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Analysis of Volatile Constituents of *Baimaohou* (*Camellia sinensis* L.) by Gas Chromatography-Mass Spectrum

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Volatile oil of *Baimaohou* (*Camellia sinensis* L.) was obtained by simultaneous distillation-solvent extraction. Following, the essential oil was analyzed by gas chromatography-mass spectrum. 48 components at least were identified, constituting approximately 74% of the oil. The main constituents of the essential oil were phytol (16.4%) and 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2-(4H)-benzofuranone (10.6%), a very expensive flavour material.

Key Words: *Baimaohou* (*Camellia sinensis* L.), Essential oil, SDE, GC-MS.

INTRODUCTION

Baimaohou (*Camellia sinensis* L.) often goes by the name of Pekoe, White Monkey Green Tea or White Hair Monkey. Two kinds of *Baimaohou* (*Camellia sinesis* L.) or *Maohou* so called, described in Chinese Tea Dictionary[1]. The plant is short and small in size and open in form, but its branches are close. And the leaves are middle in length and width, round in figure, smooth and hairy in face, yellow to green in colour. It belongs to the clone group, frutex type.

The tea of Baimaohou (*Camellia sinensis* L.) tastes full of sweetness, lasting after taste. It was said the tea could provide a man refreshment, reducing blood fat and body weight, as well as clearing away liver-fire to treat eye disease based on the traditional Chinese medicine. However, few descriptions and inspection data were reported about it in the pharmacognosy[2, 3] and analytical chemistry[4–7] area.

In this paper, constituents extracted by simultaneous distillation-solvent extraction (SDE) and analyzed by GC-MS from the commercial tea of *Baimaohou* (*Camellia sinensis* L.) cultured and cured at Xiping, Anxi County, Fujian Province, China have been reported.

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EXPERIMENTAL

The leaf tea, commercial tea from market, is made from the top two leaves and the bud of new season growth (late March/early April, 2003) from Xiping, Anxi County, Fujian Province, China.

20 g of collective samples of dry aerial parts of *Baimaohou* (*Camellia sinensis* L.) were subjected to SDE (50 mL CH_2Cl_2 as solvent in a 250 mL round bottom flask) in a conventional Likens-Nickerson simultaneous distillation-solvent extraction device for 4 h. The extracted oil was filtered, dried over anhydrous sodium sulphate for over 10 h and concentrated to 0.25 mL. A clear light-yellow-coloured liquid was obtained.

Gas chromatography-mass spectrometry: GC-MS analyses were carried out on an Agilent HP6890 GC/5973 MSD gas chromatohraph coupled with 5973N mass spectrum system equipped with a DB-wax fuse silica column (length 30 m, 0.25 mm i.d., film thickness 0.25 μm). Oven temperature was held at 40°C for 2 min, programmed to 250°C at a rate of 3°C/min later on and then held isothermal at 250 °C for 10 min. Transfer line temperature, 280°C; lasting time, 3 min; injector temperature, 250°C; sample volume, 2 μL; split ratio, 20 : 1. The carrier gas was helium, with a flow rate of 1 mL/min; scan range, 35–550 amu.

Identification of constituents: The constituents of the essential oil were identified by comparing the linear retention indices of the peaks on DB-wax column with literature values[8–10], computer matching against the library spectra and finally confirmed by comparison of mass spectra of peaks with published data[11–13]. Whenever possible, the constituents were matched by co-injection with authentic compounds. The relative amounts of individual components are based on peak area obtained without consideration of the FID calibration factors (*i.e.*, F = 1.00 for all compounds). The retention indices were calculated using a homologous series of *n*-alkanes (C_8–C_{28}) on a DB-wax column.

RESULTS AND DISCUSSION

This is the first report on the composition of the essential oil of *Bainaohou* (*Camellia sinensis* L.). The volatile oil obtained by simultaneous distillation-solvent extraction of commercial leaf tea, was found to be a light yellow liquid.

In the GC-MS analysis of the oil, 48 compounds at least, representing 74.64% of the total oil, were characterized. The relative concentrations of the volatile components identified are presented in Table-1 according to their elution order on the DB-wax column.

One thing should be mentioned that a compound found in the oil, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone, is a very expensive flavour material. It could be isolated from the tea maybe.

