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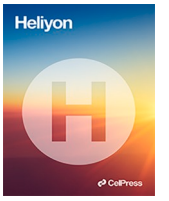

Research article

Chemical composition of organic extracts of *Phyla nodiflora* L. in Syria by GC-MS

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ABSTRACT

Introduction: *Phyla nodiflora* L. is a perennial herbaceous plant belonging to the Verbenaceae family. It is widely used as an herbal drink to treat many diseases. It has antioxidant, antifungal and anti-inflammatory properties. In traditional medicine, it is used to treat skin infections. However, there is little information on the chemical composition of organic plant extracts. Therefore, the aim of this study was to determine the chemical composition of organic extracts of *P. nodiflora* L.

Methods: In this study, organic extracts were prepared using a continuous Soxhlet extractor and four different solvents with increasing polarity from nonpolar to polar solvents (petroleum ether, chloroform, ethyl acetate, and isopropanol) to ensure the possibility of extracting a wide range of compounds. GC–MS analysis was performed to determine the chemical constituents of the organic extracts.

Results: Nineteen compounds were identified in the petroleum ether (Et) extract, 14 in the chloroform (Ch) extract, 18 in the ethyl acetate (Ea) extract and 15 in the isopropanol (Is) extract. The most important compounds in the Et extract were 1,1-diethoxyethane (33.9 %) and nonadecane (19.9 %). The most important compound in the Ch extract was octacosane (37.4 %). The most important compounds in the Ea extract were 3-hydroxy-dodecanoic acid (17.7 %) and geranyl isovalerate (15.5 %). The most important compound in the Is extract was behenic acid alcohol (18.6 %). The chemical structures of the major compounds were confirmed by mass spectrometry by studying their fragmentation mechanism and comparing the molecular weights of the resulting fragments with the molecular weights of the peaks present in each mass spectrum.

Conclusions: The results of this study show that the dominant compounds in nonpolar extracts (petroleum ether and chloroform) are hydrocarbons, ethers, epoxides, and silicon compounds, while the dominant compounds in moderately polar extracts (ethyl acetate and isopropanol) are alcohols, carbonyl compounds, and oxygenated terpenes.

1. Introduction

Since the beginning of human civilization, medicinal plants have been used as a source of a wide range of bioactive compounds. They have been used as raw plant material or as pure natural compounds isolated from plants to treat various diseases because they contain natural biologically active compounds [1,2]. Their various natural compounds have inspired the development of a large

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number of pharmaceuticals. Many plants produce organic compounds such as phenolic acids, flavonoids, coumarins, tannins, catechins, quinones, essential oils and terpenoids [3]. These compounds exhibit a broad spectrum of biological activities, including anticancer, anti-inflammatory, antioxidant and antimicrobial effects [3]. Due to their high efficacy even at low concentrations, these products are becoming increasingly important in medicine. With the continuous increase in global biodiversity, natural products play an important role in meeting this need [1,2]. *P. nodiflora* L. is a fast-growing creeping perennial plant [4] with small pink or white flowers [5] that belongs to the family Verbenaceae [4,5] and is found in humid areas and moisture-rich soils [6]. Its habitat is South America, India, Sri Lanka and Africa [7]. It has good biological and medicinal properties. It has antibacterial [8], antitumor [9], anti-inflammatory [10], antioxidant [11], and antidiabetic [12] properties. It also has antiseptic and anthelmintic properties [13] and antitussive and antipyretic properties [14] and is also used for treating joint pain and respiratory diseases [15].

Previous studies have shown that *P. nodiflora* contains glycosidic flavonoids [16], alkaloids, resins, tannins and terpenes [17]. Researchers were able to isolate flavonoid compounds (nodifloretin, 4′-hydroxywogonin, cirsiliol, 5,7,8,4′-tetrahydroxy-3′-methoxyflavone and eupafolin) with antioxidant activity from the methanolic extract of the aerial parts of the plant *P. nodiflora* from Taiwan [18]. The chemical composition of the methanolic extract of the Pakistani *P. nodiflora* plant was investigated, and the results of GC–MS analysis showed that the extract contained glycosidic flavonoids (6-methoxytaxifolin, luteolin 7-rhamnosyl (1->6) galactoside, isovitexin 7-*O*-rhamnoside, maysin, grossamide, torosaflavone D), diterpenes (betavulgaroside X, betavulgaroside VI) and triterpenes (periandrin V, medicoside H, spinacoside D, spinacoside C) [19]. A new flavonoid, 5-hydroxy-3′,4′,7-trimethoxyflavone, was isolated from the methanolic extract of Indian *P. nodiflora* and showed high antioxidant activity according to the DPPH method [20]. The chemical composition of the essential oil extracted from the aerial parts of the *P. nodiflora* plant revealed the presence of monoterpenes, the most important of which are β-pinene, 2,6-dimethyloctane, 1-methyl-4-isopropylcyclohexane, *p*-cymene, β-ocimene, terpinolene, γ-terpinene, linalool, *p*-cymen-8-ol, α-terpineol, carvone, thymol, carvacrol and eugenol, and sesquiterpenes (α-copaene, β-caryophyllene, α-bergamotene, β-bisabolene, δ-cadinene, 4,10-dimethyl-7-isopropylbicyclo-[4.4.0]-1,4-decadiene and calamenene) [17]. The chemical components of the essential oil of *P. nodiflora* include monoterpenes and triterpenes, the most important of which are limonene, carvone, piperitone, verbenone, calarene and murolene [21].

Due to the lack of chemical studies related to the plant *P. nodiflora* and the lack of chemical studies in Syria, this research aimed to analyse the chemical composition of organic extracts (petroleum ether, chloroform, ethyl acetate and isopropanol) of aerial parts of *P. nodiflora* using GC–MS technology. The fragmentation pathways of the resulting key compounds were studied by matching the mass spectra of the compounds to standard mass spectra from Wiley and the NIST library database (Supplementary Material).

2. Materials and methods

2.1. Chemicals and solvents

GC–MS (Shimadzu - 17A/QP5050), Soxhlet-type apparatus (BÜCHI), laboratory heating (Heraeus), sensitive scale (Sartorius), rotary evaporator (Büchii), laboratory glassware (Isolab), petroleum ether (S.C.P), chloroform (Merck), ethyl acetate (P.R.S Panreac), isopropanol (Honeywell), sodium sulphate and filter paper (ZELPA) were used.

2.2. Preparation of organic extracts

The aerial parts of the plant *P. nodiflora* were collected in July 2023 in the governorate of Latakia in Syria. The aerial parts were cleaned of dust and suspended impurities, dried for one month in the dark, well ventilated at room temperature (25 °C) and then crushed.

