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Chemical profiling of two aromatic weeds, *Cyathocline purpurea* and *Blumea lacera*

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ABSTRACT

In the present investigation chemical constituents of *Cyathocline purpurea* (Buch.-Ham. ex D. Don) Kuntze and *Blumea lacera* (Burm.f.) DC. (Family-Compositae) were studied by using gas chromatography coupled with mass spectrometry (GC/MS). These two weeds are small herbs and well known for their potent medicinal properties. Total 17 and 27 compounds were identified from *C. purpurea* and *B. lacera* respectively. The major constituents in both the extracts were pentadecanoic acid, 14-methyl-, methyl ester (30.56%), cis-phytol (21.26%), α -cadinol (7.87%), γ -cadinene (7.13%), neophytadiene (3.81%) and α -cubebene (1.82%). GC/MS analysis revealed the presence of various bioactive compounds such as fatty acids, sesquiterpenoids, phenols, etc. in the acetone extracts of both the plants. The identified compounds have various biological activities.

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INTRODUCTION

Cyathocline purpurea (Buch.-Ham. ex D. Don) Kuntze and *Blumea lacera* (Burm.f.) DC. are commonly found as weed and widely distributed in South Asia, which belongs to the medicinally important Compositae family [1-3]. These plants are small herbs with strong odor and well known for their various medicinal properties which are due to presence of various bioactive compounds [4]. *C. purpurea* is known for various medicinal properties such as antimicrobial, anthelmintic, anticancer and hypotensive [5-7]. Various phytochemicals of *C. purpurea* showed anti-inflammatory, antioxidant potential, anti-arthritis activity and stomach relieving properties [8-10]. The plant parts were used in herbal remedy to treat tuberculosis, malaria, bleeding, swelling, rheumatism and a wide range of biological activities including mutagenic, genotoxic, cytotoxic and antitumor actions [7,11]. Previously various chemical constituents were reported from this plant such as guaianolide, eudesmanolide, sesquiterpene lactones, isoavangustin and guaianolide [12]. Many sesquiterpene lactones have shown significant antineoplastic or cytotoxic effects [6].

B. lacera is also valuable medicinal plant in many popular systems of medicine including Ayurveda, Homoeopathy and Unani. There is a heavy demand of different parts (fresh and dry both) of this

weed in national and international drug markets [13]. Leaf juice is used as astringent, stimulant, anthelmintic, liver tonic, bleeding piles, diuretic, bronchitis and blood diseases [14,15]. The plant also acts as a good stomachic and antispasmodic activity [16]. It is used in folk medicine for the treatment of cough, bronchitis, dysentery and wound healing potential [17,18].

Despite the fact that, these plants can be best used for its medicinal benefits. No research is available on GC/MS profiling of weed extract of selected plants. The objective of the present study was to assess and generate the phytochemical profile of both the selected medicinally important plants by using gas chromatography techniques.

MATERIAL AND METHODS

Plant Material and Extract Preparation

Plant samples (500 g) were collected from the Western Ghats of Maharashtra during flowering stages (August-September 2018). Plant samples of *C. purpurea* and *B. lacera* were collected from Bhimashankar (19°4'19.09"N, 73°32'8.5"E) and Savitribai Phule Pune University campus (18°32'53.9"N, 73°49'28.9"E) respectively. The plants were identified and authenticated from the herbarium of Department of Botany, Savitribai Phule Pune

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University, Pune (sweetgum.nybg.org) and assigned voucher number for *C. purpurea* is Bot/DNM/51/2020 and for *B. lacera* is Bot/DNM/52/2020.

The plant materials was carefully brought to the laboratory and cleaned with distilled water. The leaves were separated from the plants and spread on a filter paper for shade drying at room temperature (27 ± 2 °C). The dried leaves were grounded into fine powder using Wiley mill. The powder obtained was passed through 2 mm sieve. The fine powder (10 g) mixed in 100 ml of acetone (extract has been repeated thrice) and kept in shaker overnight at 25 °C at 60 rpm. The sample was filtered using Whatman filter paper no. 1 and the solvent from filtrate extract was removed on rotary vacuum evaporator (RVE) at 35-40 °C [19]. After RVE 5 g of crude extract was obtained and the obtained crude extract was greenish in colour. The extract was soluble in ethanol, methanol, chloroform and acetone. For GC/MS analysis 10 μ L of crude extract was dissolved in 1 mL of acetone was used. Each experiment was performed in triplicate and mean was calculated.

