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Data Article

# Chemical composition of steam and solvent crude oil extracts from *Azadirachta indica* leaves

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ABSTRACT

This work identifies the chemical components of *Azadirachta indica* (neem plant) leave extracts. *A. indica* is a vascular plant which belongs to the Meliaceae family and its use as herb in folk medicine is widely acclaimed. Essential oils were extracted from leaves of *A. indica.* Steam and solvent extraction methods were used with two solvents: Ethanol and Hexane. The crude oil extracted using both extraction methods were analyzed using GC–MS. The result of the analyses show that the major constituents were Eicosane (9.7662%), Diacenaphtho[1,2-j:1′,2′-l]fluoranthene (11.301%), Phenol, 4-[[(4-methoxyphenyl)methylene]amino]- (11.84%) and (3Ar,6S,9ar)-1,2,3,4,5,6,7,9a-octahydro-8-methyl-3a,6-methano-3ah-cyclopentacycloocten-10-one (36.883%) in steam extracted oil; Eicosane (10.259%), Diacenaphtho[1,2-j:1′,2′-l]fluoranthene (13.51%) and Butanamide, N-(2-methoxyphenyl)-3-oxo- (16.615%) in the ethanol extracted oil, and (3Ar,6S,9ar)-1,2,3,4,5,6,7,9a-octahydro-8-methyl-3a,6-methano-3ah-cyclopentacycloocten-10-one (10.72%), n-Hexadecanoic acid (14.688%) and 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- (34.719%) in the hexane extracted *A. indica* essential oil.



## Specifications Table

| | |
|---|---|
| Subject area | *Chemical Engineering, Biochemistry* |
| Compounds | *Active Ingredient* |
| Data category | *data of bioactive compounds in crude essential oil from neem and lemon plants* |
| Data acquisition format | *Mass spectra* |
| Data type | *Raw, analyzed* |
| Procedure | Oil samples were analyzed using a gas chromatography-mass spectrometry analyzer, Agilent technologies 7890B GC system, operating at ionization energy of 70 eV with a HP-5MS capillary column (30 m × 0.25 mm; film thickness 0.50 µm). 1 µl of essential oil was injected in split/split less mode at a split ratio of 20:1 and an inlet temperature of 250 °C. The carrier gas used to aid the analysis of the essential oils was helium at a constant pressure mode of 9.4 psi. The oven was programmed to have a 3 °C/min incremental raise until it reached 240 °C from 60 °C. The mass spectrometry analyser was operated at a scan mode in 40–400 m/z range with an ion source and transfer line temperature at 230 and 300 °C respectively. ChemStation software was used in the analysis of the data acquired from the GC–MS. The constituents of the essential oils was determined based on their Kovats indices (KI), retention time (RT) and mass spectra with NIST. |

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| | |
|---|---|
| Data accessibility | *A detailed data of compounds identified by GC–MS analysis of crude essential oil extracts from neem, lemon grass and commercial essential oil is provided in this article* |

## 1. Rationale

It has long been observed that plants' roots, flowers, seeds and leaves contain some active ingredients. Some are being extracted with organic solvent such as ether while some are odoriferous and very volatile [1–3]. *Azadirachta indica* is a vascular perennial plant belonging to the family Meliaceae and has *A. excelsa* as its only congener. It is a fast growing evergreen tree. Its leaves are pinnate and consist of 20–30 serrated leaflets which are dark green in colour when they are matured. *A indica* adapts to tropical and subtropical climates and grows best where annual rainfall is between 450–1200 mm. Although *A. indica* can grow within soil pH of 5.0–8.0 and is known to survive in variety of soil types, it is best adapted to deep, permeable sandy soil and soil pH between 6.2–7.0 [4]. *A. indica* extracts are used in cosmetics, insecticides and repellents. The plant is also known to have diverse medicinal values. Constituents of extracts from the leaves and other parts of the plant have been reported to exhibit antidiabetic, immunomodulatory, diuretic, antiseptic, anti-inflammatory, antipyretic, antihyperglycaemic, antiulcer, antiarthritic, antimalarial, spermicidal, antifungal, antibacterial, hypoglycemic, antioxidant, antimutagenic and anticarcinogenic properties [5–8]. *A. indica* leave extracts and some other leaves are active against certain dermatophytes, microorganisms and parasitic insects such as bacteria, fungi and mosquitoes [9–11]. The wide range of bioactive constituents and the versatility of the use of *A. indica* plant extracts have positioned the plant as one of the most important herbal and medicinal plants [12].