Four chemical extracts of the plant were prepared using different solvents with increasing polarity from nonpolar to polar solvents (petroleum ether (Et), chloroform (Ch), ethyl acetate (Ea) and isopropanol (Is)) via a continuous Soxhlet extractor by placing 50 g of the plant in a cartridge and adding 300 ml of petroleum ether to a 500 ml round bottom flask. The extraction process took 18 h. The extraction process was repeated with the other solvents on the same plant sample (the plant sample was dried in an oven at 40 °C before each extraction with a different solvent). The solvents were evaporated with a rotary evaporator at a temperature of 45 °C and then dried in a desiccator. The dried extracts were weighed, and the percentage yield was calculated using the following relationship:

$$\text{Yield } \% = (\text{weight of dry extract} / \text{weight of plant material used for extraction}) \times 100$$

2.3. GC–MS analysis

The analysis was performed by injecting 2 μl of each sample into a SHIMADZU GC–MS instrument, model GCMS-17A/QP5050, using a nonpolar capillary column (BP5MS, 5 % phenylpolysilphenylene siloxane) with dimensions of 30 m × 0.25 mm, i.d. 0.25 μm, and the carrier gas was helium with a purity of 99.9999 % at a flow rate of 1 ml/min. Chloroform was used as the solvent for injecting the samples.

The thermal programme started at 80 °C for 4 min and then increased by 10 °C per minute until 200 °C was reached. This temperature was maintained for 5 min, after which the temperature was increased from 200 °C by 7 °C per minute to 300 °C, after which the temperature was maintained for 15 min. The total run time was 50.3 min. Mass spectra were recorded from 42 *m/z* to 600 *m/z* in 70 eV ionization energy mode, and the ionization source temperature was set to 280 °C.

2.4. Identification of the components

The chemical compounds present in each extract were identified based on the interpretation of the GC–MS mass spectrum using the NIST and WILEY databases by comparing the mass spectrum of the analysed compound with the spectrum of known compounds stored in the libraries available on the instrument's computer (Nist 05a. L, Nist 02. L, Wiley 7.1).

3. Results and discussion

Chemical extracts from the aerial parts of the plant *P. nodiflora* were obtained using different solvents of increasing polarity (petroleum ether, chloroform, ethyl acetate, and isopropanol) with the aim of obtaining a wide range of compounds. The extracts were weighed, and the yield was calculated as shown in Table 1.

The GC/MS chromatogram of the petroleum ether (Et) extract (Fig. 2) showed the presence of 19 different compounds, which accounted for 90.2 % of the total composition of the extract, with nonpolar compounds dominating the extract. Petroleum ether extract (Et) consists mainly of four ether compounds (41.6 %), six hydrocarbon compounds (30.8 %), seven ester compounds (16.9 %) and two silicon compounds (0.9 %). The most abundant compound obtained was ether 1,1-diethoxyethane (33.9 %), followed by the aliphatic hydrocarbon nonadecane (19.9 %), n-butyl methacrylate (5.9 %), dibutyl phthalate (5.8 %), the terpene compound anethole (5.5 %), cetene (4.4 %) and ethyl dodecanoate (2.7 %). The remaining compounds were present in trace amounts of less than 2 %. Table 2 shows the chemical composition of the petroleum ether (Et) extract of the aerial parts of *P. nodiflora* using GC–MS. Fig. 3 shows the main chemical formula of the petroleum ether (Et) extract.

The GC–MS chromatogram of the chloroform extract (Ch) (Fig. 4) revealed 14 different compounds accounting for 94.9 % of the total composition of the extract. The chloroform extract (Ch) consisted mainly of two hydrocarbon compounds (40.1 %), seven silicon compounds (31.8 %) and two chlorine compounds (3.1 %). The oxygen compounds (19.9 %) included carbonyl compounds and phthalic acid esters. The most abundant compound was the hydrocarbon compound octacosane (37.4 %), followed by hexamethylcyclotrisiloxane (22.5 %), 3-methyl-2-cyclohexen-1-one (13.6 %), 4-chloromethylene-2-phenyl-4,5-dihydrooxazol-5-one (5.5 %), dodecamethylcyclohexasiloxane (3.5 %), heptacosane (2.7 %), octamethylcyclotetrasiloxane (2.1 %) and decamethylcyclopentasiloxane (2 %). The remaining compounds were present in smaller trace amounts (2 %). The chemical composition of the chloroform extract (Ch) of *P. nodiflora* is shown in Table 3. The main chemical formula of the chloroform extract (Ch) is shown in Fig. 5.

The GC–MS chromatograms of the ethyl acetate (Ea) extract (Fig. 6) revealed 18 different compounds accounting for 91.8 % of the total composition of the extract. The A3 ethyl acetate extract consists mainly of terpenoids (38.7 %), fatty acids (20.7 %), alcohols (10.7 %) and phthalic acid esters (11.1 %), as well as other compounds in minor proportions. These include fatty acids and esters. The most abundant compound was 3-hydroxydodecanoic acid (17.7 % of the total). Table 4 shows that the extract (Ea) contains two monoterpenes, geranyl isovalerate (15.5 %) and isopulegol (8.9 %), a single sesquiterpene compound called hexahydrofarnesyl acetone (10.6 %) and a single oxygen diterpene, phytol (3.7 %). The extract also contained a good percentage (9.6 %) of butyl octyl-1,2-benzenedicarboxylate and (6.3 %) of 1,2,3-propanetriol-1-acetate. The other compounds were present in lower amounts (4.5 %). Table 4 shows the chemical composition of the ethyl acetate (Ea) extract of *P. nodiflora*. Fig. 7 shows the main chemical formula of the ethyl acetate (Ea) extract.

The GC–MS chromatogram of the isopropanol (Is) extract (Fig. 8) revealed 15 different compounds accounting for 97.4 % of the total composition of the extract. The isopropanol (Is) extract consisted mainly of alcohols (28.4 %, carbonyl compounds (27.6 %), phthalic acid esters (16.3 %) and fatty acids and their esters (13.3 %). The most abundant compound was behenic alcohol (18.6 %), followed by bis(2-methylpropyl) phthalate (12.5 %) and the aldehyde (*E*) 2-decenal (10.3 %). The extract also contained a good percentage (8.3 %) of the compound 1-tetradecanol, 8.1 % of the compound 2-methyl-2-cyclohexen-1-one and 7.5 % of the compound ethyl hexadecanoate. Isopropanol extract also contains the steroid derivative (3β) cholest-5-en-3-ol tetradecanoate (6.5 %) and oleic acid (5.8 %). The chemical composition of the isopropanol extract (Is) of *P. nodiflora* is shown in Table 5. Fig. 9 shows the main chemical formulas of the isopropanol extract (Is).

