Chemical composition of Essential oil from the leaves of two species of *BaiJiangCao*, *Patrinia scabiosaefolia* Fisch and *Patrinia villosa* (Thunb.) Juss.

Jian Wu, Ying Xu, Zheng Xiang*

Center of Research on Life Science and Environmental Science, Harbin University of Commerce,

No. 138 Tongda Street, Daoli District, Harbin 150076, China;

Address correspondence: rainbowaftersnow@hotmail.com

Keywords: *Patrinia scabiosaefolia* Fisch, *Patrinia villosa* (Thunb.) Juss., essential oil, GC-FID, monoterpene, sesquiterpene.

Abstract: The essential oil obtained by the hydrodistillation of the leaves of *Patrinia scabiosaefolia* Fisch and *Patrinia villosa* (Thunb.) Juss were analyzed by a combination of capillary GC-FID and GC/MS analytic techniques. 51 components comprising 94.56% of essential oil in leaves of *P. scabiosaefolia* Fisch and 33 components comprising 89.87% of oil in leaves of *P. Villosa* Juss were identified, respectively. The principal ingredients of oil from *P. scabiosaefolia* Fisch were 3-Methylbutanoic acid, Palmitic acid, Hexanoic acid and *cis*-Anethol and the principal ingredients of oil from *Patrinia villosa* (Thunb.) Juss were Camphogen, 2-Methyl-6-hydroxyquinoline, β-Damascenone and β-Ionone. Nine common components were confirmed in the essential oil of *P. scabiosaefolia* Fisch and *P. Villosa* Juss.

Introduction

Patrinia, which belongs to family Valerianaceae, is a widely distributed plant grown in East Asia and North America. The genus included more than 20 species, 10 of which growing in China (1). Usually, *Patrinia* species are used as leaves vegetables in some areas of China, and research also revealed its leaves with pharmacological properties, especially the species of *Patrinia scabiosaefolia* Fisch and *Patrinia villosa* (Thunb.) Juss..

The *P. scabiosaefolia* Fisch and *P. villosa* (Thunb.) Juss., two species that have been recorded in Chinese Pharmacopoeia with the same name "*BaiJiangCao*" in Chinese, are important ancient herbal medicines widely used for more than 2000 years from *ShenNongBenCaoJing*, a famous ancient Chinese medicinal literary. *BaiJiangCao* is heat-clearing, antipyretic, detoxicant, anti-inflammatory, and is used traditionally in the treatment of wound healing, abdominal pain and intestinal carbuncle, including acute appendicitis, abscess of the liver, dysentery in enteritis, carbuncle and deep-rooted ulcer (2, 3).

Previous research on the chemical constituents of *BaiJiangCao* have revealed that it contains several compound classes. Triterpenoid saponins, iridoids, flavonoids, flavonones and polysaccharides are the dominant bioacitve constituents in the leaves of *P. Villosa* Juss and *P. scabiosaefolia* Fisch, which displayed potential ability of anti-tumor and anti-inflammatory (4, 5, 6, 7, 8, 9). Other components, such as sterols and fatty acids were also confirmed (6, 10, 11, 12).

Essential oil are the bioactive components possess the activity of antitumor, antibiosis and

antioxidant. However, there are no reports on the essential oil composition of the leaves of *P. Villosa* Juss. As such, the objective of the present study was to characterize the essential oil components in *P. Villosa* Juss leaves, and also to make a comparision of the essential oil costituents from leaves of *P. Villosa* Juss and *P. scabiosaefolia* Fisch for the first time

Experimental

Plant materials: The *P. villosa* Juss. leaves were purchased from Hebei Qixin Traditional Chinese Medicine Pellets Co., Ltd., P. R. China, *P. scabiosaefolia* Fisch leaves were purchased from Anhui Yonggang Traditional Chinese Medicine Pellets Co., Ltd., P. R. China. All the leaves were identified by Dr. Jian Wu, Harbin University of Commerce. And voucher specimens (NO.PVJ20130821 and PSF20130816) were deposited at the Pharmacognosy Laboratory, Harbin University of Commerce.

Dried leaves of *P. Villosa* Juss and *P. scabiosaefolia* Fisch were submitted to hydrodistillation in a Clerenger-type apparatus for 4 hours. After distillation the oil was collected, dried with anhydrous Na_2SO_4, and kept in a vial at a temperature of -4^oC for further analysis.

