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CHEMOTYPICAL VARIABILITY OF LEAF OILS IN *Elephantopus scaber* FROM 12 LOCATIONS IN CHINA

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The chemical constituents of leaf oils of Elephantopus scaber *L. from 12 locations in Southern China, including three provinces and Hong Kong, were investigated using GC/MS. A total of 24 compounds were detected, of which 20 were identified by their mass spectra fragmentation patterns. The major compounds include hexadecanoic acid (8.19–39.22%), octadecadienoic acid (trace – 29.22%), five alkane homologues, i.e., n-tetradecane (1.19–5.26%), n-pentadecane (3.22–12.05%), n-hexadecane (2.38–16.26%), n-heptadecane (2.48–15.32%), and n-octadecane (1.39–9.59%), as well as tetramethylhexadecenol (2.06–4.31%). Hierarchical cluster analysis classified the leaf oils into two groups. Two main chemotypes of leaf oils in* E. scaber *were thus identified, one rich in hexadecanoic acid and octadecadienoic acid, and the other rich in the five alkane homologues.*

Key words: *Elephantopus scaber*, leaf oil, GC/MS analysis, chemotype.

The genus *Elephantopus* L. (family Compositae) comprises approximately 30 species distributed in the neotropics and the Old World [1–3]. In China, there are two species, i.e., *E. scaber* L., the lectotype species of this genus, and *E. tomentosus* L., both occurring in southern and southwestern regions as well as Hong Kong and Taiwan. In particular, *E. scaber* is a perennial herb 10~50 cm in height and widely used in Chinese traditional medicine in the treatment of nephritis, edema, colds, chest pain, fever and cough of pneumonia, scabies, and arthralgia due to trauma [4–6]. It has also been popular as a medicinal herb in many countries of Southeast Asia, Latin America, and Africa [7, 8], e.g., infusions and the decoction of the whole plant are used to stimulate diuresis, reduce fever, and eliminate bladder stones in Brazil [1, 9].

Recently, we analyzed the essential oil of *E. scaber*, growing in China, for the first time [10]. The major constituents identified were hexadecanoic acid, isopropyl dimethyl tetrahydronaphthalenol, β-sesquiphellandrene, octadecadienoic acid, and phytol. Since the habitats of *E. scaber* have greatly changed during the past several decades due to increasing human activities such as rapid urbanization, a further comparative study of *E. scaber* in China from different locations is needed. In particular, most wild plants of *E. scaber* for medical use (herba *Elephantopi*, or Chinese common name "Ku-di-dan") are recently harvested in Guangdong and Hainan Island in Southern China.

A total of 24 compounds in the leaf oils of *E. scaber* from 12 locations in Southern China were detected, of which 20 were identified by their mass spectra fragmentation patterns (Table 1). The major compounds include hexadecanoic acid (8.19–39.22%), octadecadienoic acid (trace – 29.22%), *n*-tetradecane (1.19–5.26%), *n*-pentadecane (3.22–12.05%), *n*-hexadecane (2.38–16.26%), *n*-heptadecane (2.48–15.32%), *n*-octadecane (1.39–9.59%), and tetramethylhexadecenol (2.06–4.31%). In particular, *n*-tetradecane, *n*-pentadecane, *n*-hexadecane, *n*-heptadecane, and *n*-octadecane, which are alkane homologues, ranged from 10.66% to 58.48% in the 12 locations.

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TABLE 1. Composition of Leaf Oils from the 12 Locations of *E. scaber*, %

