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Chemical Composition and Antioxidant Activity of the Seeds Oil of *Vitex kwangsiensis* C. Pei

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Abstract: The chemical constitution of the seeds essential oil of *Vitex kwangsiensis* C. Pei and *in vitro* antioxidant activity have been investigated. The essential oil was isolated by hydrodistillation method then analyzed by GC-MS. Fifty-six compounds were identified, representing 93.1% of the oil. The main components identified were methyl linoleate (11.2%), caryophyllene oxide(10.3%), β-eudesmol (9.1%) and methyl palmitate (8.1%). The antioxidant activity was tested by DPPH method and it showed weak antioxidant activity. The composition and bioactivity of *Vitex kwangsiensis* seeds oil are described for the first time.

Keywords: *Vitex kwangsiensis*; essential oil; antioxidant activity.

1. Plant Source

Ripe seeds of *Vitex kwangsiensis* were collected from Jinchengjiang district, Guangxi province, China, and were identified to be the *Vitex kwangsiensis* by Associated Prof. Hong Zhao of the Marine College, Shandong University at Weihai. The voucher specimen (No. VK201109) is deposited at Herbarium of Shandong University, Weihai. Plant samples were air-dried prior to hydrodistillation.

2. Previous Studies

The genus of *Vitex* contains about 250 species distributed widely in tropical and temperate zones[1,2]. There are 14 species and 7 varieties growing mainly in south of Yangtaze River, China. The Vitex family is traditional Chinese herb that the fruits, leaves, especially seeds were used for healing and recent study showed that the extract possess antitumor, antimicrobial and antioxidant activities[3]. It has been reported that sabinene, 1,8-cineole in the fruits, seeds, flowers of *Vitex agnus-castus*[4,5]; butylated hydroxytoluene (BHT), phytol, β-caryophyllene in the leaves of *Vitex megapotamica* [6]; β-pinene , β-caryophyllene and β-elemene in the leaves of *Vitex quinata* [7].*Vitex kwangsiensis* C. Pei is endemic to China and is used for relieving cough and heavy pant. As far as we know, there is no former study on the essential oil of *Vitex kwangsiensis* seeds and its biological activity.

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3. Present Study

The ripe seeds of *Vitex kwangsiensis* (200g) were dried at room temperature. The essential oil was extracted by hydrodistillation in a Clevenger type apparatus for 3h. The obtained oil was stored at 4℃ until future tests.

Table 1. Chemical composition of essential oil of *Vitex kwangsiensis seeds*

No	Compound Name	%	RI	Identification Method
1	1,8-Cineole	2.7	1035	RRI,MS
2	2-Butoxyethyl acetate	0.6	1087	MS
3	8-Hydroxylinalool	0.5	1105	RRI,MS
4	4-Terpineol	3.1	1186	MS
5	α-Terpineol	0.6	1198	RRI,MS
6	5-Caranol	0.9	1202	MS
7	*p*-Menth-4-en-3-one	0.2	1258	MS
8	2,3-Camphanediol	0.2	1263	MS
9	Geraniol acetate	0.4	1288	RRI,MS
10	Isoborneol ethyl ester	2.7	1294	MS
11	β-Methylnaphthalene	0.2	1307	RRI,MS
12	Elixene	0.1	1347	RRI,MS
13	α-Terpineol acetate	1.3	1356	RRI,MS
14	α-Cubebene	0.3	1359	RRI,MS
15	2-Butanone, 4-(7-methoxy-7-methyl-2-oxepanylidene)	0.2	1369	MS
16	Cedrene	0.3	1389	RRI,MS
17	β-Elemene	0.9	1403	RRI,MS
18	Cyperene	0.4	1432	RRI,MS
19	α-Guaiene	0.1	1426	RRI,MS
20	γ-Caryophyllene (*cis*-Caryophyllene)	3.1	1438	MS
21	Thujopsene	0.3	1451	RRI,MS
22	Ledene	0.3	1455	RRI,MS
23	α-Himachalene	0.6	1472	MS
24	1ξ,6ξ,7ξ-Cadina-4,9-diene	1.1	1492	RRI,MS
25	β-Selinene	1.4	1506	RRI,MS
26	β-Bisabolene	2.1	1517	RRI,MS
27	Eremophilene	1.3	1522	RRI,MS
28	β-Guaiene	2.2	1531	RRI,MS
29	δ-Cadinene	2.7	1538	RRI,MS
30	β-Himachalene	1.9	1547	RRI,MS
31	Selina-3,11-diene-2,14-diol	0.6	1554	MS
32	α-Calacorene	1.0	1561	RRI,MS
33	Caryophyllene oxide	10.3	1574	RRI,MS
34	calamenene	0.8	1581	MS