TABLE-1
PERCENTAGE COMPOSITION OF *BAIMAOHOU* (*CAMELLIA SINENSIS* L.) ESSENTIAL OIL

No.	Compounds	RI*	Area %	Identification method
1.	Furfural	833	0.61	RI, MS.Col
2.	5,5-Dimethyl-1-ethyl-1,3-cyclopentadiene	860	0.74	RI, MS
3.	2-Hexenal	884	4.75	RI, MS, Col
4.	2-Hexen-1-ol	902	0.32	RI, MS
5.	2-Hydroxy-2-cyclopenten-1-one	911	0.53	RI, MS
6.	Heptanal	920	0.33	RI, MS, Col
7.	2-Pentyl-furfural	945	0.5	RI, MS, Col
8.	3-Methyl-1,2-butadiene	956	0.39	RI, MS
9.	2,2,6-Trimethyl-cyclohexanone	976	0.17	RI, MS
10.	Phthalan + benzeneacetaldehyde	989	0.39	RI, MS
11.	*Cis*-5-ethenyltetrahydro-5-trimethyl-2-furanmethanol	1037	0.29	RI, MS
12.	3,7-Dimethyl-1,6-octadien-ol	1054	1.14	RI, MS
13.	3,5,5-Trimethyl-2-cyclohexen-1-one	1059	0.43	RI, MS
14.	4-Trimethyl-3-cyclohexene-1-methanol	1098	0.4	RI, MS, Col
15.	2,6,6-Trimethyl-1,3-cyclohexadiene-1-carboxaldehyde	1103	0.32	RI, MS
16.	1,3,4-Trimethyl-3-cyclohexene-1-carboxaldehyde	1112	0.71	RI, MS
17.	2-Methoxy-4-vinylphenol	1155	1.12	RI, MS, Col
18.	2,2-Dimethyl-3-(2-methyl-1-propenyl)-cyclopropanecarboxylic acid	1210	0.2	RI, MS
19.	Caryophyllene	1241	0.45	RI, MS
20.	2,4,5,6,7,7a-Hexahydro-4,4,7a-trimethyl-*cis*-2-benzofuranmethanol	1260	0.24	RI, MS
21.	5-Methoxy-6,7-dimethyl-benzofuran	1269	0.37	RI, MS
22.	4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	1277	1.17	RI, MS
23.	*Bis*(1,1-dimethylethyl)-phenol	1311	0.25	RI, MS, Col
24.	5-Amino-1-ethylpyrazole	1336	1.36	RI, MS
25.	5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-2(4H)-Benzofuranone	1355	10.64	RI, MS
26.	Cedrol	1367	2.1	RI, MS
27.	3,3-Dimethyl-hexane	1480	0.24	RI, MS, Col
28.	Adamantane-1-carboxylic acid	1513	0.56	RI, MS
29.	3,7,11-Trimethyl-1-dodecanol	1522	0.47	RI, MS
30.	3,4-Dihydro-2H-1,4-benzoxazine	1540	0.27	RI, MS
31.	Phenanthrene + Diphenylethyne + 9-methylene-9H-fluorene	1574	0.24	RI, MS
32.	6,10,14-Trimethyl-2-pentadecanone	1769	3.46	RI, MS
33.	Bis(2-methylpropyl) 1,2-benzenedicarboxylate	1861	2.67	RI, MS
34.	1-Formyl-2,2-dimethyl-3-*cis*-(2-methyl-but-2-enyl)-6-methylidene-cyclohexane	1873	1.76	RI, MS

No.	Compounds	RI*	Area %	Identification method
35.	Methyl hexadecanoate + methyl 14-methyl-pentadecanate	1924	0.76	RI, MS
36.	Isophytol + *cis*-3-methylpent-3-ene-5-ol	1958	1.51	RI, MS
37.	Dibutyl phthalate	2009	3.45	RI, MS
38.	Pentadecanoic acid	2085	0.9	RI, MS, Col
39.	*n*-Hexadecanoic acid	2091	0.2	RI, MS, Col
40.	1,2-Dimethyl-cyclohexene	2164	1.1	RI, MS
41.	Methyl 11,14,17-Eicosatrienoate + cyclododecyne + 1,3-cyclooctadiene	2175	1.05	RI, MS
42.	2-(5-Oxohexyl)-cyclopentanone	2189	0.96	RI, MS
43.	Phytol	2205	16.43	RI, MS
44.	4,8,12,16-Tetramethylheptadecan-4-olide	2256	1.46	RI, MS
45.	1-Methylidene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)cyclohexane	2293	0.35	RI, MS
46.	Dioctyl phthalate + bis(2-ethylhexyl) phthalate + diisooctyl 1,2-benzenedicarboxylate	2361	0.27	RI, MS
47.	9-Octyl heptadecane	2394	1.7	RI, MS, Col
48.	Triacontane	2451	4.91	RI, MS
	Total		74.64	

RI = retention indices in elution order from DB-Wax column; MS = mass spectroscopy; Col = co-injection.

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