Compound	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12
Dimethyldecane	0.20	Tr.	Tr.	Tr.	0.20	Tr.	0.15	0.82	0.29	Tr.	Tr.	Tr.
Trimethyldodecane	0.68	1.32	0.58	0.74	0.73	0.22	0.50	2.34	0.87	0.32	0.20	0.58
Methylpropylnonane	0.20	0.34	1.05	0.23	0.20	Tr.	0.15	Tr.	0.29	0.16	Tr.	0.23
Dimethyldodecane	0.47	0.11	0.47	0.51	0.53	Tr.	0.35	1.75	0.77	0.24	0.16	0.47
n-Tetradecane	1.35	2.40	5.26	1.71	1.73	3.51	1.19	3.15	1.26	2.09	3.11	3.37
Caryophyllene	1.08	0.63	Tr.	0.11	0.40	0.37	0.45	2.34	1.45	0.32	0.44	2.56
β-Sesquiphellandrene	0.61	1.20	2.46	0.97	1.00	0.88	0.79	Tr.	1.74	0.88	1.16	1.28
n-Pentadecane	4.26	6.35	12.05	5.74	5.26	7.60	3.22	10.16	6.39	5.62	8.02	8.84
Unknown 1	1.08	2.00	2.34	1.19	1.46	1.54	0.94	3.04	1.94	1.04	0.64	1.05
n-Hexadecane	3.92	7.20	16.26	5.69	4.52	10.82	2.38	8.29	5.91	6.18	12.05	9.42
Unknown 2	Tr.	Tr.	Tr.	Tr.	Tr.	Tr.	Tr.	2.92	Tr.	Tr.	Tr.	Tr.
n-Heptadecane	4.19	7.66	15.32	5.69	4.52	10.53	2.48	9.81	7.45	8.43	11.61	10.70
z-Methylheptadecane	0.95	1.60	1.52	1.08	1.40	0.66	0.84	2.45	1.94	0.40	1.00	1.40
Myristic acid	2.23	1.26	2.81	2.05	2.73	2.63	2.18	Tr.	4.74	2.89	2.23	3.60
n-Octadecane	2.70	4.80	9.59	3.64	2.66	7.02	1.39	5.14	4.26	4.65	7.62	6.51
Unknown 3	9.20	6.29	9.01	7.11	8.92	12.72	9.87	10.75	1.16	8.83	9.26	9.88
Tetramethylhexadecene	1.01	1.14	1.05	0.85	1.26	0.95	0.89	Tr.	Tr.	1.04	1.08	1.74
Unknown 4	1.62	1.60	2.11	1.42	1.73	2.49	1.44	2.22	1.55	1.77	2.08	2.21
Tetramethylhexadecenol	2.91	2.06	3.27	2.27	2.93	4.31	2.78	3.62	2.32	2.97	3.63	3.84
n-Nonadecane	1.83	0.74	6.43	2.50	2.00	4.39	0.94	3.50	3.10	3.05	4.79	4.30
Hexadecanoic acid	39.22	28.93	8.19	31.50	36.59	21.42	36.11	14.14	35.91	32.83	24.58	24.30
n-Eicosane	Tr.	Tr.	Tr.	Tr.	Tr.	Tr.	Tr.	1.75	Tr.	Tr.	Tr.	Tr.
Phytol	0.34	1.37	0.23	1.59	2.13	0.15	1.74	5.26	0.29	0.16	0.28	0.35
Octadecadienoic acid	19.95	20.98	Tr.	23.42	17.10	7.82	29.22	6.54	16.36	16.05	6.07	3.37

Tr.: trace quantities (< 0.1% detected).

Chemical variability of the leaf oils of *E. scaber* was also analyzed by using hierarchical cluster analysis. Two groups were formed: Group 1, formed by five locations (P3, P6, P8, P11, and P12), showed relatively high concentrations of *n*-tetradecane (between 3.11% and 5.26%, with an average value of 3.68%), *n*-pentadecane (7.60–12.05%, average 9.33%), *n*-hexadecane (8.29–16.26%, average 11.37%), *n*-heptadecane (9.81–15.32%, average 11.59%), and *n*-octadecane (5.14–9.59%, average 7.18%). Group 2, formed by seven locations (P1, P2, P4, P5, P7, P9, and P10), is characterized by high concentrations of hexadecanoic acid (28.93–39.22%, average 34.44%) and octadecadienoic acid (16.05–29.22%, average 20.44%), and very low concentrations of *n*-tetradecane (1.19–2.40%, average 1.68%), *n*-pentadecane (3.22–6.39%, average 5.26%), *n*-hexadecane (2.38–7.20%, average 5.11%), *n*-heptadecane (2.48–8.43%, average 5.77%), and *n*-octadecane (1.39–4.80%, average 3.44%). The two main chemotypes of leaf oils in *E. scaber* were thus identified by the characteristic concentrations of seven major compounds, one rich in hexadecanoic acid and octadecadienoic acid, and the other rich in the five alkane homologues.

EXPERIMENTAL

Elephantopus scaber L. from 12 locations in Southern China, including three provinces and Hong Kong (indicated by codes from P1 to P12), were collected from April 2004 to July 2004. Voucher specimens have been deposited in the Ministry of Education Key Laboratory for Biodiversity Science and Ecological Engineering, Fudan University, Shanghai, China.

The compounds were extracted from dried leaf samples (0.2 g) with CH_2Cl_2 (1 mL) overnight at room temperature and filtered. The extracts were then stored in a 2 mL glass vial at –20°C until analyzed.

The GC/MS analysis was performed on a combined GC-MS instrument (Finnigan Voyager, San Jose, CA, USA) using an HP-5 fused silica gel capillary column (30 m length, 0.25 mm diameter, 0.25 μm film thickness). A 1 μL-aliquot of oil was

injected into the column using a 10:1 split injection, whose temperature was set at 250°C. The GC program was initiated with the column temperature set at 60°C for 2 min and increased to 250°C at a rate of 10°C/min, and held for 10 min. Helium was used as the carrier gas (1.0 mL/min). The mass spectrometer was operated in the 70 eV EI mode with scanning from 41 to 450 amu at 0.5 s, and the mass source was set at 200°C.

Identification of the components was done by comparison of the GC retention indices (RI) relative to C_8 to C_{20} *n*-alkanes and computer matching of their mass spectral fragmentation patterns with those stored in the spectrometer database using the National Institute of Standards and Technology Mass Spectral database (NIST-MS, 1998). Relative percentage amounts of the identified components were calculated from the total ion chromatograms by a computerized integrator.

An average Euclidean distance matrix based on the composition percentages of leaf oils from the 12 locations of *E. scaber* was calculated. Hierarchical cluster analysis based on the distance matrix was performed with the unweighted pair-group method using an arithmetic average (UPGMA) [11], using the NTSYSpc version 2.02 [12].

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