## ESSENTIAL OIL COMPOSITION OF *Hibiscus sabdariffa* FROM YUNNAN, CHINA

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The genus *Hibiscus* L. (Malvaceae) provides a soft drink, usually named red tea (*Hibiscus sabdariffa* L.) [1]. Red tea is widely cultivated in the South of China (such as Yunnan, Hainan) and has been used in food and medicine for a long time. For food applications, it is used as a vegetable and even as a meat substitute [2]. It is also used for protection against sunlight-induced free radicals [3]. Red tea also has biological activities [4–7], such as antibacterial, antifungal, insecticidal, and antioxidant properties.

The calyces and drinks made from *Hibiscus sabdariffa* L. were reported to contain carbohydrates, iron, ascorbate, and  $\beta$ -carotene from analysis using colorimetric methods and as reported by the AOAC (Association of Official Analytical Chemists) [8]. The aim of this study is to extend our knowledge and report preliminary results on the oil composition of red tea's 47 components, representing 97% of the oil. The results are listed in Table 1, where the compounds are arranged in the order of elution on the RTX-5MS silica capillary column. Esters are found to be the main components (31.42%), and this fraction is dominated by tributyl phosphate (18.63%), benzyl benzoate (3.40%), and diisooctyl ester (3.37%). It also includes alkyls (29.19%), acids (9.85%), aromatic compounds (9.34%), ketones (9.32%), hydroxyketone (4.91%), alkene (2.04%), and aldehyde (0.93%).

**Plant Material**. Red tea was collected in Nov. 2005 from Yunnan, China. The plant was authenticated in the Key Laboratory of Medicinal Plant Resources and Nature Pharmaceutical Chemistry, Ministry of Education, Xi'an, China. A voucher specimen of the samples has been deposited in the School of Life Sciences, Shaanxi Normal University, Shaanxi, China.

**Oil Isolation**. The sample (100 g) was cut into small pieces and subjected to hydrodistillation at 95°C for 5 h, using a Clevenger-type apparatus as recommended by the British Pharmacopoeia [9]. The essential oil was dried over anhydrous sodium sulfate and stored at 4°C in the dark pending analysis by GC/MS.

GC/MS Analysis. The volatile compound analysis was performed on a GC/MS instrument (Shimadzu GC/MS-QP2010, Japan). The compounds were separated on an RTX-5MS fused-silica capillary column (30 m length, 0.25 mm diameter, 0.25 µm film thickness) coated with 5% diphenyl and 95% dimethylpolysiloxane.

GC/MS (EI) conditions: helium was used as the carrier gas (1.46 mL/min). 2  $\mu$ L oil was injected into the column with a split ratio of 50:1 and injector port temperature of 250°C. The GC program was initiated at a column temperature of 80°C, then increased to 140°C, 160°C, 210°C, and 250°C at a rate of 15°C/min, 10°C/min, 5°C/min, and 20°C/min, respectively, and then kept constant at 250°C for 5 min.

Temperatures of the ion source and interface were 200°C and 250°C, respectively. The mass spectrometer was operated (full scan mode) with the EI-mode at 70 eV.

GC/MS (CI) conditions: the PCI and NCI mass spectra were recorded on the same apparatus equipped with the same column and specific ionization chemical source. Ionizing gas: methane (CH<sub>4</sub>); other experimental conditions were as those in the EI analysis.

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## TABLE 1. Composition of the Essential Oil of Hibiscus sabdariffa

Compound	%	Compound	%
α-Isophoron	0.35	2-Pentadecanone	2.01
Benzoic acid	0.56	8-Octadecenal	0.53
Nonanoic acid	0.45	Tetradecanoic acid	0.79
2-Isopropenyl-5-methyl-4-hexenal	0.93	Benzyl benzoate	3.40
2-Undecanone	0.86	2-Pentadecanone, 10,14-trimethyl-	0.57
Citronellic acid	0.71	Benzoic acid, 2-phenylethyl ester	0.61
Salicylic acid, isopropyl ester	0.97	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	0.73
Decane, 2,3,5,8-tetramethyl-	0.53	Nonadecane	1.03
Geranic acid	1.26	Farnesyl acetone	1.52
<i>n</i> -Decanoic acid	0.45	6-Octen-1-ol, 3,7-dimethylpropanoate	0.83
Eugenol	4.62	<i>n</i> -Hexadecanoic acid	2.23
4-Methyl-1-undecene	0.74	Dibutyl phthalate	1.07
Benzene, 1,2-dimethoxy-4-(2-propenyl)-	7.97	Eicosane	0.59
5,9-Undecadien-2-one, 6,10-dimethyl-	0.24	Heneicosane	8.62
2-Tridecanone	3.24	9,12-Octadecadienoic acid (Z,Z)-	0.87
Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-	1.37	Octadecanoic acid	1.90
4-Dihexylcarbamoyl-butyric acid	0.63	Docosane	1.12
3,8-Dimethylundecane	1.30	9-Tricosene, (Z)-	1.30
Diethyl phthalate	1.16	Nonacosane	11.84
Tetradecanal	0.55	Tetracosane	0.37
1-Methyldodecyl acetate	0.65	1-Pentacosanol	0.29
Pentadecane, 2,6,10,14-tetramethyl-	1.00	Pentacosane	1.15
Tributyl phosphate	18.63	1,2-Benzenedicarboxylic acid, diisooctyl ester	3.37
Heptadecane	1.09		

**Qualitative and Quantitative Analyses.** The unambiguous identification of most of the compounds was done by comparing their fragmentation pattern in the EI mass spectra with those of the Mass Spectral database (NIST05 and NIST05s); as for those without adequate assurance, the identification was based on joint information from the EI and CI mass spectra. Some of them were further confirmed by comparing their fragmentation pattern in the EI mass spectra with those of authentic compounds available in our laboratory or from literature data [10–11]. Relative amounts (percent) of the individual components were calculated based on GC peak areas without response factor correction.

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