Analysis of Volatile Oils from Different Parts of *Rabdosia rubescens* from Guizhou

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Abstract The volatile chemical components of flowers, leaves, stems, and roots of *Rabdosia rubescens* were extracted by solid-phase microextraction method, and the extracts were analyzed by gas chromatography-mass spectrometry. A total of 40 chemical constituents were identified from the essential oils of the roots, stems, leaves, and flowers of *R. rubescens*. Among them, 15, 24, 15, and 17 chemical components were identified from the roots, stems, leaves, and flowers of . *rubescens* respectively. In the roots, camphene (38.29%), calarene (7.25%), o-cymene (5.31%), elsholtzia ketone (4.49%) were identified as the major constituents. In the stems, the main components were benzaldehyde (37.81%), elsholtzia ketone (26.14%), β-caryophyllene (5.03%). The leaves were characterized primarily by elsholtzia ketone (73.85%), β-caryophyllene (5.95%) and benzaldehyde (3.31%). In the flowers, elsholtzia ketone (63.18%), β-caryophyllene (10.68%), bicyclogermacrene (4.90%) and benzaldehyde (4.58%) were identified to be the predominant compounds. These results indicate that the essential oils from different organs of *R. rubescens* exhibit distinct chemical compositions. The differences were particularly between the aboveground and belowground organs.

Key words *Rabdosia rubescens*, Volatile oil, GC-MS

0 Introduction

Rabdosia rubescens (Hemsl.) Hara is distributed in Guizhou, Sichuan, Guangxi, Henan, Zhejiang, and Hubei and other provinces of China. It commonly grows in hillsides, shrublands, forest margins, and along roadsides[1]. Modern pharmacological studies have shown that *R. rubescens* exhibits antitumor, cardiovascular protective, antibacterial, anti-inflammatory, and immunomodulatory activities. It is also widely used in traditional folk medicine in Guizhou Province. These biological activities are mainly associated with its chemical constituents, such as terpenoids and flavonoids, which are non-volatile compounds[4-6]. In particular, its antibacterial and anti-inflammatory effects may also be related to its volatile constituents. Previous studies have indicated that the volatile chemical components in *R. rubescens* is influenced by its geographical origin[7-11]. Therefore, it is necessary to investigate the volatile chemical constituents of *R. rubescens* from Guizhou. This study provides fundamental data on the volatile composition of *R. rubescens* in Guizhou.

1 Experiment

1.1 Materials The samples were collected from Liuzhi County, Guizhou Province, they were identified as *R. rubescens* (Hemsl.) Hara (Lamiaceae) by Prof. Liu Shaohuan from Guizhou Medical University.

1.2 Instrument HP 6890/5975C gas chromatography-mass spectrometry (GC-MS) system (Agilent Technologies, USA), 50/30 μm DVB/CAR/PDMS StableFlex solid-phase microextraction (SPME) fiber (1 cm; Supelco, USA).

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1.3 Sample preparation Approximately 2.0 g of fresh flowers, leaves, stems, and roots of *R. rubescens* were cut into small pieces and placed in SPME vials. The SPME fiber was inserted into the vial and exposed to the headspace above the sample. Extraction was performed at 90 ℃ for 50 min. The fiber was then immediately inserted into the GC injection port at 250 ℃ and desorbed for 3.0 min[12].

1.4 GC-MS analysis A TG-5MS capillary column (30 m × 0.25 mm × 0.25 μm) was used for chromatographic separation. The injection port temperature was 250 ℃, and it was introduced in splitless mode. High-purity helium was used as the carrier gas at a flow rate of 1 mL/min. The oven temperature was set at 40 ℃ and held for 2 min, increased to 250 ℃ at a rate of 5 ℃/min, and maintained at 250 ℃ for 5 min.

Electron ionization (EI) was used as the ion source. The ion source temperature was set at 250 ℃, and the ionization energy was 70 eV. The interface temperature was maintained at 300 ℃. The solvent delay time was 1.5 min. The mass scanning range was 30 -450 m/z.