The aim of the extraction procedure (serial exhaustive extraction method) with different polar solvents (starting with the nonpolar solvent petroleum ether up to the most polar solvent isopropanol) on the same plant sample was to first extract the nonpolar compounds (in the petroleum ether and chloroform extracts) and then extract the medium polar compounds (in the ethyl acetate and isopropanol extracts). The predominant compounds in the petroleum ether and chloroform extracts were saturated and unsaturated hydrocarbons, ethers, epoxides and silicon compounds, while the predominant compounds in the ethyl acetate and isopropanol extracts were alcohols, carbonyl compounds and oxygenated terpenes. The results presented in Tables 2 and 3 show that the petroleum ether and chloroform extracts contained no (polar) alcoholic compounds, while the results presented in Tables 4 and 5 demonstrate the

Table 1
Color and yield of the obtained organic extracts.

Symbol	Extract	Color	Yield %
Et	Petroleum ether extract	Pale yellow	1.77
Ch	Chloroform extract	Dark green	2.15
Ea	Ethyl acetate extract	Dark yellow	1.54
Is	Isopropanol extract	Brown	3.17

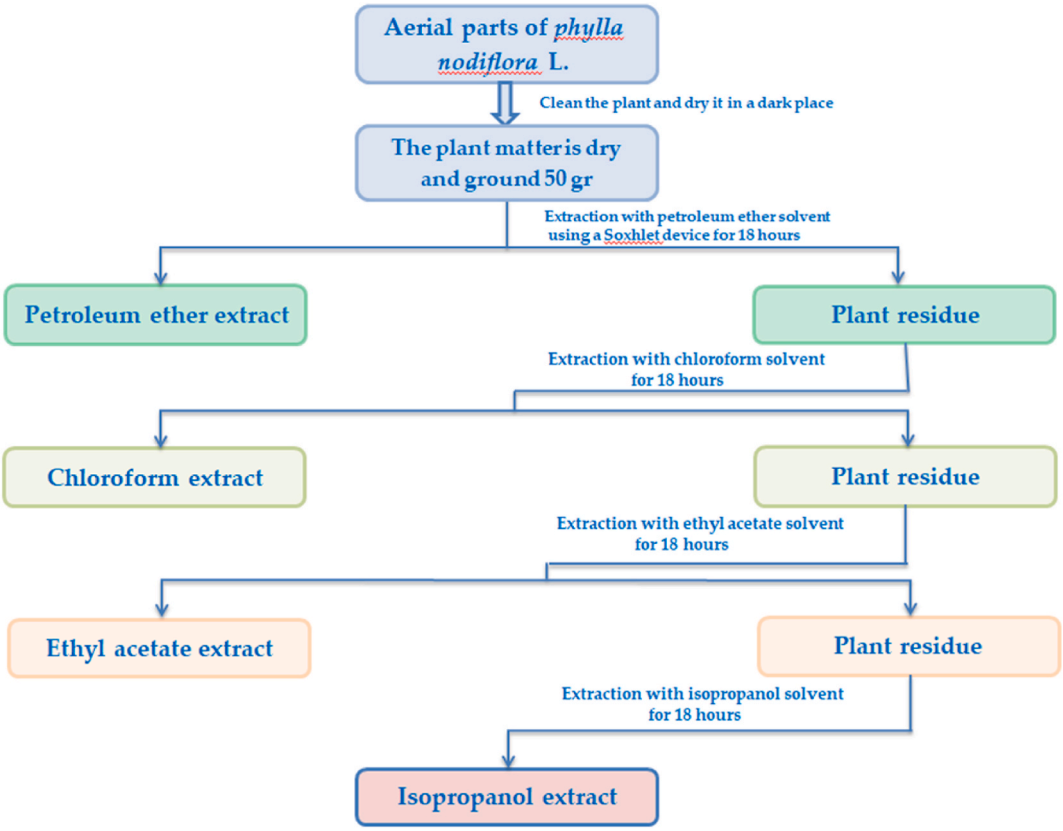

Fig. 1. General scheme for the extraction of aerial parts of *P. nodiflora* using polar gradient solvents.

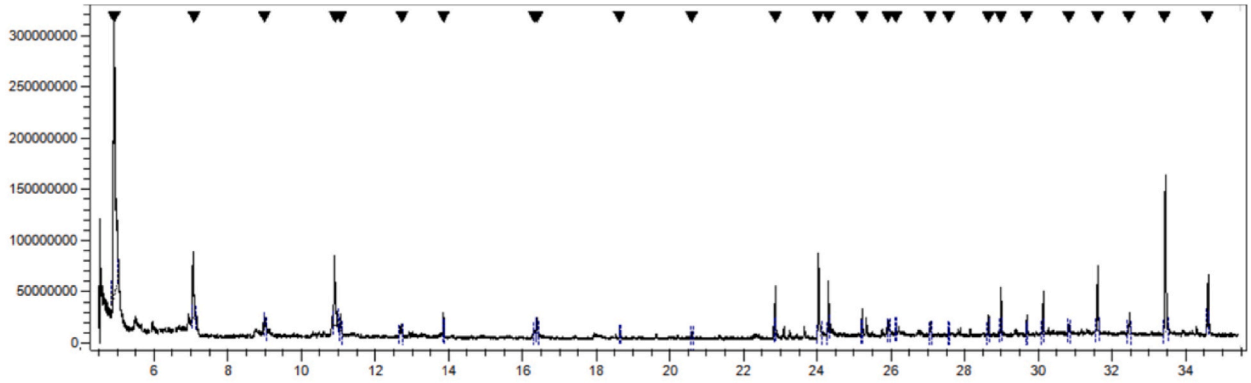

Fig. 2. GC–MS chromatogram of petroleum ether extract (Et) of aerial parts of *P. nodiflora*.

absence of hydrocarbons and silicon compounds (nonpolar compounds). This is evidence of good extraction using serial solvents of different polarities.

Ether compounds in petroleum ether (Et) constitute a large percentage (41.6 %). The compound 1,1-diethoxyethane is used in the fields of manufacturing pharmaceuticals and the perfume industry [22]. As hydrocarbon compounds constitute a large percentage of Et extract, nonadecane compounds have antioxidant, antimicrobial, and antimalarial biological activities and have cytotoxic effects [23–27]. Chloroform extract (Ch) contains a high proportion of hydrocarbons, accounting for more than 40 % of the total content of the extract. Octacosan has an antioxidant effect and is used in wound healing [28]. The percentage of monoterpenes in the ethyl acetate (Ea) extract was good (24.4 %). According to previous studies, terpenes have anti-inflammatory, antioxidant, antimicrobial and antihypertensive pharmacological properties. The compound geranyl isovalerate, for example, has good anticancer activity [29]. The sesquiterpene derivative hexahydrofarnesyl acetone has medicinal antioxidant and antimicrobial properties [30]. Alcohols are the main components of isopropanol extract (Is) (28.4 %). The compound tetradecanol is used in cosmetics because it brightens and

Table 2
Chemical components of petroleum ether extract (Et) of aerial parts of *P. nodiflora* by GC–MS.

