COMPOSITION OF THE ESSENTIAL OIL OF *Adiantum flabellulatum*

W. Y. Kang,[1,2*] Z. Q. Ji,[1,2] J. M. Wang[1,2]

UDC 547.913

The genus *Adiantum*, belonging to the Adiantaceae family, is found in mild tropical and subtropical regions. The genus consists of 200 species widespread throughout the world, mainly in South America and about 30 species in China. *A. flabellulatum* is a well-known traditional Chinese medicinal herb in the south of China [1].

Phytochemical research showed that the genus *Adiantum* contained triterpenoids and flavonoids [2–5], and pharmacological investigations showed that some important *Adiantum* species had antimicrobial activity [6]. No research has so far been conducted concerning the chemical constituents of the essential oil of the genus.

In order to identify the chemical constituents of the essential oil in the roots and leaves of *A. flabellulatum* and to illuminate the difference between them, we report on the essential oil of *A. flabellulatum* using the HS-SPME technique subsequently analyzed by GC-MS for the first time.

The chemical composition of the oils in roots and leaves are presented in Table 1. Forty-two compounds in the roots of *A. flabellulatum* were identified, which comprised 94.6% of the volatile fraction. The main constituents of the oil in the roots were *n*-decanoic acid (11.44%), 6,10,14-trimethyl-2-pentadecanone (11.23%), diethyl phthalate (8.63%), and nonanoic acid (6.15%). Thirty-eight compounds in the leaves of *A. flabellulatum* were identified, which comprised 91.64% of the volatile fraction. The main constituents were *n*-decanoic acid (11.77%), 2-isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene (10.63%), [1*R*-(1α,7β,8aα)]-1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-naphthalene (9.88%), α-panasinsen (8.11%), 4-tetradecyne (6.63%), β-pinene (5.16%), and nonanoic acid (4.01%).

Nineteen compounds were identified in both roots and leaves of *A. flabellulatum*, and this shows that there are some obvious similarities between the essential oil in roots and leaves of *A. flabellulatum*, but they are different from each other fundamentally.

Some main compounds, such as 2-isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalene, [1*R*-(1α,7β,8aα)]-1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-naphthalene, and α-panasinsen, were only detected in the leaves, and other main compounds, such as 6,10,14-trimethyl-2-pentadecanone and diethyl phthalate, decreased in amount from the roots to the leaves of *A. flabellulatum*. *n*-Decanoic acid, as the main component, was detected in both the roots and leaves of *A. flabellulatum*.

ACKNOWLEDGMENT

This work was supported by the Key Foundation of Science and Technology, Henan Hygienics Bureau of China (No. 2006038), The Project of Basic and Forefront of Henan Province Office of Science and Technology (No. 0723004502), and the Fund of Henan University (No. 06YBZR085).

1) Pharmaceutical College of Henan University, Kaifeng, Henan, 475004, P. R. China, fax +86 378 3880680, e-mail: kangweny@hotmail.com; 2) Institute of Natural Products, Henan University, Kaifeng, Henan, 475004, P. R. China. Published in Khimiya Prirodnykh Soedinenii, No. 4, pp. 485–486, July–August, 2009. Original article submitted January 8, 2008.

0009-3130/09/4504-0575

TABLE 1. Chemical Constituents of the Essential Oil in Roots and Leaves of *A. flabellulatum*