2 Results and analysis

The volatile chemical constituents from four different parts of *R. rubescens* were extracted by solid-phase microextraction and analyzed by GC-MS. A total of 40 chemical constituents were preliminarily identified in the volatile oils of the different plant organs. The detailed results are shown in Table 1. The volatile oils from the flowers, leaves, stems, and roots of *R. rubescens* were analyzed, and a total of 40 volatile compounds were identified. The results are as follows.

2.1 Volatile chemical components of flowers 17 compounds were isolated and identified from the volatile oil of the flowers of *R. rubescens*, accounting for 99.34% of the total volatile oil content. The major constituents were elsholtzia ketone (63.18%),

β-caryophyllene (10.68%), bicyclogermacrene (4.90%), benzaldehyde (4.58%). 2,2-dimethyl-3-heptanone and 3,7,7-trimethylbicyclo[4.1.0] hept-3-ene-2,5-dione were detected only in the flowers, indicating that they are characteristic volatile constituents of the flowers of *R. rubescens*.

2.2 Volatile chemical components of leaves 15 compounds were identified in the fresh leaves of *R. rubescens*, accounting for 91.63% of the total oil. The main constituents were Elsholtzia ketone (73.85%), β-caryophyllene (5.95%) and benzaldehyde (3.31%).

2.3 Volatile chemical components of stems 24 compounds were identified in the fresh stems of *R. rubescens*, accounting for 86.15% of the total oil. Among of them, benzaldehyde (37.81%), elsholtzia ketone (26.14%), β-caryophyllene (5.03%) were the main constituents. β-Pinene, isobutyl isovalerate, 2-ethyl-1-hexanol, nonanal, (E)-4,8-dimethylnona-1,3,7-triene, piperitone, 3,5,5-trimethyl-2-cyclopenten-1-one, α-bergamotene, (E)-β-Famesene were detected only in the stem.

2.4 Volatile chemical components of roots From the roots of *R. rubescens*, 24 compounds were identified, accounting for 81.60% of the total oil. Camphene (38.29%), calarene (7.25%), o-cymene (5.31%), elsholtzia ketone (4.49%) were the main constituents of roots. Eight volatile compounds including nonane, tricyclene, camphene, (E)-2-octenal, bornyl acetate, cyclosativene, (-)-aristolene, and calarene were found exclusively in the roots.

