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Essential Oil Constituents of *Swertia chirata* Buch.-Ham.

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Abstract

The essential oil of *Swertia chirata* Buch.-Ham. was extracted by solvent extraction (n-pentane:diethylether, 1:1) method using simultaneous distillation-extraction (SDE) apparatus and analyzed by gas chromatography-mass spectrometry (GC/MS). The yield of essential oil obtained from *S. chirata* was 236.47 mg/kg. Seventy seven compounds of the essential oil belonging to chemical classes of acid (4), alcohol (21), aldehyde (15), ester (3), furan (3), hydrocarbon (7), ketone (17) and miscellaneous (7) were tentatively identified. The major volatile compounds ranged in content order were as follows: undecanoic acid (28.63%), 2-buten-2-one (20.42%), camphor (18.40%), 2-heptadecanone (14.72%), and cedrol (13.07%).

Key words: *Swertia chirata*, essential oil, volatile compounds

INTRODUCTION

Among the 170 species of the genus *Swertia* (Gentianaceae), twenty nine species are found in Nepal and nine species are being traded in the country (1). A species, *Swertia chirata* Buch.-Ham., locally known as 'Chiriato', found in the temperate Himalayan region between 1,200 and 3,000 m, plays a dominant role in the trade covering about 80% of total traded volume of *Swertia* species in the country (2). This species has been used in traditional medicine against asthma, stomachic, antidiarrhoetic, dyspepsia, piles, hepatitis, typhoid fever and liver disorders (3). Pharmacological studies of this plant reported the multidirectional clinical applications including anti-inflammatory, hepatoprotective and anti-leishmanial activities (4,5). Phytochemical investigations resulted in the isolation of xanthonoids, flavonoids, alkaloids, triterpenoids, and lignans (6-8).

Essential oils, obtained from medicinal plants, have played an important role as a source of pharmacologically active substances. Therefore, there has been a considerable interest in the study of the essential oils of medicinal wild plants. With growing attention in the use of essential oils of medicinal plants in the food, aromatherapy and pharmaceutical industries, an examination of the components of the essential oil of these plants has become increasingly important for their chemical safety and clinical acceptability. The chemical basis for the use of essential oil of *chirata* is far from clear, and it is difficult to research the pharmacological activities in detail without access to a relatively explicit chemical data base, which is not currently available. The identification of the useful volatile organic compounds from this plant for widespread consideration as elements of health care systems will be an interesting topics for research. Therefore, we interested to study the profile of volatile compounds of the 'Chiriato' growing in Nepal, for which no data have been previously reported.

MATERIALS AND METHODS

Materials

Swertia chirata Buch.-Ham.: Commercially available sample of *S. chirata,* locally called 'Chiriato' in Nepal, was collected in July 2006 from Kathmandu, Nepal. Vacuum packing of the samples was carried out by removing air from the package and stored at -18°C before the experiment.

Reagents: The regents were purchased from Sigma Co. (USA) and Fisher Scientific (USA). HPLC grade organic solvents (*n*-pentane & diethylether) used for extraction and chromatography were redistilled using a spiral packed double distilling apparatus (Normschliff Geratebau, Wertheim, Germany) and Milli-Q water that was generated with a water purification system (Millipore Corporation, Bedford, USA).

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Methods

Extraction of volatile organic compounds : Fifty grams of sample were homogenized in a blender (MR 350CA, Braun, Spain) and mixed with 1 L of distilled water. After adjusting to pH 6.5 with 1% NaOH, 1 μL *n*-butylbenzene was added as an internal standard. The resultant slurry was used for extraction of volatile organic compounds with 200 mL redistilled *n*-pentane:diethylether (1:1, v/v). The extraction of volatile organic compound was carried out for 2 hr, using simultaneous distillation-extraction (SDE) apparatus of Nikerson and Likens (9) type as modified under atmospheric pressure by Schultz et al. (10). The solvent, containing compounds extract, was dehydrated for 12 hr using 10 g anhydrous Na_2SO_4 and then concentrated to approximately 1.5 mL using the vigreux column. This concentrate was further concentrated to 0.5 mL under gentle stream of N_2 gas and used for gas chromatography-mass spectrometry (GC/MS) analysis.