As there are renewed interests in herbal based medications in order to forestall the side effects of synthetic drugs, the quest to find new and unique molecular structures of plant origin as major constituents of some natural products, and those of *modern drugs* as means of combating recalcitrant diseases is also on the increase [13–15]. Inasmuch as essentials oils and other plant extracts are principally products of complex biological processes; and genetics and environment play crucial role in determining the morphology, chemical composition and ultimately the properties of herbal and medicinal plants [16,17], expanded knowledge rooted in holistic scientific research will open up a wealth of possibilities. As demand for plant based medication increases, studies on taxonomy, toxicity, chemical analysis and pharmacology of plant secondary metabolites will among other things, prevent problems associated with indiscriminate use caused by incorrect identification, improper documentation and lack of standardization of plant based extracts and their products. This work presents the chemical components of essential oils from *A. indica* leaves of Nigerian origin, extracted using steam, ethanol and hexane for the purpose of further scientific investigations.

## 2. Procedure

### *2.1. Source of raw materials*

Several *A. indica* trees are found within the premises of Covenant University, Ota, Ogun State, Nigeria. Ota is on latitude 6.41 $^{o}$N and longitude 3. 41 $^{o}$E, has a tropical climate and a mean annual rainfall of 1280 mm. Fresh leaves were plucked from one of the *A. indica* trees found on sandy - loam soil within the academic area of the University, air dried and partly ground to powder.

### *2.2. Extraction of the essential oil by steam distillation*

The air dried leaves was placed in a conical flask with distilled water at the bottom of the flask and an electrically powered hot plate with a control dial to set the temperature as desired served as the heat source for generating the required steam for the extraction process. A T-connector, having a thermometer at one end and a condenser at the other was attached to the conical flask with the aid of a cork. The condenser had an L-connector at its other end by which it was attached to a flat bottom flask with a cork. The mixture of extracted essential oil and water flowed from the conical flask to the flat bottom flask.

### *2.3. Solvent extraction of the essential oil*

Using the Soxhlet apparatus, essential oil was extracted from the plant material with hexane and ethanol. The ground plant material was placed in a muslin cloth material and put in the extraction chamber of the Soxhlet apparatus. Hexane or ethanol was placed in the flat bottom flask; 300 ml of each of the solvent was used to cause a siphoned flow in the apparatus without totally evaporating from the flat bottom flask. As the solvent is evaporated from the flat bottom flask at a temperature between 50–70 °C for hexane and 78.24 °C for ethanol, it goes through the distillation path through which it gets to the middle section of the Soxhlet apparatus before the vapour flows to the condenser at the top of the apparatus. The vapour condenses and falls back into the middle section of the Soxhlet apparatus where it comes in contact with the plant material placed there. Based on the design of the apparatus, the solvent has enough retention time in the middle