No.	Compound name	Molecular formula	Mw (g/mol)	R_t	Area %
1	1,1-Diethoxy ethane	$C_6H_{14}O_2$	118.17	4.92	33.9
2	Styrene	C_8H_8	104.14	8.99	1.6
3	n-Butyl methacrylate	$C_8H_{14}O_2$	142.19	10.91	5.9
4	1,1,3-Triethoxy propane	$C_9H_{20}O_3$	176.25	12.72	1.1
5	Anethole	$C_{10}H_{12}O$	148.20	16.32	5.5
6	Tetradecamethyl cycloheptasiloxane	$C_{14}H_{42}O_7Si_7$	519.077	18.62	0.4
7	Hexadecamethyl cyclooctasiloxane	$C_{16}H_{48}O_8Si_8$	593.23	20.59	0.5
8	Dibutyl phthalate[a]	$C_{16}H_{22}O_4$	278.34	24.03	5.8
9	Ethyl dodecanoate	$C_{14}H_{28}O_2$	228.39	24.31	2.7
10	Propyl hexadecanoate	$C_{18}H_{36}O_2$	299.39	25.22	1.2
11	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	$C_{16}H_{28}O_3$	268.39	25.91	0.8
12	2,6,10-Trimethyltetradecane	$C_{17}H_{36}$	240.30	27.07	0.8
13	Methyl 2,6,10,14-tetramethyl pentadecanoate	$C_{20}H_{40}O_2$	312.23	26.13	0.2
14	Tetrahydro-6-nonyl-*2H*-pyran-2-one	$C_{14}H_{26}O_2$	226.42	27.56	0.3
15	Heptadecane	$C_{17}H_{36}$	240.15	28.65	0.7
16	Cetene	$C_{16}H_{32}$	224.42	29.21	4.4
17	Tetradecyl oxirane	$C_{16}H_{32}O$	240.42	29.68	1.1
18	Nonadecane	$C_{19}H_{40}$	268.52	32.45	19.9
19	Tetracosane	$C_{24}H_{50}$	338.65	34.59	3.4
Hydrocarbons					**30.8**
Silicon compounds					**0.9**
Ester compounds					**16.9**
Other oxygenated compounds (ethers and epoxides)					**41.6**
Total identified compounds					**90.2**

M.F.: Molecular formula; M.W.: Molecular weight; R_T: Retention time (minutes); Area %: Percentage peak area.
[a] Phthalate derivatives contaminations.

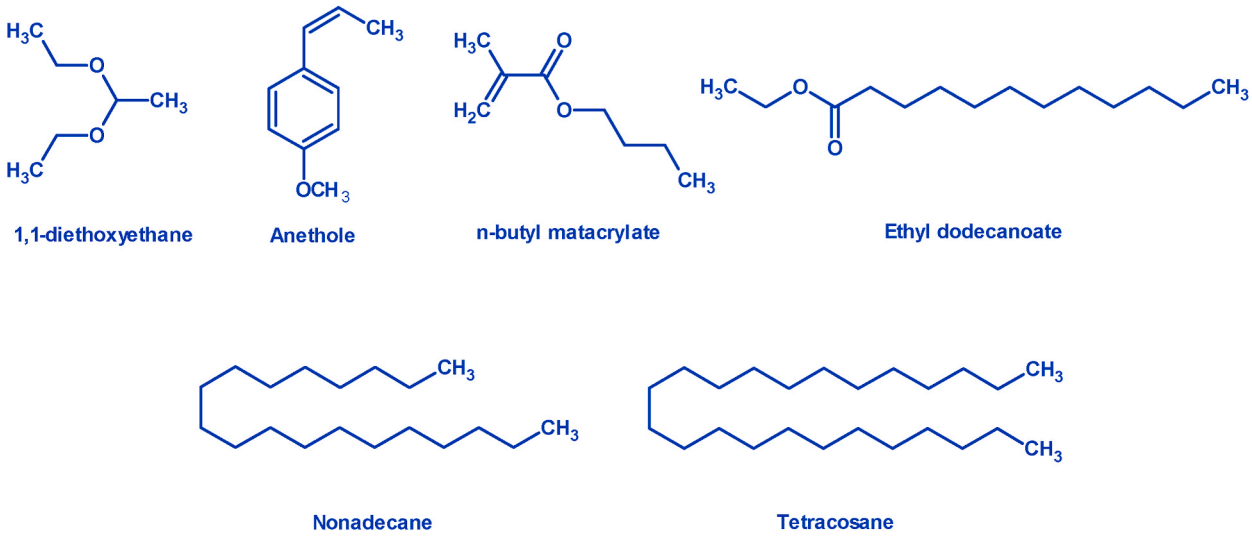

Fig. 3. The main chemical formulas of the petroleum ether (Et) extract.

moistens the skin [31]. It is also used to treat gingivitis [32,33]. In general, the unique chemical composition of organic extracts of *P. nodiflora* indicates good therapeutic and medicinal potential.

The presence of phthalic acid esters (phthalates) has been observed in organic extracts of the plant *P. nodiflora*, although they are not natural (synthetic) compounds that are widely used in the plastics and paints industry, plasticizers, or the cosmetics industry. However, there are many studies in which phthalic acid esters were found, whether in essential oils or in organic extracts of other plants. Surveys revealed the presence of phthalate compounds in various parts of sixty plant species belonging to 38 families, and their percentages ranged between 1 and 32 % in some plants. This is attributed to the accumulation of phthalates in a variety of medicinal plants, especially those growing in rivers, because plant roots are exposed to contaminated wastewater, as these pollutants are able to be absorbed from water and soil into plant roots [34–44]. Phthalate derivatives cause obvious toxicity to living organisms, including humans, which leads to serious diseases, including hypothyroidism; liver, kidney and lung infections; and asthma [45,46]. Some studies have also indicated that phthalic acid esters can be biosynthesized within plants via the shikimic acid pathway. Other studies