Chromatographic analysis : Chromatographic analysis was carried out using a Shimadzu GC/MS (QP-5000, Shimadzu Co., Kyoto, Japan) in EI mode. The ionization voltage was 70 eV and temperatures of ion source and injector were 230°C and 250°C, respectively. The capillary column used was a DB-WAX (60 m×0.2 mm, i.d., 0.25 μm, film thickness; J&W, USA). The oven temperature programmed at 40°C (Isothermal for 3 minutes) was ramped to 150°C at 2°C/min and to 220°C at 4°C/min (20 min) followed by 230°C at 5°C/min. Helium was used as the carrier gas at a flow rate of 1 mL/min, with injector volume of 1 μL using 1:20 split ratio.

Identification of volatile organic compounds : Qualitative analysis of volatile compounds was carried out by identif ication of compounds from mass spectra with the aid of mass spectral data book (11,12). The spectrum of each volatile compound agreed with that present in the mass spectrum library of WILLY 139, NIST 12 and NIST 62. The content of the volatile flavor compounds was calculated on a dry weight basis by comparing with peak area percent of the internal standard. The mass spectrometer scanned was ranged from 41 to 450 *m/z*.

RESULTS AND DISCUSSION

The essential oil of *S. chirata* was extracted by solvent extraction (P:E,1:1) method for 2 hr using SDE apparatus and analyzed by GC/MS. The result obtained by qualitative and quantitative analysis of volatile organic compounds of *S. chirata* was listed in Table 1 and chromatogram was shown in Fig. 1. Investigation confirmed that the yield of essential oil was 236.47 mg/kg. Seventy seven compounds of the essential oil belonging to chemical classes of acid (4), alcohol (21), aldehyde (15), ester (3), furan (3), hydrocarbon (7), ketone (17), and miscellaneous (7) were tentatively identified. Ketones were detected as dominant chemical class with highest proportion (28.58%). The major compounds belonging to ketone group were 3-buten-2-one, camphor, 2-heptadecanone, 3-ethenyl cyclohexenone and (*Z*)-geranylacetone. Most of the compounds, related to ketone group, were aliphatic compounds with lower than 1% concentration. Alcohol group containing 27.44% was characterized as second major chemical group. Cedrol was the most abundant alcohol compound while patchoulol, β-eudesmol, isothujol, *p*-cymen-3-ol, linalool, farnesol were also detected by high amount. All of these compounds are terpene alcohols.

Table 1. Relative content of functional groups of volatile organic compounds identified in *Swertia chirata* Buch.-Ham. extract

Functional groups	Relative peak area percentage (%)	Number of compounds
Acids	17.54	4
Alcohols	27.44	21
Aldehydes	11.12	15
Esters	3.3	3
Furans	1.38	3
Hydrocarbons	2.64	7
Ketones	28.58	17
Miscellaneous	8.00	7
Total	100	77

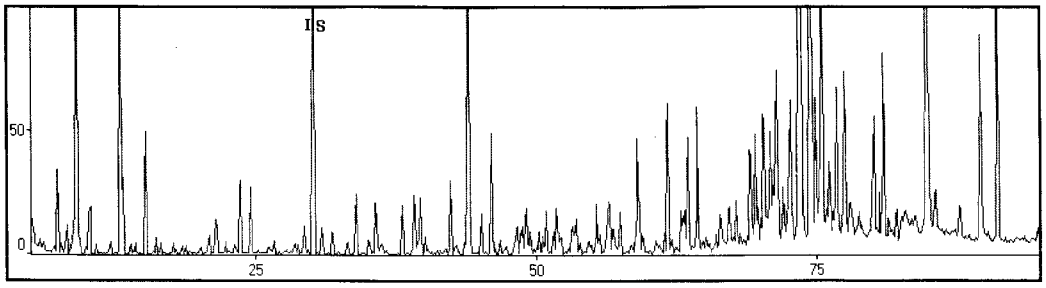

Fig. 1. Total ion chromatogram of volatile organic compounds of *Swertia chirata* Buch.-Ham. extract.