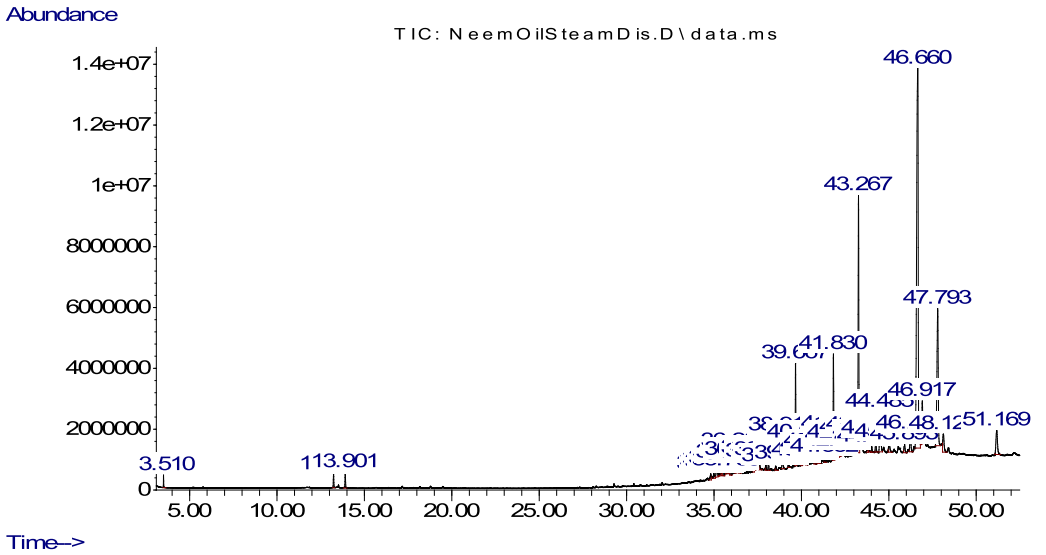


**Fig. 1.** Gas chromatogram of steam extracted essential oil from *A. indica* leaves.

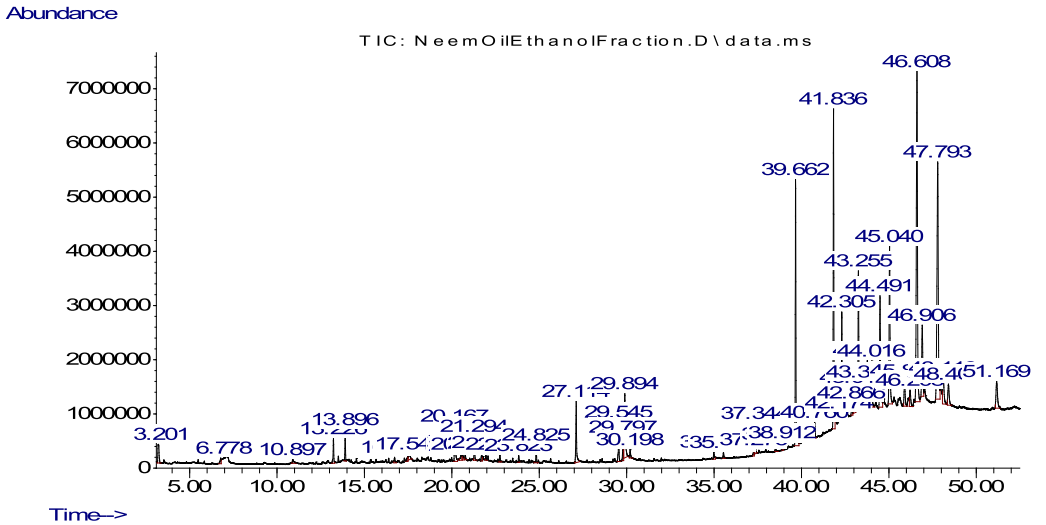


**Fig. 2.** Gas chromatogram of ethanol extracted essential oil from *A. indica* leaves.

section to enable it to extract the desired substances from the plant material there before it is siphoned back into the flat bottom flask.

### *2.4. Oil extract analysis*

The composition of the oil extracts was determined with the use of a gas chromatography-mass spectrometry analyser, Agilent technologies 7890B GC system, operating at ionization energy of 70 eV with a HP-5MS capillary column (30 m × 0.25 mm; film thickness 0.50 µm). 1 µl of essential oil was injected in split/splitless mode at a split ratio of 20:1 and an inlet temperature of 250 °C. The carrier gas used to aid the analysis of the essential oils was helium at a constant pressure mode of 9.4 psi. The oven was programmed to have a 3 °C/min incremental raise until it reached 240 °C from 60 °C. The mass spectrometry analyser was operated at a scan mode in 40–400 m/z range with an ion source and transfer line temperature at 230 and 300 °C respectively. ChemStation software was used in the analysis of the data acquired from the GC–MS. The constituents of the essential oils was determined based on their Kovats indices (KI), retention time (RT) and mass spectra with NIST.

