Note

Essential Oil of *Scutellaria baicalensis* G[†]Katsuya FUKUHARA, Takane FUJIMORI,
Hitoshi SHIGEMATSU and Akio OHNISHICentral Research Institute, Japan Tobacco Inc.,
6-2, Umeokaoka, Midori-ku, Yokohama,
Kanagawa 227, Japan

Received November 17, 1986

"Ohgon", a dried preparation of the roots of *Scutellaria baicalensis* Georgi, is one of the tentative Chinese herbs. It was been used for the treatment of various inflammatory diseases and diarrhoea in Chinese traditional medicine.

Up to now, thirty-eight flavonoids including baicalein and wogonin, 3 sterols and 14 amino acids have been isolated from *S. baicalensis* G.^{1~3)} Baicalein and wogonin have been reported to exhibit anti-inflammatory and anti-allergic actions.^{4,5)}

However, there have been no reports on the essential oil of *S. baicalensis* G. The oil has a good note, and a sweet and aromatic floral odor as well as a medicinal one.

We report here on the components of the essential oil obtained from *S. baicalensis* G.

Crushed and powdered roots, 1200 g (*S. baicalensis* G purchased at a Japanese market), was extracted with ether in a simultaneous distillation extractor (SDE). The ether extract was evaporated to remove the solvent, which afforded the essential oil. A gas chromatogram of the essential oil is presented in Fig. 1. The essential oil (13.6 g) was chromatographed on a column of silica gel (Merck; silica gel 60, 70~230 mesh), eluted an *n*-hexane-ether solvent system as an eluate to afford 25 fractions. The respective fractions were eluted with *n*-hexane (fr. 1~4, 480 mg), 2% ether-*n*-hexane (fr. 5~8, 310 mg), 5% ether-*n*-hexane (fr. 9~12, 360 mg), 10% ether-*n*-hexane (fr. 13~16, 660 mg), 50% ether-*n*-hexane (fr. 17~20, 800 mg), ether (fr. 21~24, 370 mg) and methanol (fr. 25, 300 mg). Each fraction was analyzed by GC/MS on a fused silica capillary column (HP 5996A; methyl silicone, 25 m × 0.2 mm i.d.; 100°C→280°C, 3°C/min; ionization vol., 70 eV).

Consequently, 81 compounds were identified, as shown in Table I. They were classified into 10 groups as follows: hydrocarbons (21), acids (10), ketones (13), phenols (9), lactones (7), aldehydes (5), alcohols (6), esters (3), ethers (4) and *N*-containing compounds (3). The major constituents of the essential oil were acetophenone (Fig. 1, peak No. 60), (*E*)-4-phenyl-3-buten-2-one (123), 1-phenyl-1,3-butanedione (132), palmitic acid (246) and oleic acid (270).

The essential oil has a medicinal-like odor with a chemical-tone as well as an aromatic floral odor with a sweet-note. Fractions 6 to 16 (ether; 2~10%) had a medicinal-like chemical odor. Fractions 13 to 17 (ether;

FIG. 1. Gas Chromatogram of the Essential Oil from *Scutellaria baicalensis* G.

Conditions: Shimadzu GC-9A; methyl silicone, 25 m × 0.2 mm i.d.; 100°C→280°C (3°C/min); He (1.0 ml/min); FID.

[†] This paper was presented at the Annual Meeting of the Agricultural Chemical Society of Japan, Kyoto, April 1986.