Table 2. Volatile organic compounds of *Swertia chirata* Buch.-Ham. extract

No.	RI[1)]	Compound name	Amount (mg/kg)	Relative peak area (%)	No.	RI	Compound name	Amount (mg/kg)	Relative peak area (%)
1	803	Ethyl formate	0.19	0.08	39	1595	[*E*]-Caryophyllene	1.41	0.60
2	864	Ethyl acetate	1.58	0.67	40	1601	6-Undecanone	0.64	0.27
3	878	2-Butanone	0.12	0.05	41	1641	α-Humulene	1.37	0.58
4	893	2-Methylbutanal	0.27	0.11	42	1643	Decanal	0.77	0.33
5	898	3-Methylbutanal	0.59	0.25	43	1647	Acetophenone	0.33	0.14
6	917	2-Methyl-1-propen-1-one	0.20	0.08	44	1698	α-Terpineol	1.01	0.43
7	923	Ethanol	1.02	0.43	45	1719	[*Z,E*]-α-Farnesene	1.84	0.78
8	932	3-Buten-2-one	20.42	8.63	46	1725	[*Z*]-β-Farnesene	0.26	0.11
9	939	2-Ethyl furan	0.23	0.10	47	1736	Carvone	1.15	0.49
10	967	3-Methyl-2-butanone	0.87	0.37	48	1764	[*E*]-3-Nonen-2-ol	4.32	1.83
11	971	Pentanal	1.25	0.53	49	1773	α-Curcumene	0.35	0.15
12	1037	2-Butenal	8.70	3.68	50	1794	Butyrophenone	0.27	0.11
13	1041	Methyl butenol	1.81	0.77	51	1816	3-Ethenyl cyclohexenone	4.59	1.94
14	1079	Hexanal	2.68	1.13	52	1843	2-Methylbutyl cyclohexane	0.96	0.41
15	1102	β-Pinene	0.18	0.08	53	1850	[*E*]-Geraniol	0.89	0.38
16	1122	3-Penten-2-one	0.24	0.10	54	1856	[*Z*]-Geranylacetone	2.49	1.05
17	1180	2-Heptanone	0.25	0.11	55	1874	Safrol	3.78	1.60
18	1182	Heptanal	0.74	0.31	56	1913	β-Phenylethanol	0.21	0.09
19	1214	2-Hexenal	1.74	0.74	57	1924	Dodecanol	1.17	0.49
20	1228	2-Pentylfuran	1.48	0.63	58	1963	1,2,3-Trimethoxybenzene	1.49	0.63
21	1253	Pentanol	0.16	0.07	59	2031	Tetradecanal	4.50	1.90
22	1286	Octanal	0.23	0.10	60	2048	3,4,5-Trimethoxytoluene	2.53	1.07
IS[2)]	*1310*	*Butylbenzene*	–	–	61	2056	Octanoic acid	1.45	0.61
23	1321	2,3-Octanedione	0.88	0.37	62	2065	Isothujol	4.35	1.84
24	1335	6-Methyl-5-methylideneheptane-2-one	0.50	0.21	63	2079	Hexadecanal	1.28	0.54
25	1355	Hexanol	0.30	0.13	64	2097	3,4,5-Trimethoxybenzaldehyde	4.97	2.10
26	1367	2,4-Dimethylfuran	1.56	0.66	65	2112	6,10,14-Trimethyl-2-pentadecanone	14.72	6.22
27	1382	4-Methylhexanol	0.26	0.11	66	2116	Cedrol	13.07	5.53
28	1390	Nonanal	1.46	0.62	67	2130	Nonanoic acid	6.43	2.72
29	1427	[*E*]-2-Octenal	1.09	0.46	68	2134	Eugenol acetate	6.05	2.56
30	1444	Limonene oxide	1.65	0.70	69	2140	*p*-Cymen-3-ol	4.04	1.71
31	1453	Hexen-3-ol	1.42	0.60	70	2151	Patchoulol	8.29	3.51
32	1459	Furfural	0.25	0.11	71	2161	Farnesol	2.77	1.17
33	1492	2-Ethylhexanol	2.10	0.89	72	2173	β-Eudesmol	4.64	1.96
34	1511	Pyrrole	0.54	0.23	73	2184	Decanoic acid	5.30	2.24
35	1517	Camphor	18.40	7.77	74	2250	[*E*]-Propenyl guaiacol	4.24	1.79
36	1535	Octanol	0.91	0.38	75	2375	Undecanoic acid	28.63	12.11
37	1549	Linalool	3.46	1.45	76	2393	Hexadecanol	1.29	0.55
38	1584	2,6-Nonadienal	0.68	0.29	77	2549	Octadecanol	8.26	3.49
								236.47	100