Organic solvents for the experiment were purchased from Kermel Chemical Co. (Tianjin, China)

***Analysis of the essential oils*:** The oil samples analysis were performed on an Agilent 6890 Gas Chromatograph with an Elite-1 capillary column (cross bond 100% dimethyl polysiloxane, non-polar, 30 m × 0.32 mm × 0.25 mm) fitted with Flame Ionisation Detector.

Helium was used as the carrier gas at flow rate of 1mL/min. The column temperature was programmed from 55 to 265^oC at a rate of 5^oC/min. The injector and detector temperatures were programmed at 220^oC and 250^oC, respectively. The analysis was performed three times and relative percentages of components as mean values were calculated from the peak area-percent of GC-FID data. GC/MS analyses of the oils were performed by splitless injection of 1.0 mL of the oil on a Hewlett Packard 6890 gas chromatograph fitted with a cross-linked 5% PH ME siloxane HP-5 capillary column, 30 m × 0.32 mm × 0.25 mm coating thickness, coupled with a model 5973 mass detector. GC/MS operation conditions: injector temperature 220^oC; transfer line 290^oC; oven temperature programme 60 to 246^oC (3^oC/min); carrier gas: He at 1.0 mL/min. Mass spectra: Electron Impact (EI^+) mode 70 eV with a mass range of 40 to 450 m/z, ion source temperature 250^oC. Individual components were identified by Wiley 275.L and NIST 05a.L database matching and by comparison of retention times and mass spectra of constituents with published data (13). Identification was also done by comparison of MS with those of pure and authentic standards.

Results and discussion

The chemical composition of the essential oil of *P. scabiosaefolia* Fisch and *P. Villosa* Juss were shown in Table 1 and the gas chromatogram of the essential of two species of *Patrinia* were shown in Figure 1 and 2.

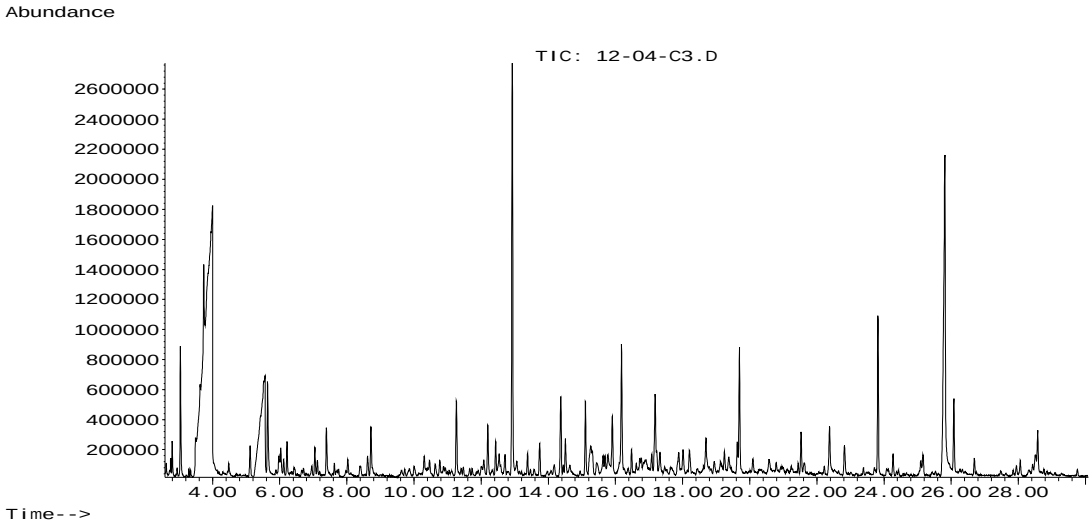

Figure 1. Typical gas chromatogram of the essential oil of *P. scabiosaefolia* Fisch.