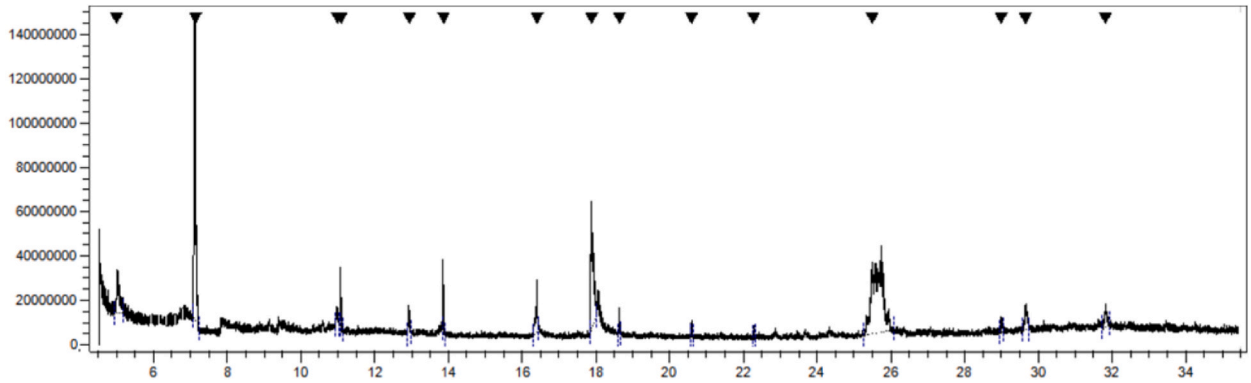

Fig. 4. GC–MS chromatogram of the chloroform extract (Ch) of the aerial parts of *P. nodiflora*.

Table 3
Chemical components of the chloroform extract (Ch) of the aerial parts of *P. nodiflora* determined by GC–MS.

No.	Compound name	Molecular formula	M.W. (g/mol)	R_t	Area %
1	4-Chloromethylene-2-phenyl-4,5-dihydrooxazol-5-one	$C_{10}H_6ClNO_2$	207.61	5.01	5.5
2	Hexamethyl cyclotrisiloxane	$C_6H_{18}O_3Si_3$	222.46	7.14	22.5
3	Pentachloro ethane	C_2HCl_5	202.29	10.99	1.3
4	Octamethyl cyclotetrasiloxane	$C_8H_{24}O_4Si_4$	296.61	11.08	2.1
5	Hexachloro ethane	C_2Cl_6	236.73	12.94	1.8
6	Decamethyl cyclopentasiloxane	$C_{10}H_{30}O_5Si_5$	370.76	13.87	2.0
7	Dodecamethyl cyclohexasiloxane	$C_{12}H_{36}O_6Si_6$	444.92	16.40	3.5
8	3-Methyl-2-cyclohexen-1-one	$C_7H_{10}O$	110.15	17.88	13.6
9	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	$C_{18}H_{52}O_7Si_7$	576.36	18.63	0.9
10	3TMS derivative (β)-epinephrine	$C_{17}H_{34}O_3Si_3N$	384.24	20.59	0.5
11	1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethyl heptasiloxane	$C_{14}H_{44}O_6Si_7$	505.09	22.28	0.3
12	Octacosane	$C_{28}H_{58}$	394.76	25.49	37.4
13	Diundecyl 1,2-benzenedicarboxylate[a]	$C_{30}H_{50}O_4$	474.71	28.99	0.8
14	Heptacosane	$C_{27}H_{56}$	380.73	29.65	2.7
Hydrocarbons					40.1
Silicon compounds					31.8
Chlorine compounds					3.1
Other oxygenated compounds					19.9
Phthalic acid esters					0.8
Carbonyl compounds					19.1
Total identified compounds					**94.9**

[a] Phthalate derivatives contaminations.

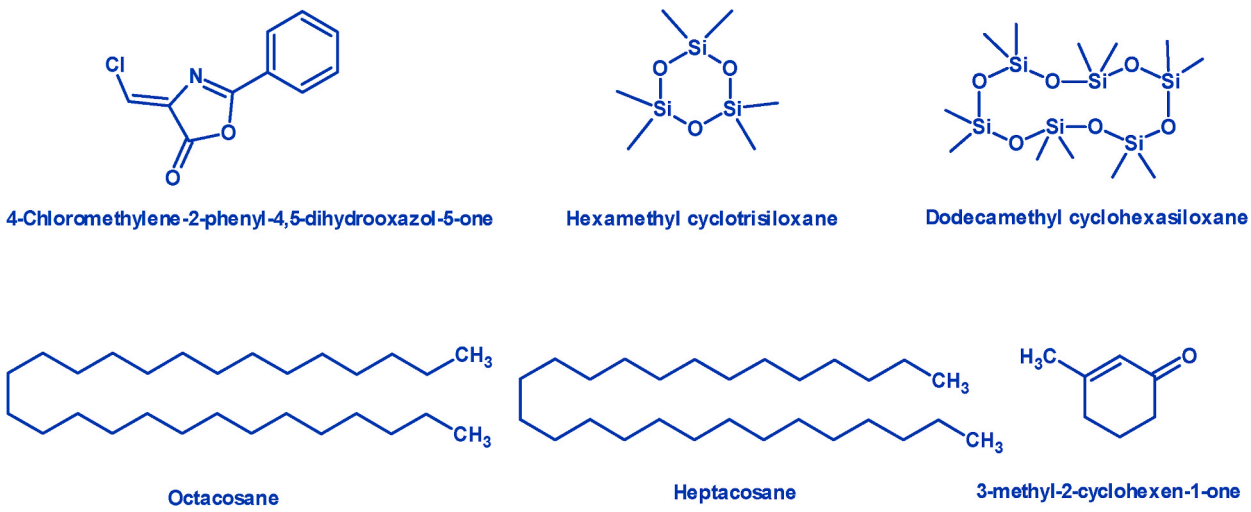

Fig. 5. The main chemical formulas of the chloroform (Ch) extract.

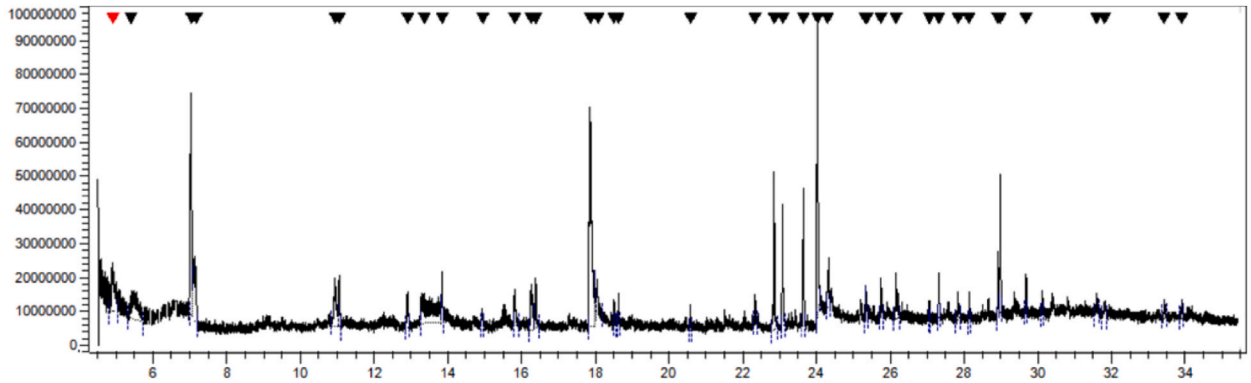

Fig. 6. GC–MS chromatogram of the ethyl acetate extract (Ea) of the aerial parts of *P. nodiflora*.