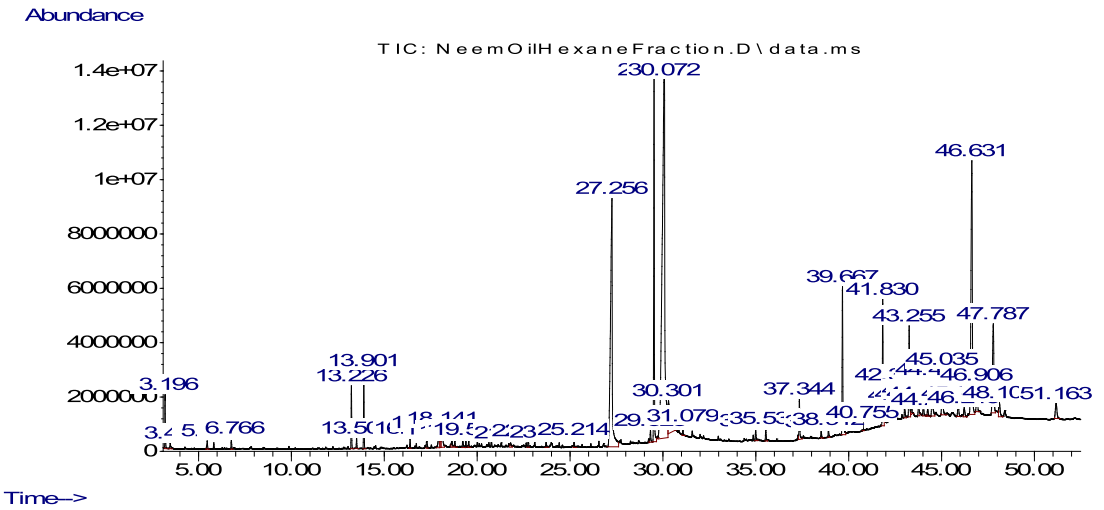


**Fig. 3.** Gas chromatogram of hexane extracted essential oil from *A. indica* leaves.

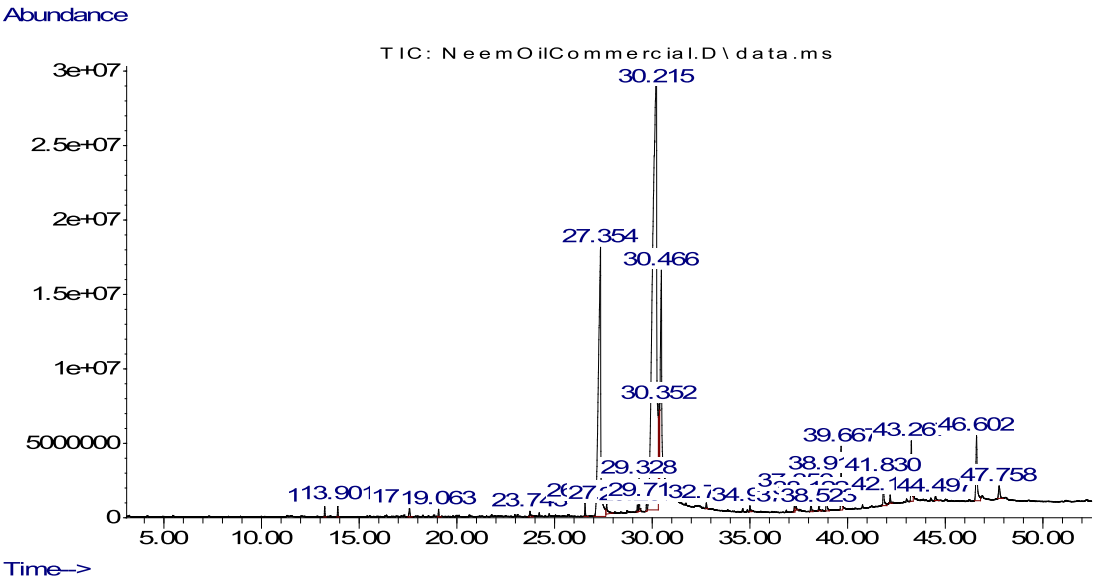


**Fig. 4.** Gas chromatogram of commercial neem oil.

## 3. Data, value and validation

The chemical components of neem essential oil from commercial source and those extracted from *A. indica* leaves with steam, ethanol and hexane are presented in Table 1 and the gas chromatograms are shown in Figs. 1–4.