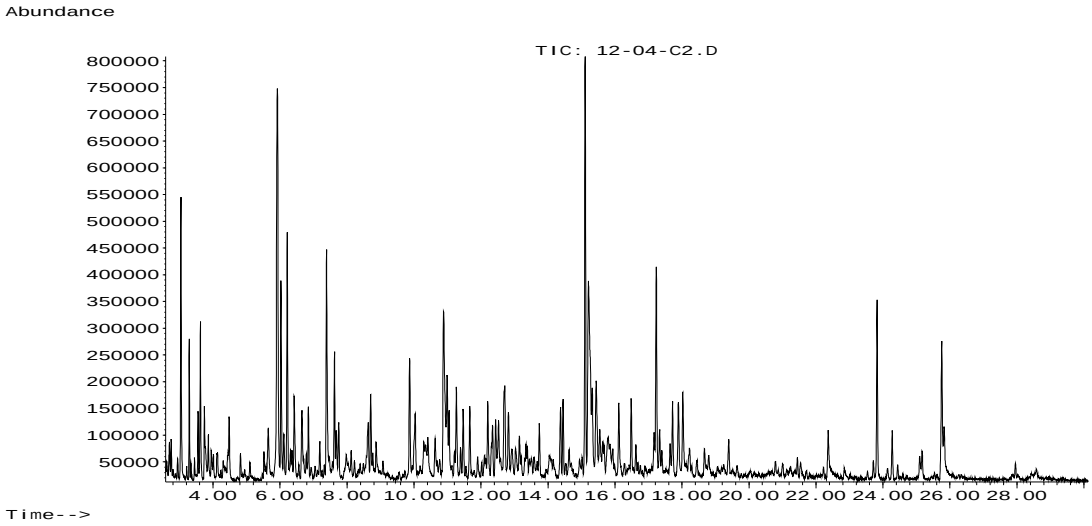

Figure 2. Typical gas chromatogram of the essential oil of *P. Villosa* Juss.

Table 1. Volatile constituents derived from *P. Villosa* Juss and *P. scabiosaefolia* Fisch

	P. Villosa Juss		*P. scabiosaefolia* Fisch	
NO.	Compound	%composition	Compound	%composition
1	Hexanal	3.39±0.37	Toluene	0.19±0.04
2	2,4-Dimethyl-heptane	1.3±0.17	Methyl isovalerate	0.38±0.06
3	2,4-Dimethyl-1-heptene	0.7±0.12	Hexanal	1.85±0.24
4	1,3-Cyclopentadiene	1.93±0.22	Furfural	0.82±0.13
5	2-Hexenal	1.24±0.18	Hexanoic acid	9.25±0.98
6	Camphogen	10.72±1.17	3-Methylbutanoic acid	25.11±2.26
7	(E)-5-Pentyloxy-2-pentene	2.85±0.29	(1S)-(-)-alpha-Pinene	0.52±0.08
8	2-Pentylfuran	3.94±0.51	3-Methyl pentanoic acid	2.98±0.42
9	(1H)Imidazole-4-acetonitrile	1.49±0.25	Benzaldehyde	1.94±0.24
10	3-Ethyl-1,4-hexadiene	1.21±0.18	(1S)-(1)-beta-Pinene	0.32±0.05
11	4-Methyldecane	0.96±0.17	2,5-Octanedione	0.66±0.11
12	Benzeneacetaldehyde	3.92±0.32	2-Pentylfuran	0.54±0.09
13	2,4,6-Trimethyldecane	1.43±0.11	D-Limonene	0.45±0.07
14	1-Nonanal	2.48±0.15	Benzeneacetaldehyde	1.01±0.15