TABLE I. IDENTIFIED COMPOUNDS

Peak No.	Compounds	Evidence			Peak No.	Compounds	Evidence		
		GC	MS	NMR			GC	MS	NMR
Hydrocarbons (21)					Esters (3)				
36	1,3,5,7-Cyclooctatetraene		+		239	Methyl palmitate	+	+	
77	1,3-Butadienyl benzene		+		242	Dibutyl phthalate	+	+	
85	Dodecane	+	+		316	Diocetyl phthalate	+	+	
117	Tridecane	+	+		Phenols (9)				
134	α -Cubebene		+		46	Phenol	+	+	
137	β -Elemene		+		57	<i>o</i> -Cresol	+	+	
140	Tetradecane	+	+		61	<i>m</i> or <i>p</i> -Cresol	+	+	
145	<i>trans</i> -Caryophyllene		+		64	Guaiacol	+	+	
165	Pentadecane	+	+		112	4-Ethenyl guaiacol	+	+	+
183	Hexadecane	+	+		125	Eugenol	+	+	
104	Heptadecane	+	+		145	Isoeugenol	+	+	
211	Octadecane	+	+		155	BHA		+	
238	Nonadecane	+	+		163	BHT	+	+	
250	Eicosane	+	+		Acids (10)				
269	Heneicosane	+	+		20	Acetic acid	+	+	
280	Docosane	+	+		58	Heptanoic acid	+	+	
292	Tricosane	+	+		77	Benzoic acid	+	+	
304	Tetracosane	+	+		79	Octanoic acid	+	+	
315	Pentacosane	+	+		102	Nonanoic acid	+	+	
324	Hexacosane	+	+		172	Decanoic acid	+	+	
338	Heptacosane	+	+		210	Tetradecanoic acid	+	+	
Ketones (13)					246	Palmitic acid	+	+	
60	Acetophenone	+	+	+	270	Oleic acid	+	+	
68	Maltol		+		274	Stearic acid	+	+	
77	2-Hydroxyacetophenone		+		Lactones (7)				
95	4-Phenyl-2-butanone		+		54	4-Hexanolactone		+	
100	(<i>Z</i>)-4-Phenyl-3-buten-2-one		+	+	184	Butyl phthalide		+	
121	4-Methoxyacetophenone	+	+		189	Butylidenephthalide		+	+
132	(<i>E</i>)-4-Phenyl-3-buten-2-one	+	+		193	Cnidilide		+	+
132	β -Damascone		+		198	Senkyunolide		+	
132	1-Phenyl-1,3-butanedione	+	+	+	200	Neocnidilide		+	
142	Paeonol		+		202	Ligustilide		+	
147	Geranyl acetone	+	+		Alcohols (6)				
164	Ochracin		+		58	2-Methyl benzylalcohol		+	
222	Hexahydrofanesylacetone		+		68	Linalool	+	+	
Ethers (4)					69	Phenylethylalcohol	+	+	
49	2-Pentyl furan		+		83	4-Terpineol	+	+	
87	2,3-Dihydro benzofuran		+		190	β -Eudesmol		+	
111	3-Phenyl furan		+		290	Ferruginol		+	
169	Elemicine		+		Aldehydes (5)				
N-Compounds (3)					45	5-Methyl-2-furaldehyde	+	+	
47	2-Formyl pyrrole	+	+		56	Phenylacetaldehyde	+	+	
57	Acetyl pyrrole	+	+		96	4-Methoxybenzaldehyde	+	+	
103	(1 <i>H</i>)-Indole	+	+		101	3-Phenyl-2-propenal	+	+	
					130	Vanillin		+

FIG. 2. Gas Chromatogram of Fr. 16.

Compounds: (44) benzaldehyde (tr*); (56) phenylacetaldehyde (0.6); (60) acetophenone (16.0); (75) 2-methyl benzylalcohol (0.1); (83) 4-terpineol (tr); (87) 2,3-dihydrobenzofuran (0.1); (95) 4-phenyl butanone (0.1); (100) (Z)-4-phenyl-3-butene-2-one (0.9); (101) 3-phenyl propenal (0.3); (103) (1*H*)-indole (0.8); (112) 4-ethenyl guaiacol (7.1); (125) eugenol (0.9); (132) 1-phenyl-1,3-butanedione (9.1); (142) paeonol (1.3); (145) isoeugenol (0.1); (155) BHA (0.1); (202) ligus-tilide (1.8); (242) dibutyl phthalate (2.6).
(*), ratio of each peak area to the total peak area.

10~50%) had an aromatic floral odor. Notably, fr. 16 (ether; 10%, 130 mg) had a similar odor to that of the total essential oil. So, the components of fr. 16 were further investigated in order to clarify the key compounds of the odor of *S. beicalensis* G, and 18 compounds were identified (Fig. 2). They comprised 6 ketones, 4 aldehydes, 4 phenols and 4 others. The major constituents of the fraction were acetophenone (Fig. 2, peak No. 60), 4-ethenyl guaiacol (112) and 1-phenyl-1,3-butanedione (132), the odors of the respective major compounds being hawthron-like, herbaceous and floral. However, no key compound that had the same odor as the essential oil itself was found contribute to the characteristic odor of the essential oil.

REFERENCES

- 1) T. Tomimori, H. Jin, Y. Miyaichi, S. Toyofuku and T. Namba, *Yakugaku Zasshi*, **105**, 148 (1985).
- 2) M. Takido, M. Aimi, S. Takahashi, S. Yamanouchi, H. Torii and M. Dohi, *Yakugaku Zasshi*, **95**, 108 (1975).
- 3) S. Takagi, M. Yamaki and K. Inoue, *Yakugaku Zasshi*, **100**, 1221 (1980).
- 4) M. Kubo, H. Matsuda, M. Tanaka, Y. Kimura, H. Okuda, M. Higashino, T. Tani and K. Namba, *Chem. Pharm. Bull.*, **32**, 2724 (1984).
- 5) A. Koda, H. Nagai and H. Wada, *Folia Pharmacol. Japan*, **66**, 471 (1970).