Respectively, a total of 39, 44, 44 and 25 compounds were identified in essential oil extracted using steam, ethanol, hexane and the commercial neem oil. 2,6-Octadienal, 3,7-dimethyl-, (Z)-; Citral; Eicosane and 1,2-Bis(trimethylsilyl)benzene were found to be common chemical components of essential oils from steam extraction, ethanol extraction, hexane extraction and the commercial neem oil. *Eicosane* is known to possess antifungal, antibacterial, antitumor and cytotoxic properties [18]. Anticancer, antimicrobial, antioxidant and hyperchloesteralemic properties of *9,12,15-Octadecatrienoic acid*, (Z,Z,Z)- have been reported [19]. Several *fatty acids* like *oleic acid* and *hexadecanoic acid* exhibit antibacterial and antifungal activities [20]. *Octadecanoic acid* is also known to possess antitumor activity in addition to antibacterial and antifungal activities [18,21]. The roles of minor components in increasing the activity of essential oils and providing synergistic effects have been shown [22]; hence, probable contributions of minor components to the overall properties of essential oils should not be underestimated. As an antioxidant, *Vitamin E* has the capability to protect organisms from oxidative stress [23].

**Table 1**
Constituents of crude oils extracts from *Azadirachta indica* leaves and a commercial source as identified by GC–MS analysis.

