene oxide	1195-92-2	1
(Z)-beta-ocimene	3338-55-4	1
Linalyl isobutyrate	78-35-3	1
(+)-Camphene	5794-03-6	1
2,4-Thujadiene	36262-09-6	1
alpha-Pinene oxide	1686-14-2	1
2-Isopropenyltoluene	7399-49-7	1
Menthone	89-80-5	1
4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran	494-90-6	1
Dl-Menthyl acetate	16409-45-3	1
2-Isopropylidene-5-methylcyclohexanone	15932-80-6	1
Citral*	5392-40-5	1
2,5-Diethyl tetrahydrofuran	41239-48-9	1
(R)-(+)-pulegone	89-82-7	1
cis-1,2-Dimethylcyclopropane	930-18-7	1
Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	242794-76-9	1
Propylene glycol	57-55-6	1
Methyl salicylate	119-36-8	1
gamma-Terpineol	586-81-2	1
beta-Terpineol	138-87-4	1

Dihydrocarveol	619-01-2	1
Butyl butyrate*	109-21-7	1
Isobutyl butyrate	539-90-2	1
Methyl benzoate	93-58-3	1
Isomenthone	491-07-6	1
Citronellyl formate	105-85-1	1
Methyl formate*	107-31-3	1
Nonanal	124-19-6	1
1-Hexanol*	111-27-3	1
gamma-Murolene	30021-74-0	1
Ethyl formate*	109-94-4	1
Ethylbenzene*	100-41-4	1
gamma-Octalactone	104-50-7	1
Heneicosane	629-94-7	1
gamma-Nonanolactone	104-61-0	1
(+)-(E)-limonene oxide	6909-30-4	1
D,l-Menthol	15356-70-4	1
Iso-amyl-senecioate	56922-73-7	1
Ethyl acetate*	141-78-6	1

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Supplementary Table 5: VOCs emitted from all "regular" essential oils (n=12).

Compound	CAS #	Prevalence (# of essential oils)
Acetaldehyde*	75-07-0	10
Linalool	78-70-6	9
1-(2-Methoxy-1-methylethoxy)propan-2-ol	20324-32-7	9
alpha-Pinene	80-56-8	8
Limonene*	138-86-3	8
Acetone*	67-64-1	8
Ethanol*	64-17-5	8
1-(2-Methoxypropoxy)propan-2-ol	13429-07-7	6
4-tert-Butylcyclohexyl acetate	32210-23-4	6
alpha-Phellandrene	99-83-2	5
beta-Myrcene	123-35-3	5
Camphene	79-92-5	5
Benzyl acetate	140-11-4	5
2-(1-Methoxypropan-2-yloxy)propan-1-ol	55956-21-3	5
3-Carene	13466-78-9	4
Eucalyptol	470-82-6	4
beta-Phellandrene	555-10-2	4
Dihydromyrcenol	18479-58-8	4
Ethyl acetate*	141-78-6	4
2-(2-Hydroxypropoxy)-1-propanol	106-62-7	4
Methyl acetate*	79-20-9	4
gamma-Terpinene	99-85-4	3
beta-trans-Ocimene	3779-61-1	3
m-Cymene	535-77-3	3
Methanol*	67-56-1	3
Terpinolene	586-62-9	3
Camphor	76-22-2	3
Ethyl formate*	109-94-4	3
3,5,5-Trimethylhexyl acetate	58430-94-7	3
2-Methylpropene*	115-11-7	3
1,1'-dimethyldiethyleneglycol	110-98-5	3
2,2'-Oxydipropanol	108-61-2	3
2-Butanol,3,3'-oxybis	54305-61-2	3
cis-3,7-Dimethyl-2,6-octadien-1-ol*	106-25-2	3