Compound	RI*	Roots, %	Leaves, %
1*R*-α-Pinene	931	–	1.04
β-Pinene	973	–	5.16
2-Pentylfuran	990	0.97	–
Nonanal	1104	4.18	2.95
(*E*)-2-Nonenal	1160	0.46	–
2,6,6-Trimethyl-1,3-cyclohexadiene-1-carboxaldehyde	1199	0.26	–
Octanoic acid	1210	–	0.45
(*E*)-2-Decenal	1263	1.2	–
Nonanoic acid	1309	6.15	4.01
2,6,10-Trimethyldodecane	1373	0.42	–
Tetradecane	1397	2.59	–
n-Decanoic acid	1410	11.44	11.77
(*E*)-4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	1430	0.7	–
β-Humulene	1442	–	1.94
(*E*)-2-Tridecenoic acid	1447	2.51	–
(*E*)-6,10-Dimethyl-5,9-undecadien-2-one	1456	1.68	0.54
4,8-Dimethylundecane	1462	2.17	–
2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	1483	–	10.63
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	1488	1.97	–
[1*R*-(1α,7β,8aα)]-1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-naphthalene	1493	–	9.88
Pentadecane	1498	2.28	1.09
α-Panasinsen	1518	–	8.11
(1*S*-*cis*)-1,2,3,4-Tetrahydro-1,6-dimethyl-4-(1-methylethyl)-naphthalene	1525	0.72	0.48
5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone	1538	1.91	0.54
2-Methylpentadecane	1563	0.46	0.35
6,10,14-Trimethylpentadecan-2-ol	1571	1.05	–
N-Methyl-4-chlorobenzenesulfonamide	1577	–	0.55
Hexadecane	1599	2.63	1.85
Diethyl phthalate	1603	8.63	0.85
2-Bromododecane	1649	2.29	1.53
2-Methylhexadecane	1663	0.36	–
(1α,4aβ,8aα)-(+/–)-1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-naphthalene	1668	–	3.57
3-Methylhexadecane	1670	0.52	–
2-Hexyl-1-decanol	1677	3.67	–
1-Nonadecene	1678	–	0.8
Cyclododecane	1683	1.14	–
1,6-Dimethyl-4-(1-methylethyl)-naphthalene	1684	–	0.8
bis(2-Methylpropyl) ester hexanedioic acid,	1689	0.98	0.56
Heptadecane	1700	2.51	1.48
2,6-Dimethylheptadecane	1705	2.29	2.06
N-[4-Bromo-*n*-butyl]-2-piperidinone	1716	–	0.77
Hexadecyloxirane	1717	1.02	–
7-Tetradecene	1742	1.33	–
Butyl ester 6-tetradecanesulfonic acid	1752	–	0.29
3-Methylheptadecane	1771	–	0.21
1-Nonadecene	1785	1.31	–
Octadecane	1800	0.97	0.75
2,6,10,14-Tetramethylhexadecane	1809	0.98	1.13
Diazinon	1814	0.45	–
6,10,14-Trimethyl-2-pentadecanone	1849	11.23	1.7
bis(2-Methylpropyl) ester 1,2-benzenedicarboxylic acid	1874	–	1.11
Diisobutyl phthalate	1874	1.5	–

TABLE 1 (continued)

Compound	RI*	Roots, %	Leaves, %
1-Hexadecyne	1899	–	0.93
4-Ethyl-cyclohexanone	1923	2.24	–
Methyl ester hexadecanoic acid	1928	–	0.36
Oxacycloheptadecan-2-one	1936	0.98	–
di-*n*-Butylphthalate	1969	0.7	0.61
n-Hexadecanoic acid	1983	3.15	2.23
Eicosane	1998	0.6	–
Methyl 2-octylcyclopropene-1-heptanoate	2106	–	1.93
4-Tetradecyne	2164	–	6.63
Total, %		94.6	91.64

*Retention indices calculated against *n*-alkanes.

REFERENCES

1. Institute of Botany, Chinese Academy of Sciences, *Iconographia Cormophytorum Sinicorum* (Tomus I), Science Press, Beijing, 1972, p. 167.
2. G. Brahmachari and D. Chatterjee, *Fitoterapia*, **73**, 363 (2002).
3. K. Tsuzuki, A. Ohashi, Y. Arai, K. Masuda, A. Takano, K. Shiojima, H. Ageta, and S. Q. Cai, *Phytochemistry*, **58**, 363 (2001).
4. V. L. Niranjan Reddy, V. Ravikanth, T. Prabhakar Rao, P. V. Diwan, and Y. Venkateswarlu, *Phytochemistry*, **56**, 173 (2001).
5. M. Sarwar Alam, Neeraj Chopra, Mohammad Ali, and Masatake Niwa, *Phytochemistry*, **54**, 215 (2000).
6. M. Singh, N. Singh, P. B. Khare, and A. K. S. Rawat, *J. Ethnopharmacol.*, **152**, 327 (2008).