Chromatographic Analysis

For preliminary screening of phytochemicals, acetone extracts of both the plants were subjected to GC/MS. GC was done by using Agilent 7890B while MS on Agilent 5977A MSD. The HP-5ms capillary column (30 m \times 0.25 mm \times 25 μ m) was used for the sample analysis. Helium (99.999 %) was used as a carrier gas at a flow rate of 1 mL/min. The temperature for GC/MS analysis was as follows: the injector temperature was kept at 250 °C, the initial temperature in oven was kept at 50 °C for 3 minute and was increased at a rate of 5 °C per minute until 175 °C. This temperature was maintained for 2 minute, with a total time of analysis of 30 min. MS data were recorded at 70 eV with a mass range of m/z of 45-600 amu. Single quadrupole mass spectrometer detector (150 °C) was used in MS analysis. The

information generated in GC/MS was used for quantification of compounds. For this purpose, an external standard method was used [20,21].

Identification of Compounds

The compounds were identified by the comparison of retention indices and mass spectra of most of the compounds with those of authentic compounds available in the database of National Institute Standard and Technology (NIST) and Wiley libraries. The identification was further supported by the calculation of their retention indices (RI) under identical experimental conditions using *n*-alkanes (C10- C40) and the calculated indices were then compared to those reported in the literature [22]. The assignments made were further confirmed by co-injection of authentic samples (Sigma-Aldrich) of the identified compounds, wherever possible [23].

RESULTS AND DISCUSSION

Preliminary analysis of phytochemicals revealed the presence of metabolites of diverse chemical nature in both the plant extracts. Among the 17 compounds identified in *C. purpurea* extract, the major compounds are pentadecanoic acid, 14-methyl-, methyl ester (30.56%), methyl oleate (9.56%), methyl stearate (9.15%), 2',5'-dimethoxypropiofenone (8.64 %), α -cadinol (7.87 %), along with some significant important compounds such as α -cubebene (2.69%), α -cadinene (1.98%), δ -cadinene (1.98%), nonadecanoic acid (1.84 %), β -cubebene (1.62 %), γ -cadinene (0.98 %) are abundantly present (Table 1 and Figure 1).

Whereas in *B. lacera* extract total 27 compounds were identified by GC/MS. The major constituents are cis-phytol (21.26%), 13-octadecenoic acid (7.64%), γ -cadinene (7.13%), 2- methyldocosane (6.42 %), bis (2-ethylhexyl) phthalate (5.02 %), trans-phytol (4.45 %), neophytadiene (3.81 %) beside