| No | RT | Compound | Area% for extraction methods considered | | | Area% for commercial essential oil |
|---|---|---|---|---|---|---|
| | | | Steam | Ethanol | Hexane | |
| 1 | 3.2014 | Toluene | ND | 1.0011 | 0.8454 | ND |
| 2 | 3.476 | Cyclopentanol, 1-methyl- | ND | ND | 0.369 | ND |
| 3 | 3.5103 | Silanediol, dimethyl- | 0.2081 | ND | ND | ND |
| 4 | 5.4672 | 3-Pentanol, 2-methyl- | ND | ND | 0.2057 | ND |
| 5 | 6.7776 | 1,2,3,4-Butanetetrol, [S-(R*,R*)]- | ND | 0.251 | ND | ND |
| 6 | 10.898 | 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- | ND | 0.2448 | ND | ND |
| 7 | 13.226 | 2,6-Octadienal, 3,7-dimethyl-, (Z)- | 0.4485 | 0.744 | 1.1123 | 0.1863 |
| 8 | 13.507 | Geraniol | ND | ND | 0.1885 | ND |
| 9 | 13.896 | Citral | 0.5734 | 0.7511 | 1.4285 | 0.2286 |
| 10 | 16.385 | 2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- | ND | ND | 0.1808 | ND |
| 11 | 16.722 | Undecane | ND | 0.1974 | ND | ND |
| 12 | 17.289 | Caryophyllene | ND | ND | 0.3518 | ND |
| 13 | 17.483 | Cyclopentaneundecanoic acid | ND | 0.224 | ND | ND |
| 14 | 17.546 | N-acetyl-4-fluoroamphetamine | ND | 0.4074 | ND | ND |
| 15 | 17.575 | 1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)- | ND | ND | ND | 0.2578 |
| 16 | 17.947 | Diethylmalonic acid, di(3-chlorobenzyl) ester | ND | ND | 0.659 | ND |
| 17 | 18.021 | 1-Decanol, 2-hexyl- | ND | ND | 0.2578 | ND |
| 18 | 18.141 | 4,5-Dimethyl-3-heptanol | ND | ND | 0.7893 | ND |
| 19 | 18.645 | Octanal, 7-hydroxy-3,7-dimethyl- | ND | ND | 0.2364 | ND |
| 20 | 18.799 | Pentadecane | ND | ND | 0.1359 | ND |
| 21 | 19.063 | .beta.-Bisabolene | ND | ND | ND | 0.1402 |
| 22 | 19.223 | Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)- | ND | ND | 0.2427 | ND |
| 23 | 19.549 | 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl- | ND | ND | 0.1652 | ND |
| 24 | 20.167 | 1-Piperidinethiocarboxamide | ND | 1.3956 | ND | ND |
| 25 | 20.528 | Imidazole-2-carboxylic acid, 4-methyl- | ND | 0.4337 | ND | ND |
| 26 | 20.631 | Hexadecane, 1-(ethenyloxy)- | ND | 0.2265 | ND | ND |
| 27 | 20.768 | Hexadecane | ND | 0.1809 | ND | ND |
| 28 | 21.294 | Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]- | 0.4568 | 0.6594 | ND | ND |
| 29 | 21.706 | .alpha.-Cadinol | ND | 0.3012 | ND | ND |
| 30 | 21.798 | l-[-]-4-Hydroxy-1-methylproline | ND | ND | 0.1621 | ND |
| 31 | 21.952 | 1,4-Methano-1H-indene, octahydro-1,7a-dimethyl-4-(1-methylethenyl)-, [1S-(1.alpha.,3a.beta.,4.alpha.,7a.beta.)]- | ND | 0.224 | ND | ND |
| 32 | 22.748 | 1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethylidene)-, [1R-(1.alpha.,4a.beta.,8a.alpha.)]- | ND | 0.2223 | ND | ND |
| 33 | 22.753 | Pentadecane, 2,6,10,14-tetramethyl- | ND | ND | 0.1602 | ND |
| 34 | 23.709 | Tetradecanoic acid | ND | ND | 0.1533 | 0.1998 |
| 35 | 23.823 | N-Benzhydrylimidazole | ND | 0.2007 | ND | ND |
| 36 | 24.825 | 2-Naphthalenemethanol, 1,2,3,4,4a,5,6,8a-octahydro-.alpha.,.alpha.,4a,8-tetramethyl-, (2.alpha.,4a.alpha.,8a.alpha.)- | ND | 0.514 | ND | ND |
| 37 | 25.214 | 2-Pentadecanone, 6,10,14-trimethyl- | ND | ND | 0.1843 | ND |
| 38 | 26.558 | Hexadecanoic acid, methyl ester | ND | ND | ND | 0.2843 |
| 39 | 27.114 | n-Hexadecanoic acid | ND | 2.117 | 14.688 | 19.463 |
| 40 | 27.668 | Ethyl 13-methyl-tetradecanoate | ND | ND | ND | 0.4315 |
| 41 | 29.236 | 9,12-Octadecadienoic acid (Z,Z)-, methyl ester | ND | ND | ND | 0.1296 |
| 42 | 29.328 | 11-Octadecenoic acid, methyl ester | ND | ND | 0.322 | ND |
| 43 | 29.328 | 6-Octadecenoic acid, methyl ester, (Z)- | ND | ND | ND | 0.6452 |
| 44 | 29.522 | Phytol | ND | ND | 8.0087 | ND |
| 45 | 29.545 | 3H-Pyrazolo[4,3-c]quinolin-3-one, 8-fluoro-1,2-dihydro- | ND | 1.1577 | ND | ND |
| 46 | 29.711 | Methyl stearate | ND | ND | ND | 0.2046 |
| 47 | 29.797 | 9,12-Octadecadienoic acid (Z,Z)- | ND | 0.8601 | ND | ND |
| 48 | 29.894 | 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- | ND | 2.8747 | 34.719 | ND |
| 49 | 30.198 | Octadecanoic acid | ND | 0.2942 | ND | 10.187 |
| 50 | 30.215 | Oleic Acid | ND | ND | ND | 55.723 |
| 51 | 30.352 | 9-Octadecenoic acid, (E)- | ND | ND | ND | 2.2079 |
| 52 | 31.079 | Tridecanedial | ND | ND | 0.1968 | ND |
| 53 | 34.809 | Thujone | 0.4116 | ND | ND | ND |
| 54 | 34.987 | 2-Dodecen-1-yl(-)succinic anhydride | 0.396 | ND | ND | ND |
| 55 | 34.993 | 15-Hydroxypentadecanoic acid | ND | 0.3036 | 0.2885 | ND |
| 56 | 34.998 | cis-9-Hexadecenal | ND | ND | ND | 0.1752 |

(*continued on next page*)