Table 4
Chemical components of the ethyl acetate extract (Ea) of the aerial parts of *P. nodiflora* by GC–MS.

No.	Compound name	Molecular formula	Mw (g/mol)	R_t	Area %
1	Ethyl dichloro acetate	$C_4H_6Cl_2O_2$	156.99	4.92	4.3
2	Isopulegol	$C_{10}H_{18}O$	154.25	7.04	8.9
3	3,3,4,4,4-Pentachlorobutan-2-one	$C_4H_3Cl_5O$	244.62	12.91	1.3
4	1,2,3-Propanetriol 1-acetate	$C_5H_{10}O_4$	134.13	13.36	6.3
5	5-Amino pentanol	$C_5H_{13}NO$	103.16	14.95	0.5
6	(*E*) 2-Decenal	$C_{10}H_{18}O$	154.25	15.81	1.5
7	3-hydroxy dodecanoic acid	$C_{12}H_{24}O_3$	216.32	17.87	17.7
8	1-Hexadecanol	$C_{16}H_{34}O$	242.44	22.33	0.7
9	6,10,14-Trimethyl-2-pentadecanone (Hexahydrofarnesyl acetone)	$C_{18}H_{36}O$	268.47	22.85	10.6
10	Butyl octyl 1,2-Benzenedicarboxylate[a]	$C_{20}H_{30}O_4$	334.44	23.08	9.6
11	Phytol	$C_{20}H_{40}O$	296.5	23.65	3.7
12	Geranyl isovalerate	$C_{15}H_{26}O_2$	338.36	24.03	15.5
13	Ethyl cyclohexanepropionate	$C_{11}H_{20}O_2$	184.27	24.30	3.5
14	Butyl oct-3-yl phthalate[a]	$C_{20}H_{30}O_4$	334.44	25.37	1.5
15	2-Butyl-1-octanol	$C_{12}H_{26}O$	186.33	26.15	1.8
16	Z,Z-2,5-Pentadecadien-1-ol	$C_{15}H_{28}O$	224.38	27.06	0.4
17	Palmitoleic acid	$C_{16}H_{30}O_2$	254.41	28.98	3
18	Cyclododecanemethanol	$C_{13}H_{26}O$	198.34	29.68	1
Alcohol compounds					**10.7**
Oxygenated monoterpenes					**24.4**
Oxygenated diterpenes					**3.7**
Sesquiterpene					**10.6**
Carbonyl compounds					**2.8**
Fatty acids					**20.7**
Esters					**7.8**
Phthalic acid esters					**11.1**
Total identified compounds					**91.8**

[a] Phthalate derivatives contaminations.

have also indicated that algae and bacteria can synthesize phthalates [47–49].

The chemical structure of the major compounds contained in the extracts was confirmed by mass spectrometry (MS) and by comparison of the resulting mass spectra with the reference spectra in the NIST Chemistry Web Book. The mechanisms of fragmentation of the compounds were investigated and proposed (electronic supplementary material), and the molecular weights of the resulting fragments were matched with those of the mass spectra. Table 6 shows the main fragments of the chemical compounds. Figs. 1 to 53 show the proposed fragmentation pathways for the compounds (electronic supplementary material).

4. Conclusion

The study of the chemical composition of the aerial parts of *P. nodiflora* using four different solvents of increasing polarity (petroleum ether, chloroform, ethyl acetate, and isopropanol) is a new study with the aim of obtaining a wide range of compounds. We did not obtain any studies related to the extraction process with the Soxhlet device using these solvents on the *P. nodiflora* plant from the literature. Petroleum ether and chloroform were used to extract nonpolar compounds, while ethyl acetate and isopropanol were used to extract moderate polarity compounds. The resulting main compounds are hydrocarbons, ethers, epoxides, and silicon compounds in the Et and Ch extracts and alcohols, carbonyl compounds, and oxygen terpenes in the Ea and Is extracts. It was observed that the P.