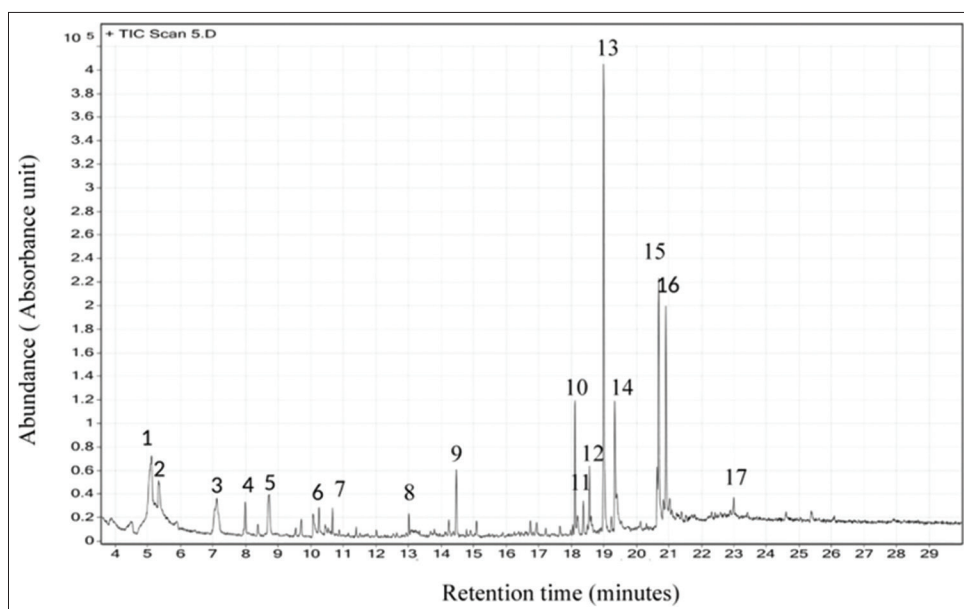
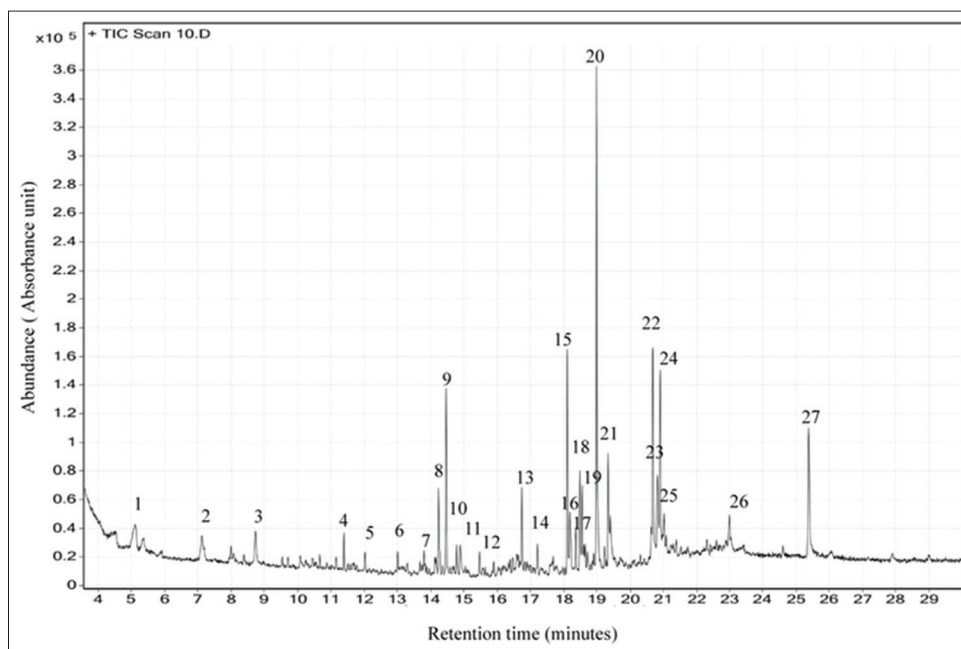


Figure 1: Gas chromatogram of *C. purpurea* extract

Table 1: Chemical composition of *C. purpurea* extract

No	Common name	RT	RI a	RI b	%	Identification
1.	α -Cubebene	5.10	1345	1348	2.69	MS, RI, CI
2.	β -Cubebene	5.34	1388	1387	1.62	MS, RI
3.	Citronellol acetate	7.11	1354	1357	0.75	MS, RI
4.	2'-Nitroacetophenone	8.11	1361	1361	0.66	MS, RI
5.	2,6-Di-Tert-butylphenol	8.71	1444	1443	0.82	MS, RI
6.	γ -Cadinene	10.14	1512	1510	0.98	MS, RI
7.	δ -Cadinene	10.73	1522	1516	1.98	MS, RI
8.	α -Cadinene	13.04	1538	1541	1.98	MS, RI
9.	α -Cadinol	14.46	1628	1626	7.87	MS, RI
10.	2',5'-Dimethoxypropiofenone	18.01	1658	1658	8.64	MS, RI
11.	Octadecane	18.30	1800	1800	1.92	MS, RI, CI
12.	Diisobutyl phthalate	18.47	1868	1871	5.48	MS, RI
13.	Pentadecanoic acid, 14-methyl-, methyl ester	19.01	1884	1884	30.56	MS, RI
14.	Pentadecanoic acid, 14-methyl-, methyl ester	19.37	1884	1884	8.84	MS, RI
15.	Methyl oleate	21.66	2085	2082	9.56	MS, RI, CI
16.	Methyl stearate	21.83	2128	2130	9.15	MS, RI, CI
17.	Nonadecanoic acid	23.10	2236	2236	1.84	MS, RI
	Fatty acids+esters	59.95				
	Sesquiterpenes hydrocarbon	9.25				
	Oxygenated sesquiterpenes	8.62				
	Aromatic acid	5.48				
	Ketone	9.3				
	Alkanes	1.92				
	Phenols	0.82				
	Oxygenated monoterpenes	0.75				
	Total	96.09				