35	Isoaromadendrene epoxide	0.8	1619	RRI,MS
36	Torreyol	1.5	1647	RRI,MS
37	Cubenol	2.0	1660	RRI,MS
38	β-Eudesmol	9.1	1677	RRI,MS
39	Methyl tetradecanoate	1.3	1719	RRI,MS
40	γ-Costol	1.1	1753	RRI,MS
41	Verrucarol	0.4	1794	MS
42	Selina-3,11-diene-2-exo,-4-ol	0.7	1805	MS
43	Hexahydrofarnesyl acetone	0.3	1840	RRI,MS
44	Methyl palmitate	8.1	1924	RRI,MS
45	Biformene	0.2	1933	MS
46	Widdrol	0.5	1945	MS
47	Ethyl hexadecanoate	0.3	1987	RRI,MS
48	Verticiol	0.2	1993	RRI,MS
49	Manool	2.3	2001	RRI,MS
50	Manoyl oxide	0.4	2010	RRI,MS
51	Methyl margarate	0.3	2020	RRI,MS
52	Methyl linoleate	11.2	2097	MS
53	Methyl elaidate	4.0	2101	MS
54	Methyl oleate	0.2	2104	MS
55	Methyl stearate	2.5	2124	RRI,MS
56	Ethyl 9,12-octadecadienoate	0.3	2158	RRI,MS
	Esters	33.3		
	Terpenes	30.7		
	Alcohols	23.1		
	Ethers	3.1		
	Aromatic compounds	2.0		
	Ketones	0.9		
	Total	**93.1**		

Concentration calculated from total ion chromatogram; RRI: Relative retention indices calculated against n-alkanes; Identification method based on the relative retention indices (RRI) of authentic compounds on a HP-5 colum; MS, identified on the basis of computer matching of the mass spectra with Nist 1.7 Mass Spectral Database and comparison with literature data.

Yellow oil with a yield of 1.21mL/100g (v/w) was obtained by hydrodistillation of *Vitex kwangsiensis*. The chemical constituents in the essential oil are esters (33.3%), terpenes (30.7%), alcohols (23.1%), ethers (3.1%), aromatic compounds (2.0%) and ketones (0.9%) which together account for 93.1% of the oil. The major components are esters (33.3%) which consist of methyl linoleate (11.2%), methyl palmitate (8.1%), methyl elaidate (4.0%), isoborneol ethyl ester (2.7%), methyl stearate (2.5%) and other 8 esters. There is a 30.5% of sesquiterpenens in the oil, including caryophyllene oxide (10.3%), γ-caryophyllene (3.1%) and δ-cadinene (2.7%) etc. The oil contains alcohols, β-eudesmol (9.1%), 4-terpineol (3.1%) and manool (2.3%) are the main component(Table 1). Esters, sesquiterpene and alcohols constitute the 86.9% of the volatile oil. The main components were methyl linoleate, caryophyllene oxide, β-eudesmol, methyl palmitate and cubenol. Some main constituents are correspond to previous studies. Caryophylene oxide was detected in the previous study, it varies among species from 2.2% in the leaves of *Vitex agnus-castus* to 27.5% , and in *Vitex kwangsiensis* the content is 11.1% [4,8]. As well as the β-

caryophyllene content range from 4.6% in the itex agnus-castus to 21.4% *Vitex negundo L*, but in our study it was 6.2% [2,9]. In the previous study, sabinene, viridiflorol, β-caryophyllene, terpinen-4-ol, epi-laurenene, humulene epoxide II, and abietadiene were detected as the major component extracted from 23 populations of *Vitex negundo L*. from India, but the composition varied depending on the origin [2]. In conclusion, the components of the oil differ in different species, even the same specie are different for the geographical differences.

The ability in quenching the stable radical 1,1-diphenyl-2-picrylhydrazyl (DPPH) was monitoring to evaluated the antioxidant activity of oil [10]. Ascorbic acid was used as the control. A maximum concentration 1mg/mL of oil was conducted and the radical scavenging rate was 26.76%, which showed weak antioxidant activity. The main constitute of the oil were fatty acid esters and lack of flavonoids, phenolic and other antioxidative components. The aromatic compounds, sesquiterpenes and diterpenes may contribute towards the antioxidant activity of the essential oil extracted from the seeds of *Vitex kwangsiensis*.

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