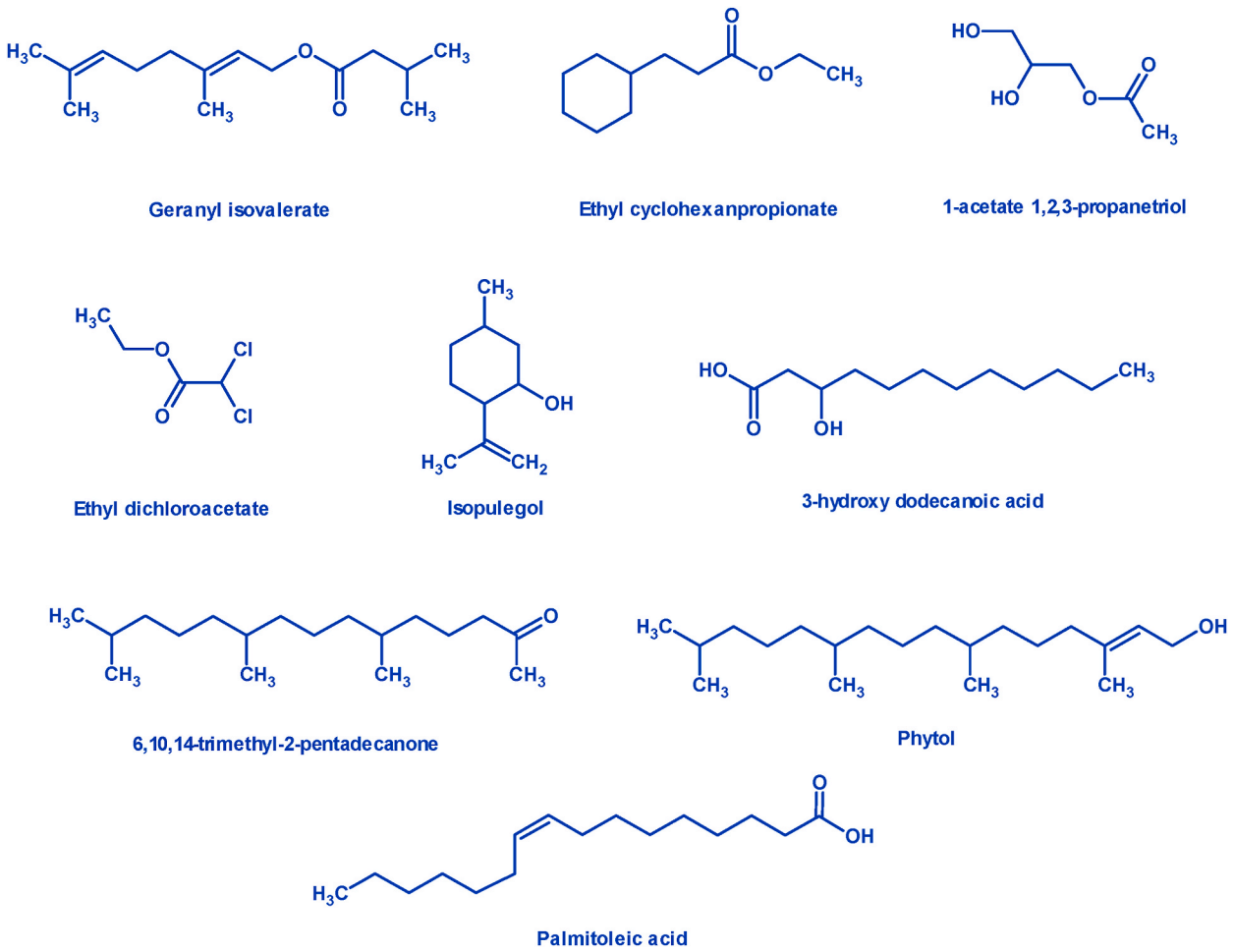

Fig. 7. The main chemical formulas of the ethyl acetate (Ea) extract.

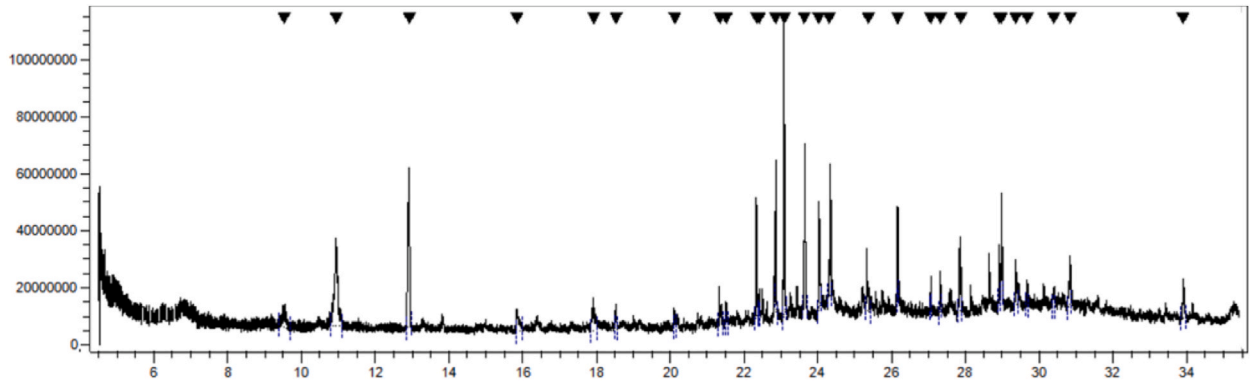

Fig. 8. GC–MS chromatogram of the isopropanol extract (Is) of the aerial parts of *P. nodiflora*.

nodiflora plant was contaminated with a good percentage of phthalate ester compounds, which causes a major problem in the field of human health, which requires more attention in both quality control and food and drug strategies by the Ministry of Health. According to the literature, the aerial parts of the plant *P. nodiflora* contain chemical compounds with biological antimicrobial, antioxidant, anticancer and antimalarial activities.

Table 5
Chemical components of the isopropanol extract (Is) of the aerial parts of *P. nodiflora* by GC–MS.

No.	Compound name	Molecular formula	Mw (g/mol)	R_t	Area %
1	(*E*) 2-Decenal	$C_{10}H_{18}O$	154.24	10.94	10.3
2	2-Methyl-2-cyclohexen-1-one	$C_7H_{10}O$	110.15	12.92	8.1
3	Dodecanal	$C_{12}H_{24}O$	184.32	21.51	0.8
4	Bis(2-methylpropyl) phthalate[a]	$C_{16}H_{22}O_4$	278.34	23.08	12.5
5	Behenic alcohol	$C_{22}H_{46}O$	326.60	23.63	18.6
6	Ethyl hexadecanoate	$C_{18}H_{36}O_2$	284.47	24.31	7.5
7	Tetradecanal	$C_{14}H_{28}O$	212.37	27.32	1.6
8	1-(Ethenyloxy) octadecane	$C_{20}H_{40}O$	296.53	27.86	5.3
9	Nonadecanol-1	$C_{19}H_{40}O$	284.52	28.92	1.5
10	Bis(2-ethylhexyl) phthalate[a]	$C_{24}H_{38}O_4$	390.56	28.98	3.8
11	1-Tetradecanol	$C_{14}H_{30}O$	214.39	29.36	8.3
12	15-Octadecenal	$C_{18}H_{34}O$	266.50	29.68	5.3
13	2-Bromo octadecanal	$C_{18}H_{35}BrO$	347.40	30.39	1.5
14	Oleic Acid	$C_{18}H_{34}O_2$	282.46	30.83	5.8
15	(3β) Cholest-5-en-3-ol tetradecanoate	$C_{41}H_{72}O_2$	597.01	33.90	6.5
Fatty acid and Esters					**13.3**
Alcohol compounds					**28.4**
Carbonyl compounds					**27.6**
Phthalic acid esters					**16.3**
Other					**11.8**
Total identified compounds					**97.4**

[a] Phthalate derivatives contaminations.