Phenylethyl alcohol	60-12-8	3
Di(propylene glycol) methyl ether	34590-94-8	3
4-Hexen-1-ol, acetate	72237-36-6	3
Acetaldehyde diethyl acetal*	105-57-7	3
2-(2-Methoxypropoxy)propan-1-ol	13588-28-8	3
-(1-ethoxyethoxy)-3-methyl-1,4-butanediol	88481-54-3	3
beta-Pinene	127-91-3	2
4-Carene	29050-33-7	2
3-Octanone	106-68-3	2
Decanal	112-31-2	2
Methyl formate*	107-31-3	2
Linalyl acetate	115-95-7	2
D,l-isobornyl acetate	92618-89-8	2
Triacetin	102-76-1	2
Diethyl phthalate	84-66-2	2
2-tert-Butylcyclohexanol	13491-79-7	2
2-Cyclohexene-1-acetaldehyde, 3-methyl-	129993-40-4	2
2-methyl-2-(4-methylpent-3-enyl)cyclopropane-1-carbaldehyde	97231-35-1	2
Methyl phenylcarbinyl acetate	93-92-5	2
Tripropylene glycol monomethyl ether	20324-33-8	2
(S)-(-)-propylene oxide*	16088-62-3	2
(Z)-rose oxide	16409-43-1	2
Hexyl acetate	142-92-7	1
alpha-Terpineol	98-55-5	1
4-Terpineol	562-74-3	1
Borneol	10385-78-1	1
Linalyl butyrate	78-36-4	1
Neryl acetate	141-12-8	1
beta-Citronellol	106-22-9	1
Octanal	124-13-0	1
Methylcyclopentane	96-37-7	1
(Z)-beta-ocimene	3338-55-4	1
(Z)-citral*	106-26-3	1
2-Methyl-2-hepten-6-one	110-93-0	1
N-butylbenzenesulfonamide	3622-84-2	1
Citral*	5392-40-5	1
cis-1,2-Dimethylcyclopropane	930-18-7	1
Nonanal	124-19-6	1
Linalyl formate	115-99-1	1
Undecane	1120-21-4	1

Carbon disulphide*	75-15-0	1
Benzyl benzoate*	120-51-4	1
2-Methyl-1-butene	563-46-2	1
Iso-camphane	473-19-8	1
1-Ethoxy-1-methoxyethane	10471-14-4	1
2-Carene	554-61-0	1
2-Butene*	107-01-7	1
Benzyl alcohol*	100-51-6	1
(-)-Camphene	5794-04-7	1
Benzaldehyde*	100-52-7	1
(R)-(-)-2-butanol*	14898-79-4	1
Geranyl bromide	35719-26-7	1
Ethyl isovalerate	108-64-5	1
Dl-2-methylbutyrate	7452-79-1	1
Diethyl malonate	105-53-3	1
Citronellyl acetate	150-84-5	1
4-Phenyl-2-butanone	2550-26-7	1
Benzyl isobutyrate	103-28-6	1
2,2,3,3-Tetramethylpentane	7154-79-2	1
Heptylhexyl ether	7289-40-9	1
1-(4-Methyl-1-cyclohex-3-enyl)ethanone	70286-20-3	1
Octanal dimethyl acetal	10022-28-3	1
beta-Ionone	79-77-6	1
alpha-Ionone	6901-97-9	1
Ethyl methyl carbonate	623-53-0	1
Propylene glycol butyl ether*	5131-66-8	1
Hexanal	66-25-1	1
trans-3-Hexenyl acetate	3681-82-1	1
Dl-4-hydroxy-3-methoxymandelic acid	928-96-1	1
Acetaldehyde dibutyl acetal	871-22-7	1
Ethyl butyrate	105-54-4	1
2-Methyl-5-propylnonane	31081-17-1	1
Ethyl 2-methylpentanoate	39255-32-8	1
4-Methylanisole	104-93-8	1
5,6-Dimethylundecane	17615-91-7	1
(+)-Camphene	5794-03-6	1
1-Octen-3-yl acetate	2442-10-6	1
Carane	554-59-6	1
Propyl 2-methyl butyrate	37064-20-3	1
Cyclohexane*	110-82-7	1
Glutaric acid dimethyl ester	1119-40-0	1
Ethyl methyl ether*	540-67-0	1

4-Methoxybenzaldehyde	123-11-5	1
p-Xylene*	106-42-3	1
Dimethyl adipate	627-93-0	1
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-2-(1-ethoxyethoxy)-3-methylbutane-1,4-diol	24555-40-6	1
88481-54-3	88481-54-3	1
alpha-Guaiene	3691-12-1	1
Dl-lactic acid	50-21-5	1
(+)-trans-Rose oxide	876-18-6	1
Diphenyl ether	101-84-8	1
2,6,11-Trimethyldodecane	31295-56-4	1
5-(2-Methylpropyl)nonane	62185-53-9	1
3,7-Dimethyldecane	17312-54-8	1
4-Methyldodecane	6117-97-1	1
2,6-Dimethyl-5-heptenal	106-72-9	1

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