15	Isodurene	3.35±0.23	Linolool oxide	0.28±0.05
16	Anethofuran	4.92±0.56	3,7-Dimethyl-1,6-octadien-3-ol	0.41±0.06
17	2,3-Dihydro-2,2,6-trimethylbenzalhyde	1.88±0.19	4,5-Dimethyl-1-hexene	1.20±0.19
18	α-Ionene	1.86±0.25	α-Ionene	0.39±0.05
19	beta-cyclocitral	1.34±0.19	1,1,4,5-Tetramethylindane	1.48±0.21
20	anti-7-Benzonorbornenol	1.59±0.21	1,2,3,4-Tetrahydro-1,6,8-trimethylnaphthalene	1.57±0.21
21	1,2,3,4-Tetrahydro-1,6,8-trimthylnaphthalene	1.84±0.13	Nonanoic acid	0.26±0.04
22	2-but-2-enyl-1,3,5-trimethylbenzene	0.79±0.14	*n*-Tetradecane	0.39±0.06
23	Pentadecan	2.46±0.26	*cis*-Anethol	7.51±0.83
24	α-Ionone	1.95±0.18	1-(1-Methylethenyl)-2,3,4,5-tetramethylbenzene	0.61±0.08
25	1,2,3,4-Tetrahydro-1,5,7-trimethylnaphthalene	1.71±0.21	1,2,3,4-Tetrahydro-1,5,7-trimethylnaphthalene	0.98±0.14
26	Dehydro-ar-ionene	2.12±0.24	3-Allyl-2-methoxyphenol	0.66±0.10
27	β-Damascenone	6.75±0.81	β-Damascenone	1.35±0.17
28	2-Methyl-6-hydroxyquinoline	7.03±0.95	Z-L-Glutamic acid	1.12±0.15
29	Propofol	3.35±0.29	1,4,6-trimethyl-1,2-dihydronaphthalene	0.52±0.09
30	β-Ionone	6.26±0.28	α-Gurjunene	0.73±0.07
31	Nerylacetone	1.56±0.19	α-Cedrene	0.94±0.10
32	2,4-Di-tert-butylphenol	1.71±0.20	(-)-Isocaryophyllene	1.31±0.21
33	5-Amino-1-ethylpyrazole	1.61±0.21	Calarene	3.16±0.38
34	5,5,8a-trimethyl-3,6,7,8-tetrahydro-2H-chromene	2.18±0.18	Geranylacetone	0.59±0.07
35	Hexahydrofarnesylacetone	3.83±0.31	(E)-a-Santalol	0.33±0.06
36	Palmitic acid	2.35±0.33	4-Hexyl-2,5-dioxofuran-3-acetic acid	1.75±0.25
37			*n*-Heptadecane	0.54±0.08
38			5-Amino-1-ethylpyrazole	0.71±0.12
39			3-(Phenylsulfanyl)-2-butanone	0.63±0.09
40			Dodecanoic acid	0.74±0.12
41			Caryophyllene oxide	0.45±0.07
42			Cedrol	0.73±0.09
43			1-(1-Adamantyl)-3-(1-methylcyclopentyl)aziridin-2-one	2.41±0.31
44			Hexadecanal	0.70±0.08
45			Tetradecanoic acid	1.09±0.14
46			Phenanthrene	0.68±0.11
47			Hexahydrofarnesylacetone	2.87±0.37
48			Diisobutyl phthalate	0.41±0.06
49			Methyl hexadecanoate	0.49±0.08
50			Palmitic acid	10.84±1.30

51		Isovaleric anhydride	1.39±0.19
52		Octadecanal	0.27±0.05
53		(E)-9-Octadecenoicacid	0.59±0.09
54		2-(5-oxohexyl)cyclopentan-1-one	0.90±0.14

Table 2. The common essential oil ingredients in leaves of *P. Villosa* Juss and *P. scabiosaefolia* Fisch (n=3).

No.	RT	Compound	Composition(%)	
			P. Villosa Juss	*P. scabiosaefolia* Fisch
1	3.04	Hexanal	3.39±0.37	1.85±0.24
2	6.22	2-Pentylfuran	3.94±0.51	0.54±0.09
3	7.39	Benzeneacetaldehyde	3.92±0.32	1.01±0.15
4	11.26	α-Ionene	1.86±0.25	0.39±0.05
5	12.21	1,2,3,4-Tetrahydro-1,6,8-trimthylnaphthalene	1.84±0.13	1.57±0.21
6	12.54	1,2,3,4-Tetrahydro-1,5,7-trimethylnaphthalene	1.71±0.21	0.98±0.14
7	15.11	β-Damascenone	6.75±0.81	1.35±0.17
8	23.83	Hexahydrofarnesylacetone	3.83±0.31	2.87±0.37
9	25.76	Palmitic acid	2.35±0.33	10.84±1.30

A total of 51 components of the essential oil of *P. scabiosaefolia* Fisch were identified, accounting to 94.56% of the total oil composition. The principal ingredients were 3-Methylbutanoic acid (25.11%), Palmitic acid (10.84%), Hexanoic acid (9.25%) and *cis*-Anethol (7.51%). 8 Monoterpenoids and 6 sesquiterpenoids, corresponding to 12.20% and 7.09%, were confirmed in the oil. A total of 33 components of the essential oil of *P. Villosa* Juss were identified, accounting to 89.87% of the volatile constituents. The main constituents were Camphogen (10.72%), 2-Methyl-6-hydroxyquinoline (7.03%), β-Damascenone (6.75%) and β-Ionone (6.26%). 6 monoterpenoids and 1 sesquiterpenoid were identified in the essential oil, corresponding to 27.87% and 2.67%, respectively.