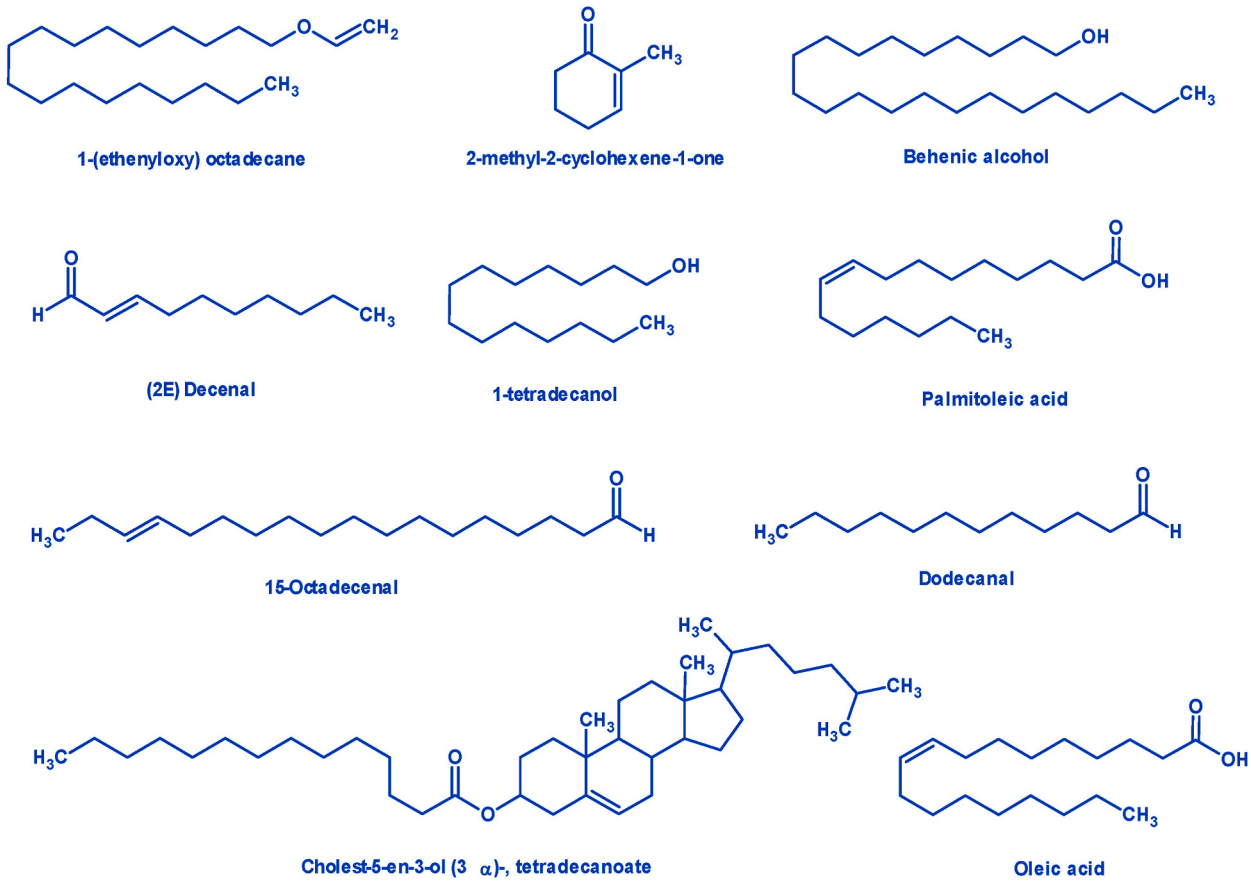

Fig. 9. The main chemical formulas of isopropanol extract (Is).

Table 6
Mass fragmentations of major compounds determined by GC–MS.

Compound name	Mw (g/mol)	Fragmentation ions [*m/z*]
1,1-Diethoxy ethane	118.17	118, 103, 73, 45
n-Butyl methacrylate	142.19	142, 113, 87, 69, 56, 41
Anethole	148.20	148, 133, 117, 105, 77, 51
Dibutyl phthalate	278.34	278, 223, 205, 149, 121, 104, 93, 76
Ethyl dodecanoate	228.39	228, 199, 183, 155, 143, 129, 101, 88, 73, 43
Cetene	224.42	224, 196, 182, 168, 154, 139, 125, 111, 97, 83, 69, 55, 43, 41
Nonadecane	268	268, 225, 211, 169, 127, 133, 99, 85, 71, 57, 43
Tetracosane	338	338, 295, 253, 225, 211, 169, 127, 99, 85, 71, 57, 43
4-Chloromethylene-2-phenyl-4,5-dihydrooxazol-5-one	207.61	207, 105, 77, 51
Hexamethyl cyclotrisiloxane	222.46	207, 191, 177, 133, 119, 103, 45
3-Methyl-2-cyclohexen-1-one	110.15	110, 82, 54
Octacosane	394.76	281, 253, 211, 169, 127, 113, 99, 85, 71, 57, 43
Heptacosane	380.73	380, 295, 253, 211, 169, 127, 99, 85, 71, 57, 43
Ethyl dichloro acetate	156.99	141, 111, 83, 73, 45
Isopulegol	154.25	154, 136, 121, 107, 95, 81, 71, 55, 41
1,2,3-Propanetriol 1-acetate	134.13	134, 103, 86, 74, 61, 43
6,10,14-Trimethyl-2-pentadecanone (Hexahydrofarnesyl acetone)	268.47	268, 250, 210, 194, 179, 165, 151, 124, 109, 95, 85, 71, 58, 43
Butyl octyl 1,2-Benzenedicarboxylate	334.44	279, 223, 205, 167, 149, 121, 104, 76, 43
Phytol	296.5	278, 123, 95, 81, 71, 57, 43
Geranyl isovalerate	338.36	238, 183, 169, 154, 136, 121, 107, 93, 85, 69, 57, 43
Ethyl cyclohexanepropionate	184.27	184, 155, 139, 121, 101, 88, 73, 55, 43
(*E*) 2-Decenal	154.24	154, 136, 121, 110, 98, 83, 70, 69, 57 55, 43, 41
2-Methyl-2-cyclohexen-1-one	110.15	110, 82, 71, 67, 54
Bis(2-methylpropyl) phthalate	278.34	287, 223, 205, 167, 149, 121, 104, 93, 76
Behenic alcohol	326.60	308, 280, 167, 139, 111, 97, 83, 71, 69, 57, 55, 43, 41
Ethyl hexadecanoate	284.47	284, 239, 199, 157, 143, 115, 101, 88, 57, 43
1-(Ethenyloxy) octadecane	296.53	296, 281, 166, 138, 111, 97, 83, 71, 69, 57, 55, 43, 41
1-Tetradecanol	214.39	196, 168, 140, 125, 111, 97, 83, 69, 55, 43
Oleic acid	282.46	282, 264, 222, 180, 151, 111, 97, 83, 69, 55, 41

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Data availability

Data will be made available on request.

CRediT authorship contribution statement

Hadi Aqel Khdera: Writing – review & editing, Writing – original draft, Visualization, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Sawsan Youseff Saad:** Supervision, Methodology, Conceptualization, Data curation, Formal analysis, Investigation, Visualization, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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None.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.heliyon.2024.e34686.

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