[1)]Retention Index. [2)]Internal standard.

Similarly acids and aldehydes containing 17.54% and 11.12% respectively were characterized as major groups. All of the compounds related to acid group were fatty acids. 2-Butenal, tetradecanal and hexanal were the important aldehydes while remaining aldehydes were quantified below 1%. Hydrocarbons (2.64%) constituted the small part of total content. Most of the hydrocarbons were related to terpene group. The complete profile of the terpenoid constituents showed 6 oxygenated monoterpenes (10.89%). Among the sesquiterpenes, 4 compounds were hydrocarbons (2.06%) and 4 compounds were oxygenated (12.16%) sesquiterpenes, while only one compound belonging to hydrocarbon monoterpene was also detected. From present finding, the major volatile compounds of *S. chirata* can be ranged in content order as follows: undecanoic acid (28.63%), 2-buten-2-one (20.42%), camphor (18.40%), 2-heptadecanone (14.72%), and cedrol (13.07%) (Table 2).

The essential oil obtained from *S. chirata* found great variety of phytochemicals having wide range of bioactivities. Some important compounds were detected and described in this study. The compounds linalool, α-terpineol, geraniol were major oxygenated monoterpenes, while cedrol, farnesol, and β-eudesmol were the major oxygenated sesquiterpene. Monoterpenes are generally regarded as safe substances, but safrole is carcinogenic. The compound of *p*-cymene, detected with high amount in this species, has anti-microbial activities as described in literature (13). Linalool, a dominant compound of this oil, is known for various pharmacological activities (14,15). Terpenoidal alcohols of α-terpineol, farnesol and β-eudesmol, detected in present study, were previously proved as myorelaxant, antispasmodic, anti-cancer, anti-epileptic and antagonistic activities (16-18). Compound cedrol, major constituent of this oil, has parasympathetic activity, decrease blood pressure (19,20). Oxygenated monoterpenes were dominant terpene of this oil. Consequently, monoterpene phenols were previously reported to be active against fungi (21) and can be used as alternative sprout inhibitors (22). Carvone was found to be potentially good therapeutic agents against infections caused by fungus and bacteria and carvone can be also used as a good potato sprouting inhibitor (23). Furfural has a wide variety of uses such as a solvent, an ingredient of phenolic resins, chemical intermediate, weed killer, fungicide and also as a flavoring agent (24). Pharmacologically active some compounds related to hydrocarbon sesquiterpenes such as isomers of farnesene, (*E*)-caryophyllene, and α-humulene were detected in this study. The isomer of farnesene is known as electro-physiologically active component for pheromonal activities (25). (*E*)-Caryophyllene and α-humulene are likely to be the precursors of the complex menthols or resins which have been claimed to contain the antibacterial, antifungal or antioxidant properties (13,26). Camphor, a third major compound of this oil, is well known with its pronounced antimicrobial potentials (27).

On the basis of the above results, we concluded that, *S. chirata* can yield an essential oil useful for the pharmaceutical and agricultural industries.

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