A New Caffeate from the Aerial Parts of *Anabasis aphylla*

LI Wei-lin[1, 3], WANG Zhen-zhong[2], WANG Hong-qing[1], GONG Ting[1], CHEN Ruo-yun[1*]

1. Key Laboratory of Bioactive Substances and Resources Utilization of Chinese Herbal Medicine, Ministry of Education, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China
2. Jiangsu Kanion Pharmaceutical Co., Ltd., Lianyungang 222001, China
3. Department of Pharmacology, Pharmacy College of Xinxiang Medical College, Xinxiang 453003, China

Abstract: **Objective** To study the chemical constituents from the aerial parts of *Anabasis aphylla*. **Methods** The chemical constituents were isolated and purified by silica gel column and Sephadex LH-20 column chromatography. Spectroscopic methods such as MS and NMR spectra were used for the structural identification. **Results** A new caffeate ester, named eicosyl-(*Z*)-caffeate (**1**), along with fourteen known compounds was isolated from the EtOAc part. **Conclusion** Compound **1** is a new compound and compounds **2**−**13** are isolated from the plants of *Anabasis* L. for the first time.

Key words: *Anabasis* L.; *Anabasis aphylla* L; eicosyl-(*Z*)-caffeate
DOI: 10.3969/j.issn.1674-6384.2010.04.002

Introduction

There are 184 species in 38 genera of Chenopodiaceae, mainly distributed in Gobi desert, inter-dunes, gravelly alluvial fans, sometimes on arid slopes in Gansu and Xinjiang, Western China. *Anabasis aphylla* L. is one of them, and used as a botanical agriculture pesticide (Editorial Committee of *Flora of China*, 1979; Zhu, 1995). So most studies of *A. aphylla* for the control of cabbage caterpillar, aphids, and other pests were carried out. So far, reported fake wood species containing chemical constituents are *Anabasis aphylla*, *A. salsa*, *A. setifera*, *A. articulata*, *A. hispanica*, and *A. ferganica* etc., and *A. aphylla*. Our research mainly focused on the chemical constituents of such plants rarely reported (Chen and Li, 2004). From these plants, the separation of the alkaloids (Du *et al*, 2008), investigated mainly with the anti-cholinesterase activity (Tilyabaev and Abduvakhabov, 1998) was carried on. To take full advantage of rich resources and the further search for new active natural products, we now researched ethyl acetate extracts of *A. aphylla*, and 15 compounds were isolated and identified.

Materials and methods

Mass spectra were recorded on Agilent 1100 LC/MSD Trap SL .^{1}H-NMR was taken on Varian mercury−300 and ^{13}C-NMR spectra were taken on Varian mercury−400, using TMS as internal standard. All solvent used were of analytical grade. Sephadex LH-20 (Pharmacia Biotech) and silica gel (160−200 mesh) were used for column chromatography, and silica gel GF_{254} plates used for TLC (Qingdao Marine Chemical Company).

The aerial parts of *Anabasis aphylla* L. were collected from Kashi area, Xinjiang Uygur Autonomous Region in 2009 and identified by associate professor MA Lin, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College.

The 95% ethanol extracts of the aerial parts (5.1 kg) were concentrated and suspended in water, then partitioned by petroleum ether, EtOAc, and *n*-BuOH. The EtOAc fraction (39.0 g) was subjected to silica gel column chromatography, eluted with $CHCl_3$-MeOH gradiently, to yield 10 fractions. Fr. 1 was applied to silica gel, Sephadex LH-20 column chromatography, and prep-HPLC (Luntech K501 pump, k2501 UV detector, and YMC part-ODS A column (250 mm × 20 mm, 5 μm) to afford compounds eicosyl-(*Z*)-caffeate (**1**, 8 mg), eicosyl-(*E*)-caffeate (**2**, 20 mg), trydecyl-(*E*)-caffeate (**3**, 17 mg), hexadecyl-(*E*)-caffeate (**4**, 6 mg),