P. Villosa Juss and *P. scabiosaefolia* Fisch with the same clinical purpose in traditional Chinese Medicine and even share the same chinese name *"BaiJiangCao"*, but only 9 of the common oil components were identified in leaves of *P. Villosa* Juss and *P. scabiosaefolia* Fisch (Table 2). This is the first report to make a comparison of essential oil constituents in leaves of two species of *BaiJiangCao*, which could have a distinguish between the two leaves on essential oil ingredient, and even could give a support for clinical use.

Acknowledgements

Thanks for the financial support of this work by the National Natural Science Foundation of China (81303211) and China Postdoctoral Science Foundation (2013M540301).

References

1. Y. Xie, J.Y Peng, G.R Fan, Y.T Wu. *Chemical composition and antioxidant activity of volatiles from Patrinia Villosa Juss obtained by optimized supercritical fluid extraction*. Journal of Pharmaceutical and Biomedical Analysis., **48**, 796–801 (2008). 2. H.Y Hsu, Y.P Chen, S.J Shen, C.S Hsu, C.C Chen, H.C Chang. *Oriental Materia Medica*. Oriental Healing Arts Institute, Long Beach, California, United States, pp. 238–239 (1986).

3. H.M Chang, P.P.H But. *Pharmacology and Applications of Chinese Materia Medica*. World Scientific, Teaneck, New Jersey, United States, pp. 790–792. (1987).

4. L Gao, L Zhang, N Li, J.Y Liu, P.L Cai, S.L Yang. *New triterpenoid saponins from Patrinia scabiosaefolia*. Carbohydrate Research., **346**, 2881-2885 (2011).
5. J.C Xu, X.Y Zeng, D.Q Yu. *Studies on the chemical constituents of Patrinia villosa Juss*. Acta Pharmacologica Sinica., **20**, 652-656 (1985).
6. J.Y Peng, G.R Fan, Y.T Wu. *Studies on Chemical Constituents of Patrinia villosa Juss*. Chinese Material Medica., **28**, 883-884 (2005).
7. T Zhang, Q.W Li, K Li, Y.R Li, J Li, G.J Wang, S.B Zhou. *Antitumor effects of saponin extract from Patrinia villosa (Thunb.) Juss on mice bearing U14 cervical cancer*. Phytotherapy Research., **22**, 640–645 (2008).
8. L.C.M Chiu, T.S Ho, E.Y.L Wong, V.E.C Ooi. *Ethyl acetate extract of Patrinia scabiosaefolia downregulates anti-apoptotic Bcl-2/Bcl-X_L expression, and induces apoptosis in human breast carcinoma MCF-7 cells independent of caspase-9 activation*. Journal of Ethnopharmacology., **105**, 263–268 (2006).
9. J.Y Peng, G.J Yang, G.R Fan, Y.T Wu. *Preparative isolation and separation of a novel and two known flavonoids from Patrinia villosa Juss by high-speed counter-current chromatography*. Journal of Chromatography A., **1092**, 235–240 (2005).
10. H Tagachi, Y Yokokawa, T Endo. *Studies on the constituents of Patrinia villosa Juss*. Yakugaku Zasshi., **93**, 607–611 (1973).
11. J.Y Peng, G.R Fan, Y.T Wu. *Supercritical fluid extraction of aurentiamide acetate from Patrinia villosa Juss and subsequent isolation by silica gel and high-speed counter-current chromatography*. Journal of Chromatography A., **1083**, 52–57 (2005).
12. J.Y Peng, G.R Fan, Y.T Wu. *Studies on chemical constituents of Patrinia villosa*. China Journal of Chinese Materia Medica., **31**, 128-130 (2006).
13. R.P Adams. Identification of essential oil components by gas chromatography/ mass spectrometry. Allured Publishing Corporatio, Carol Stream, IL (2007).