**Table 1** (*continued*)

| No | RT | Compound | Area% for extraction methods considered | | | Area% for commercial essential oil |
|---|---|---|---|---|---|---|
| | | | Steam | Ethanol | Hexane | |
| 57 | 35.147 | Longifolene | 0.7151 | ND | ND | ND |
| 58 | 35.29 | 2,6,10,14,18-Pentamethyl-2,6,10,14,18-eicosapentaene | 0.1915 | ND | ND | ND |
| 59 | 35.439 | 1,3,3-Trimethyl-2-hydroxymethyl-3,3-dimethyl-4-(3-methylbut-2-enyl)-cyclohexene | 1.0775 | ND | ND | ND |
| 60 | 35.536 | Phthalic acid, di(2-propylpentyl) ester | ND | ND | 0.2928 | ND |
| 61 | 35.542 | 3-OXO-18-NOR-ENT-ROS-4-ENE-15.beta.,16-ACETONIDE | ND | 0.2014 | ND | ND |
| 62 | 35.708 | 1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)- | 0.2251 | ND | ND | ND |
| 63 | 35.862 | 4-(2,2,6-Trimethyl-bicyclo[4.1.0]hept-1-yl)-butan-2-one | 0.9811 | ND | ND | ND |
| 64 | 36.206 | Tricyclo[4.3.1.1(3,8)]undecane | 0.8226 | ND | ND | ND |
| 65 | 37.276 | 7-Pentadecyne | 0.5684 | ND | ND | ND |
| 66 | 37.276 | Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl- | ND | 0.2393 | 1.4927 | ND |
| 67 | 37.281 | 6-Octadecenoic acid, (Z)- | ND | ND | ND | 0.1436 |
| 68 | 37.344 | Nonadecane | ND | ND | 1.0061 | 1.4981 |
| 69 | 37.344 | Eicosane | 9.7662 | 10.259 | 0.1472 | 1.3947 |
| 70 | 37.608 | Phenol, 4-[2,3-dihydro-7-methoxy-3-methyl-5-(1-propenyl)-2-benzofuranyl]-2-methoxy- | 0.4073 | ND | ND | ND |
| 71 | 37.968 | 2,6,10,14-Hexadecatetraen-1-ol, 3,7,11,15-tetramethyl-, acetate, (E,E,E)- | 0.4922 | ND | ND | ND |
| 72 | 38.117 | Silanol, trimethyl-, phosphite (3:1) | 0.4224 | ND | ND | ND |
| 73 | 38.123 | 2-Pyridinamine, 5-methyl- | ND | ND | ND | 0.3278 |
| 74 | 38.523 | Octadecane, 3-ethyl-5-(2-ethylbutyl)- | ND | 0.2227 | ND | ND |
| 75 | 38.912 | Squalene | 1.4021 | ND | ND | 0.8635 |
| 76 | 38.912 | Trichothec-9-en-4-ol, 7,8:12,13-diepoxy-, 2-butenoate, [4.beta.(Z),7.beta.,8.beta.]- | 0.1926 | 0.2308 | 0.1759 | ND |
| 77 | 39.662 | Heptadecane | ND | 7.5868 | ND | ND |
| 78 | 39.667 | Tetracosane | ND | ND | 3.5068 | ND |
| 79 | 40.011 | trans-Geranylgeraniol | 1.4076 | ND | ND | ND |
| 80 | 40.263 | Indolizine, 2-(4-methylphenyl)- | 0.2395 | ND | ND | ND |
| 81 | 40.755 | Octadecane, 1-iodo- | ND | 0.4477 | 0.188 | ND |
| 82 | 40.76 | Heneicosane, 3-methyl- | 0.3953 | ND | ND | ND |
| 83 | 40.966 | 4-Dehydroxy-N-(4,5-methylenedioxy-2-nitrobenzylidene)tyramine | 0.6149 | ND | ND | ND |
| 84 | 41.333 | 2-(Acetoxymethyl)-3-(methoxycarbonyl)biphenylene | 0.2009 | ND | ND | ND |
| 85 | 41.83 | Octadecane | ND | 1.6801 | 3.0339 | ND |
| 86 | 41.956 | 1,2,4-Oxadiazole, 3-(1,3-benzodioxol-5-yl)-5-[(4-iodo-1H-pyrazol-1-yl)methyl]- | 1.1733 | ND | ND | ND |
| 87 | 42.122 | 1,2-Bis(trimethylsilyl)benzene | 2.3602 | 4.4112 | 1.417 | 0.1613 |
| 88 | 42.174 | 1,4-Bis(trimethylsilyl)benzene | 1.2851 | 2.1832 | ND | ND |