RT= Retention Time, RI^a=Retention indices relative to C10-C40 *n*-alkanes on HP-5ms Column, RI^b= Retention indices reported in the literature (Adams, 2007), %= percentage composition of each compound, MS= mass spectrum of the respective compounds from the NIST and Wiley Library, RI=Reported retention indices, CI=Co-injection with the authentic sample.*Fatty acids+esters (Sr. No. 13,14,15,16,17), Sesquiterpenes hydrocarbon (Sr. No. 1,2,6,7,8), Oxygenated sesquiterpenes (Sr. No. 9), Aromatic acid (Sr. No. 12), Ketone (Sr. No. 4,10), Alkanes (Sr. No. 11), Phenols (Sr. No. 5), Oxygenated monoterpenes (Sr. No.3)

Figure 2: Gas chromatogram of *B. lacera* extract

this some important compounds such as 2,4-di-tert-butylphenol (3.81 %), palmitic acid (3.77 %), nonadecane (3.5 %), methyl oleate (3.48 %), methyl palmitate (2.78 %), stearic acid (2.01 %), α -cubebene (1.82 %), octanal (0.86 %), α -copaene (0.53 %) are profusely extant (Table 1 Figure 1).

The crude extracts of *C. purpurea* and *B. lacera* was mainly composed of fatty acids+esters (59.95 and 27.09 %) followed by sesquiterpenes hydrocarbon (9.25 and 14.48 %), oxygenated sesquiterpenes (8.62 and 25.71%), alkanes (1.92 and 5.14 %), oxygenated monoterpenes (0.75 and 1.33 %), phenols (0.82

Table 2: Chemical composition of *B. lacera* extract

No	Common name	RT	RI a	RI b	%	Identification
1.	Octanal	5.21	1001	999	0.86	MS, RI, CI
2.	2-Isooctanone	7.22	1259	1260	0.82	MS, RI
3.	α -Cubebene	8.71	1349	1350	1.82	MS, RI
4.	Citronellol acetate	11.49	1354	1357	1.33	MS, RI
5.	2'-Nitroacetophenone	12.10	1361	1361	0.52	MS, RI
6.	α -Copaene	13.10	1378	1376	0.53	MS, RI
7.	β -Caryophyllene	13.72	1442	1445	0.56	MS, RI
8.	2,4-Di-tert-butylphenol	14.29	1502	1494	3.81	MS, RI
9.	γ -Cadinene	14.46	1512	1510	7.13	MS, RI
10.	β -Sesquiphellandrene	14.71	1537	1537	0.63	MS, RI
11.	2',5'-Dimethoxypropiophenone	14.86	1658	1658	0.63	MS, RI
12.	2-(1-Phenylethyl)phenol	15.49	1721	1720	0.73	MS, RI
13.	Neophytadiene	16.78	1830	1830	3.81	MS, RI
14.	Diisobutyl phthalate	17.21	1863	1868	3.1	MS, RI
15.	Pentadecanoic acid, 14-methyl-, methyl ester	18.09	1877	1877	7.41	MS, RI
16.	Nonadecane	18.22	1900	1900	3.5	MS, RI, CI
17.	Methyl palmitate	18.40	1902	1904	2.78	MS, RI, CI
18.	Palmitic acid	18.55	1964	1963	3.77	MS, RI, CI
19.	Methyl oleate	18.61	2103	2103	3.48	MS, RI, CI
20.	cis-Phytol	19.03	2114	2113	21.26	MS, RI
21.	trans-Phytol	19.30	2122	2120	4.45	MS, RI
22.	13-Octadecenoic acid, methyl ester	20.69	2126	2125	7.64	MS, RI
23.	Stearic acid	20.78	2128	2130	2.01	MS, RI, CI
24.	2-Methyldocosane	20.91	2264	2265	6.42	MS, RI
25.	Tricosane	21.13	2300	2300	1.64	MS, RI
26.	Butoxycarbonylmethyl butyl phthalate	23.12	2403	2402	1.6	MS, RI
27.	Bis(2-ethylhexyl) phthalate	25.39	2550	2545	5.02	MS, RI
	Fatty acids+esters	27.09				
	Oxygenated Diterpene	25.71				
	Sesquiterpenes hydrocarbon	14.48				
	Aromatic acid	9.72				
	Fatty acyl	7.24				
	Alkanes	5.14				
	Phenols	4.54				
	Oxygenated monoterpenes	1.33				
	Ketone	1.15				
	Aldehyde	0.86				
	Total	97.26				