Table 1 Volatile chemical components in different parts of *Rabdosia rubescens*

No.	Compound	Retention time//min	Molecular formula	Relative content//%			
				Flower	Leaf	Stem	Root
1	nonane	8.55	C_9H_{20}	–	–	–	3.81
2	tricyclene	9.24	$C_{10}H_{16}$	–	–	–	3.85
3	Camphene	10.06	$C_{10}H_{16}$	–	–	–	38.29
4	benzaldehyde	10.39	C_7H_6O	4.58	3.31	37.81	–
5	β-pinene	10.92	$C_{10}H_{16}$	–	–	2.19	–
6	isobutyl isovalerate	11.83	$C_9H_{18}O_2$	–	–	1.21	–
7	o-cymene	12.39	$C_{10}H_{14}$	–	–	0.88	5.31
8	2-ethyl-1-hexanol	12.53	$C_8H_{18}O$	–	–	2.32	–
9	(E)-2-octenal	13.47	$C_8H_{14}O$	–	–	–	3.29
10	linalool	14.71	$C_{10}H_{18}O$	2.91	1.79	0.76	–
11	nonanal	14.82	$C_9H_{18}O$	–	–	1.15	–
12	(E)-4,8-dimethylnona-1,3,7-triene	15.20	$C_{11}H_{18}$	–	–	0.74	–
13	elsholtzia ketone	17.98	$C_{10}H_{14}O_2$	63.18	73.85	26.14	4.49
14	2,2-dimethyl-3-heptanone	18.42	$C_9H_{18}O$	1.06	–	–	–
15	piperitone	19.24	$C_{10}H_{16}O$	–	–	0.95	–
16	2-isopropyl-5-methyl-3-cyclohexen-1-one	19.27	$C_{10}H_{16}O$	2.18	0.24	–	–
17	thymol	20.08	$C_{10}H_{14}O$	0.08	–	0.21	3.41
18	bornyl acetate	20.13	$C_{12}H_{20}O_2$	–	–	–	2.66
19	naginata ketone	20.56	$C_{10}H_{12}O_2$	–	0.59	0.28	–
20	3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene-2,5-dione	20.57	$C_{10}H_{12}O_2$	2.62	–	–	–
21	3,5,5-trimethyl-2-cyclopenten-1-one	21.11	$C_8H_{12}O$	–	–	1.19	–
22	elemene isomer	21.54	$C_{15}H_{24}$	0.44	0.17	0.20	–
23	eugenol	22.01	$C_{10}H_{12}O_2$	0.10	0.27	–	–
24	Cyclosativene	22.38	$C_{15}H_{24}$	–	–	–	0.89
25	α-copaene	22.60	$C_{15}H_{24}$	–	–	–	2.78
26	β-bourbonvene	22.85	$C_{15}H_{24}$	0.23	0.56	–	–
27	(-)-aristolene	23.75	$C_{15}H_{24}$	–	–	–	1.67
28	β-caryophyllene	23.80	$C_{15}H_{24}$	10.68	5.95	5.03	–
29	α-bergamotene	24.08	$C_{15}H_{24}$	–	–	1.40	–
30	Calarene	24.09	$C_{15}H_{24}$	–	–	–	7.25
31	epi-β-santalene	24.39	$C_{15}H_{24}$	–	–	0.13	0.27
32	(E)-β-famesene	24.52	$C_{15}H_{24}$	–	–	0.44	–
33	α-humulene	24.62	$C_{15}H_{24}$	2.06	1.04	0.74	–
34	thymyl isobutyrate	25.23	$C_{14}H_{20}O_2$	–	0.16	0.55	3.33
35	germacrene D	25.29	$C_{15}H_{24}$	0.64	–	–	–
36	(Z,E)-α-farnesene	25.48	$C_{15}H_{24}$	2.77	0.65	0.33	–
37	γ-elemene	25.67	$C_{15}H_{24}$	–	–	0.95	–
38	bicyclogermacrene	25.69	$C_{15}H_{24}$	4.90	2.10	–	–
39	Caryophyllene oxide	27.77	$C_{15}H_{24}O$	0.69	0.79	0.40	–
40	neophytadiene	33.12	$C_{20}H_{38}$	0.22	0.16	0.15	0.30

3 Conclusions and discussion

The results of this study showed that the flowers, leaves, stems, and roots of *R. rubescens* had some similarities in volatile chemical composition. Two compounds, elsholtzia ketone (flowers: 63.18%, leaves: 73.85%, stems: 26.14%, roots: 4.49%) and neophytadiene (flowers: 0.22%, leaves: 0.16%, stems: 0.15%, roots: 0.3%), were detected in all four parts. Seven compounds, namely benzaldehyde (flowers: 4.58%, leaves: 3.31%, stems: 37.81%), β-caryophyllene (flowers: 10.68%, leaves: 5.95%, stems: 5.03%), linalool (flowers: 2.91%, leaves: 1.79%, stems: 0.76%), α-humulene (flowers: 2.06%, leaves: 1.04%, stems: 0.74%), caryophyllene oxide (flowers: 0.69%, leaves: 0.79%, stems: 0.40%), (Z, E)-α-farnesene (flowers: 2.77%, leaves: 0.65%, stems: 0.33%), and elemene isomer (flowers: 0.44%, leaves: 0.17%, stems: 0.2%), were found in the stems, leaves, and flowers. Differences in relative content were observed among different organs. Several volatile compounds were present in the aboveground parts, including flowers, leaves, and stems. However, their relative contents were different in each organ. The composition of the root volatile oil was clearly different from the aboveground parts.

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