| 89 | 42.179 | 5-Methyl-2-phenylindolizine | 0.4894 | ND | ND | 0.1866 |
| 90 | 42.305 | Vitamin E | 0.6673 | 3.3997 | 0.9438 | ND |
| 91 | 42.866 | Phenylacetic acid, 2-(1-adamantyl)ethyl ester | ND | 0.3971 | ND | ND |
| 92 | 43.015 | Silane, trimethyl[5-methyl-2-(1-methylethyl)phenoxy]- | ND | 1.7215 | 0.3501 | 0.5514 |
| 93 | 43.255 | Benzenamine, N-[(4-methoxyphenyl)methylene]-, N-oxide | ND | ND | 2.3849 | ND |
| 94 | 43.255 | 4-[(3-Methoxy-phenylimino)-methyl]-phenol | ND | 4.7733 | ND | ND |
| 95 | 43.267 | Phenol, 4-[[(4-methoxyphenyl)methylene]amino]- | 11.84 | ND | ND | ND |
| 96 | 43.267 | 1-Isopropoxy-2-phenylmethtylbenzene | ND | ND | ND | 1.7079 |
| 97 | 43.387 | Benzo[h]quinoline, 2,4-dimethyl- | 4.4605 | ND | 0.2026 | ND |
| 98 | 43.764 | 2,4-Cyclohexadien-1-one, 3,5-bis(1,1-dimethylethyl)-4-hydroxy- | 0.5062 | ND | ND | ND |
| 99 | 43.764 | 1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isopropyl ester | ND | 1.7602 | ND | ND |
| 100 | 43.862 | 4-(1,1-Dimethylpropyl)phenol, trimethylsilyl ether | 0.2728 | ND | ND | ND |
| 101 | 44.016 | Tris(tert-butyldimethylsilyloxy)arsane | 0.26 | ND | ND | ND |
| 102 | 44.022 | Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl- | ND | ND | 0.3901 | ND |
| 103 | 44.251 | Silicic acid, diethyl bis(trimethylsilyl) ester | 0.6732 | ND | ND | ND |
| 104 | 44.485 | .beta.-Sitosterol | 2.4735 | ND | ND | ND |
| 105 | 44.491 | .gamma.-Sitosterol | ND | 4.675 | 1.2889 | ND |
| 106 | 45.035 | Arsenous acid, tris(trimethylsilyl) ester | ND | ND | 1.5873 | ND |
| 107 | 45.04 | 2-[4-Cyclohexylbutanoylamino]-3-chloro-1,4-naphthoquinone | ND | 6.5549 | ND | ND |
| 108 | 46.602 | 5-Oxo-.delta.4-decahydrobenzindene | ND | ND | ND | 2.702 |
| 109 | 46.608 | Butanamide, N-(2-methoxyphenyl)-3-oxo- | ND | 16.615 | ND | ND |
| 110 | 46.631 | (3Ar,6S,9ar)-1,2,3,4,5,6,7,9a-octahydro-8-methyl-3a,6-methano-3ah-cyclopentacycloocten-10-one | 36.883 | ND | 10.72 | ND |

(*continued on next page*)

**Table 1** (*continued*)

| No | RT | Compound | Area% for extraction methods considered | | | Area% for commercial essential oil |
|---|---|---|---|---|---|---|
| | | | Steam | Ethanol | Hexane | |
| 111 | 46.906 | Tetrasiloxane, decamethyl- | ND | ND | 0.9463 | ND |
| 112 | 46.906 | 3-Quinolinecarboxylic acid, 6,8-difluoro-4-hydroxy-, ethyl ester | ND | 3.3455 | ND | ND |
| 113 | 46.917 | 2-Ethylacridine | 2.7375 | ND | ND | ND |
| 114 | 47.787 | Anthra[2,3-a]coronene | ND | ND | 3.8743 | ND |
| 115 | 47.793 | Diacenaphtho[1,2-j:1′,2′-l]fluoranthene | 11.301 | 13.51 | ND | ND |
| TOTAL | | | 100 | 100 | 100 | 100 |

ND-not detected.

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## Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cdc.2019.100208.

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