RT= Retention Time, RI^a=Retention indices relative to C10-C40 *n*-alkanes on HP-5ms Column, RI^b= Retention indices reported in the literature (Adams, 2007), %= percentage composition of each compound, MS= mass spectrum of the respective compounds from the NIST and Wiley Library, RI=Reported retention indices, CI=Co-injection with the authentic sample.*Fatty acids+esters (Sr. No. 15, 17, 18,19, 22, 23), Oxygenated Diterpene (Sr. No. 20,25), Sesquiterpenes hydrocarbon (Sr. No. 3, 6, 7, 10, 13), Aromatic acid (Sr. No. 14, 26

and 4.54 %), ketone (9.3 and 1.15 %), fatty acyl (7.24 %) and aldehyde (0.86 %) respectively. The majority of both the plants extracts constituents were rich in fatty acids+esters and sesquiterpenoids (Table 1 and 2).

The most important compounds are abundantly present in both the plants extracts are cubebene, cadinene, copaene, cadinol and citronellolacetate. These various sesquiterpenoids are contributing to the medicinal activities such as anticancer [24], anti-helicobacter pylori [25], antimicrobial [26-28], antifungal [29,30], antiviral, antioxidants [31], anti-inflammatory and antipyretic activities [25]. Cubebene was first isolated from *Piper cubeba* berries and abundantly present in various plants such as *Hornstedtia havilandii* [32], *Pinellia ternate* [33], *Annona glabra* L., *Annona squamosa* L., *Annona muricata* L., and *Annona reticulata* L. [34]. It has role in various plant metabolites. The copaene may act as an oviposition promoter in olive fruit fly [35]. Neophytadiene is reported to act as strong bactericidal, antifungal, antipyretic, analgesic, antioxidant and

vermifugic activities [36,37]. Phytol showed antimicrobial, anticancer and antidiuretic activity [36-38]. Palmitic acid, stearic acid and nonadecane acid were used in insect pest management [39]. Long-chain fatty acids such as hexadecanoic acid, octadecanoic acid, pentadecanoic acid, etc. have been reported several times over to possess various biological activities including antimicrobial [40].

The present study revealed that the plant extracts used contain diverse phytochemicals of different chemical nature. Many of the compounds having similar chemical nature are reported to be present in other plants extracts and found to have activities against various diseases and can be used as drugs formulations.

CONCLUSION

The crude extracts of *C. purpurea* and *B. lacera* was analysed by GC/MS and the phytochemical constituents were confirmed. Both the weeds contain diverse phytochemicals such as

sesquiterpenoids, fatty acids and phenols. These compounds may have some biological activities which may be exploited for bioprospecting in future. However, further research in this direction is required. These harmful weeds in agriculture field produce huge biomass which may be utilized as herbal pesticide, fungicide and herbicide. Considering the presence of different secondary metabolites they may be useful for treating disease and disorders which are to be explored.

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