* Corresponding author: Chen RY Tel/Fax: +86-10-8316 1622 E-mail: rych@imm.ac.cn
Received: October 20, 2010; Revised: November 3, 2010; Accepted: November 10, 2010
Fund: National Science and Technology Major Projects (2009zx09504-004)

octadecyl-(*E*)-caffeate (**5**, 11 mg), docosyl-(*E*)-caffeate (**6**, 15 mg), tetracosyl-(*E*)-caffeate (**7**, 15 mg), eicosyl-(*E*)-ferulate (**8**, 10 mg), docosyl-(*E*)-ferulate (**9**, 26 mg), tetracosyl-(*E*)-ferulate (**10**, 3mg), 4-hydroxy-acetophenone (**11**, 41 mg), *n*-tridecanoic acid (**12**, 8 mg), *n*-myristic acid (**13**, 9 mg), daucosterol (**14**, 67 mg), and β-sitosterol (**15**, 23 mg).

Results

Compound **1**: white amorphous powder. The molecular formula was determined as $C_{29}H_{48}O_4$ from the HR-ESI-MS, which showed a pseudomolecular ion peak at *m*/*z* 483.1375 $[M + Na]^+$. ^{1}H-NMR spectrum showed the signals of following protons at δ 7.58 (d, 1H, J = 12.9 Hz, H-8), and 6.32 (d, 1H, J = 12.9 Hz, H-7) for the *cis* double bond (*trans* double bond coupling constant should be higher than 15); three ABX coupling system signals at δ 7.20 (d, 1H, J = 2.1 Hz, H-2), 7.09 (dd, 1H, J = 8.1, 2.1 Hz, H-6), and 6.91 (d, 1H, J = 8.1 Hz, H-5) for the aromatic ring; one methyl proton signal at δ 0.92 (3H, t, J = 6.9 Hz, H-20'); hydrogen with oxygen signal δ 4.18 (2H, t, J = 6.6 Hz, H-1'). Therefore, the structure of compound **1** was established as eicosyl-(*Z*)-caffeate.

^{1}H-NMR (acetone-d_6, 300 MHz) δ: 8.45 (1H, s, OH), 8.21 (1H, s, OH), 7.58 (1H, d, J = 12.9 Hz, H-8), 7.20 (1H, d, J = 2.1 Hz, H-2), 7.09 (1H, dd, J = 8.1, 2.1 Hz, H-6), 6.91 (1H, d, J = 8.1 Hz, H-5), 6.32 (1H, d, J = 12.9 Hz, H-7), 4.18 (2H, t, J = 6.6 Hz, H-1'), 1.72 (2H, m), 1.32 (34H, br s), 0.92 (3H, t, J = 6.9 Hz, H-20'). ^{13}C-NMR (acetone-d_6, 100 MHz) δ: 167.3 (C-9), 148.5 (C-3), 146.1 (C-4), 145.3 (C-7), 127.5 (C-1), 122.3 (C-6), 116.2 (C-5), 115.6 (C-8), 115.0 (C-2), 64.5 (C-1'), 32.5 (C-2'), 31.3－23.2 (C-3'-C-19'), 14.2 (C-20'). Structure of compound **1** is seen in Fig. 1.

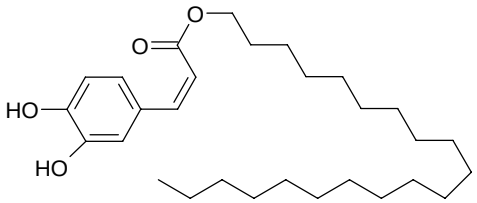

Fig. 1 Structure of compound 1

References

Chen H, Li YC, 2004. Advances in the resrarch of phytochemistry and pharmacology of *Anabasis L. Nat Prod Res Dev* 16(6): 585-589.

Du H, Wang Y, Yan C, Zhou LG, Hao XJ, 2008. Alkaloids from *Anabasis aphylla* L. *J Asian Nat Prod Res* 10(11): 1093-1095.

Editorial Committee of Flora of China, 1979. *Flora of China*. Beijing: Sciences Press.

Tilyabaev Z, Abduvakhabov AA, 1998. Alkaloids of *Anabasis aphylla* and their cholinergic activities. *Chem Nat Compd* 34: 295-297.

Zhu GL, 1995. Origin, differentiation, and geographic distribution of the chenopodiaceae. *Acta Phytotaxon Sin* 34(5): 486-504.